



**AIR POLLUTION
CONFERENCE BRAZIL**
4th CMAS SOUTH AMERICA

COMMUNITY MODELING AND ANALYSIS SYSTEM

PROCEEDINGS OF THE AIR POLLUTION CONFERENCE BRAZIL 4th CMAS SOUTH AMERICA

July 22, 23 and 24, 2019 - Belo Horizonte, Minas Gerais, Brazil.

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ISBN: 978-65-81147-00-6

SEAD, TREINAMENTOS E COACHING

Each fall for the last 18 years, the Community Modeling and Analysis System (CMAS) from the U.S has conducted its annual conference and training program in Chapel Hill, North Carolina, USA, which draws hundreds of scientists and policy makers to learn about best practices in air quality and emissions modeling. Since 2013, scientists and policy makers in South America had the opportunity to gain the modeling knowledge and skills right in their own region, when CMAS U.S was invited by the Department of Atmospheric Sciences at Brazil's University of São Paulo (USP) to host the 1st CMAS South America conference and training on emissions modeling and air quality. The Universidad Pontificia Bolivariana hosted the 2nd CMAS South America in Bucaramanga, Colombia, 2015. The Federal University of Espirito Santo hosted the 3rd CMAS South America Conference in Vitória, Espírito Santo, Brazil, 2017. Finally this year, the 4th CMAS South America was hosted by the Federal University of Minas Gerais, in Belo Horizonte City, Brazil, 2019.

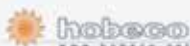
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**PROCEEDINGS OF THE
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Session 01

Air Quality, Climate and Energy

GREENHOUSE GAS EMISSIONS FROM NUCLEAR POWER GENERATION IN THE BRAZILIAN ELECTRICITY MATRIX

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Abstract: In order to meet the goal of reducing greenhouse gas emissions presented by Brazil in the 2015 United Nations Framework Convention on Climate Change (UNFCCC), while maintaining the expansion of the electricity supply system, it is essential to use energy from alternative sources, such as solar, wind, biomass and nuclear, which have played an important role in the world energy matrix. Among the thermal sources, nuclear energy has been used as a complementary source to meet the electricity generation needs of some countries such as USA, UK, Germany and Spain. Since nuclear energy is an option for the national energy mix, the present work aims to estimate greenhouse gas emissions from the historical electricity generation by nuclear power plants, Angra 1 and Angra 2 since their construction to the present and from a future scenario of nuclear electricity generation by 2050, with the introduction of Angra 3 power plant. The modeling tool, MESSAGE, was used to model the historical and future scenario of electricity generation. Results show that the greenhouse gas emissions are low when compared to nuclear generation. In 2017, while the electricity generation accounted for 2.5% of the electricity matrix, emissions were only 0.4% of total emissions of the sector. In the long term, emissions per kWh increase due to higher requirements of the fuel cycle, especially of the enrichment, but the values are still comparable to the historical electricity generation.

Keywords: Nuclear energy, greenhouse gas emissions, electricity matrix, climate change.

INTRODUCTION

Brazil pledged to reduce emissions of greenhouse gases by 37% and 43%, respectively, by 2025 and 2030 in relation to 2005. In order to achieve these goals, the government will adopt policies in several areas, including changes in the energy matrix. The country will seek efforts for a transition in the matrix using renewable sources and economy decarbonisation [1].

Although it is discussed whether or not nuclear is a clean energy, nuclear power is a low carbon technology and an option to complement the generation of renewable energies since these sources are intermittent and vary seasonally. An analysis of GHG emission estimated by the National Renewable Energy Laboratory (NREL) and published by the Intergovernmental Panel on Climate Change (IPCC) clearly places nuclear energy among the most climate-friendly and low-emission energy sources. Nuclear generation presents the fourth lowest GHG emission among all sources [2].

Most of the GHG emissions from nuclear power come from the fuel cycle stages that precede the operation of the plants. A considerable amount of energy is needed for the enrichment process, which is the stage that consumes the most energy and is responsible for the highest GHG emissions from nuclear power generation. Emissions from this stage can correspond up to 70% of the total life cycle of a nuclear power plant. Otherwise, processes such as uranium extraction, conversion,

fuel assembly, reactor construction and decommissioning, correspond from 2% to 8% of the total emissions [3]. There are two commercially available forms of enrichment: gaseous diffusion and centrifuge method. It is estimated that the energy to enrich the same amount of uranium in a gas centrifuge is about 1/10 of the energy required in the gaseous diffusion [4].

According to the sustainable development scenario presented by the IEA (2017), consistent with limiting the average global temperature increase by 2°C by 2100, renewable energy will provide about two-thirds of the emission reduction achieved in the energy sector, with carbon capture and storage (CCS) technologies providing 18% and nuclear delivering 16% of emissions reductions [5].

Therefore, the present work aims to estimate Brazilian greenhouse gas emissions from the historical electricity generation by nuclear power plants, Angra 1 and Angra 2, since their construction to the present, and from a future scenario of nuclear electricity generation up to 2050, with the introduction of Angra 3 power plant.

METHODS

Following the same methodology used by IPCC (2012) [2] and Kadiyala et al. (2016) [6], a literature review that evaluated the life cycle assessment of nuclear power generation was conducted. Several sources of data presenting life

cycle assessment studies were consulted, in a total of 22 references adding up a sample of 65 data, among them Rashad and Hammad (2000), Beerten et al. (2009), Dones et al. (2007a, 2007b), Fthenakis (2007) and Hondo et al. (2000) [7-12]. Data collected were categorized to represent the technologies and assumptions for each scenario. Finally, estimates from each case were calculated using statistical metrics - sample size (N), mean (X), standard deviation (SD), minimum (Min), maximum (Max), standard error of the mean (SE), quartile 1 (Q1), quartile 2 or median (Q2) and quartile 3 (Q3).

The data collection had to present two main characteristics to represent the technologies of reactor used in the country. The first characteristic was the type of reactor. The data were analyzed only for light water reactors (LWR) and pressurized water reactors (PWR), since the scenarios are composed only of PWR reactors. The second characteristic evaluated was the enrichment method. Among them we have gaseous diffusion (D), centrifuge (C), mixture with gaseous diffusion dominance (MD), mixture with centrifuge dominance (MC) and mixture with equivalent proportions of gaseous diffusion and centrifuge (DC).

The following cases were considered according to technologies and scenarios and modeling:

A. In order to calculate the average GHG emissions of Angra 1 and Angra 2 in the historical generation, it was considered the data whose enrichment method is based on the use of centrifuges (C, MC) or equivalent proportions of gaseous diffusion and centrifuge (DC) since most of the enrichment is done in the country using ultracentrifuges and the share of imported enrichment comes from Europe that also use gaseous diffusion.

B. For the GHG emissions of the Angra 1, Angra 2 and Angra 3 plants, it was assumed that with the increase in the need for enriched fuel by 2050, the import of enriched uranium could be increased and the enrichment could come from all enrichment methods.

The average GHG emissions were multiplied by the nuclear electricity generation in order to represent the annual emissions from the sector. For the future scenario, it was considered a capacity factor of 77.7% for Angra 1 and 89.5% for Angra 2 and Angra 3. The net capacity of Angra 1, Angra 2 and Angra 3 are 626 MW, 1275 MW, and 1245 MW, respectively.

FINDINGS AND ARGUMENT

The results of average GHG emissions for reactor technologies and their scenarios are presented in

Table 1. Since in case A the most used enrichment method is the centrifuge, the average emissions are lower than when gaseous diffusion is used, as expected.

Table 1. GHG emission estimates (g CO₂e / kWh)

Case	A	B
N	42	65
X	14.03	19.24
SD	12.31	17.90
Min	1.80	1.80
Max	54.00	84.00
SE	2.46	3.07
Q1	5.00	6.18
Q2	9.59	15.00
Q3	18.63	25.70

Therefore, considering the nuclear generation history and the future scenario with Angra 3 up to 2050 (Figure 1a), the average annual emissions of the sector is shown in Figure 1b. The decrease in generation and emissions, in 2025, followed by an increase, in 2026, are due to the decommissioning of Angra 1 and introduction of Angra 3, respectively. In 2040 occurs the decommissioning of Angra 2.

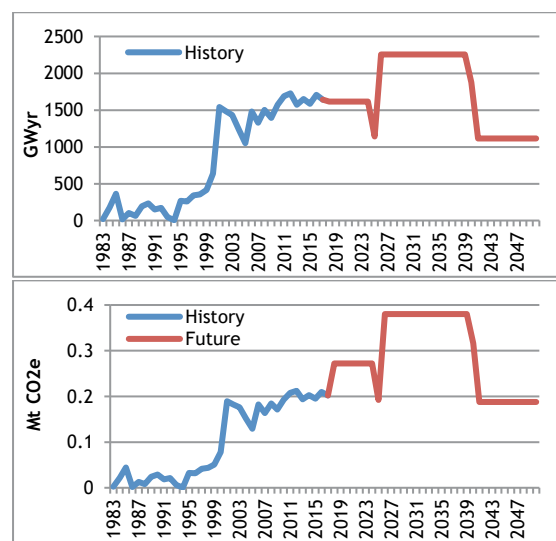


Figure 1. a) Electricity generation. b) CO₂e emissions.

On the one hand, total GHG emissions in the electricity sector have increased significantly since 2011 and in the last two years have emitted approximately 40 Mt CO₂e to the atmosphere [13]. On the other hand, the share of emissions from the nuclear sector has reduced in the same period. Maximum emissions from nuclear represented only 1.1% of total emissions in electricity generation and, in 2017, emissions were only 0.4% of total emissions of the sector (Figure 2).

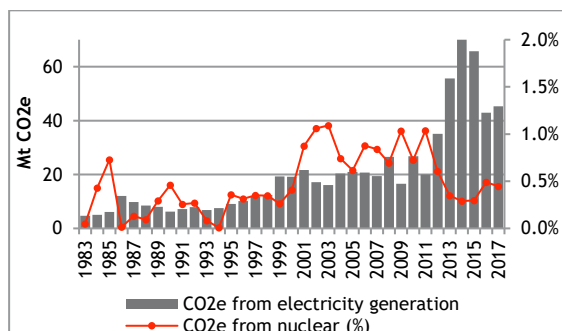


Figure 2. Emissions of CO₂e from nuclear energy in the electricity sector.

Comparing the nuclear share in the electricity matrix [14] and the nuclear participation in emissions, the impact of emissions is 2 to 8.5 times lower than the contribution in power generation. While nuclear share in generation was 2.4% in 2017, the percentage in emissions was only 0.4%. A ratio of 6 times between the share in the electricity matrix in relation to the emissions (Figure 3).

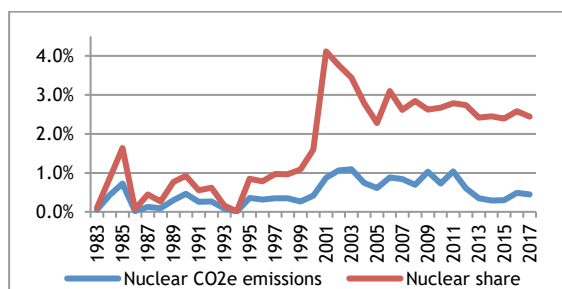


Figure 3. Nuclear share in emissions and electricity generation.

CONCLUSIONS

The largest contribution of GHG emissions from nuclear energy comes from the fuel cycle, particularly with greater contribution of the enrichment process. In the case where enrichment was considered by gaseous diffusion - more energy-intensive method - the average emissions were higher. This would imply an increase in future emissions from the national nuclear sector if the country cannot meet the needs of Angra 1, Angra 2 and Angra 3 with their ultracentrifuges.

Looking at the country's history, the contribution of nuclear emissions is relatively low when compared to its share of electricity generation. This shows the potential of nuclear energy as a low-carbon technology, which can contribute as a complementary source to renewable energy rather than fossil fuel power plants. In addition, low emissions put nuclear energy as an important option to meet the country's GHG emission

reduction targets and decarbonisation of the economy.

As emission results are estimates, for more accurate emission results for Angra 1, Angra 2 and Angra 3 it would be interesting that detailed future work of life cycle assessment was performed for these facilities.

ACKNOWLEDGEMENTS

The authors thank the Brazilian research funding agencies: FAPEMIG, CAPES, CNPq and CNEN, for their support.

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OXY-FUEL COMBUSTION AND EMPLOYMENT OF WASTE-DERIVED ALTERNATIVE FUELS IN THE CLINKERING PROCESS: MODELING AND SIMULATION

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Abstract: The cement industry is responsible for an important fraction of anthropogenic CO₂ emissions. CO₂ capture and replacement of fossil fuels by alternative fuels are important ways by which CO₂ emissions are reduced. Due to its higher capture efficiency, oxy-fuel combustion has stood out among CO₂ capture technologies. In this study, an oxy-fuel combustion model for cement clinker process is proposed and implemented in Aspen Plus®. Moreover, the employment of waste-derived alternative fuels in the CO₂ capture process for the cement industry is also studied. Five waste fuels were chosen for the analyses: used tyre, dried sewage sludge, rice husk, meat and bone, and refuse-derived fuel. Results showed that when waste-derived alternative fuels are employed with oxy-fuel combustion in the clinker process, the CO₂ concentration in the flue gas increases, allowing CO₂ capture. Under the same conditions, results showed the CO₂ generation was reduced when compared with the conventional process.

Keywords: cement clinkering, carbon dioxide emissions, carbon dioxide capture, oxy-fuel combustion, non-fossil fuels

INTRODUCTION

The cement industry is one of the world's most energy-intensive and carbon dioxide (CO₂) emitter sectors [1]. Its greenhouse gases emissions correspond to about 5% of the total anthropogenic emissions [2]. Approximately 40% of all the CO₂ produced during the cement production comes from fuel burning. The remaining (60%) originate from the raw meal calcination, electricity and transport processes [3]. The production of one thousand kilograms of cement releases about 660 - 800 kg of CO₂ [4]. This scenario highlights the importance of adopting practices to reduce the CO₂ emissions. Over the years, the cement industry has established a number of measures to reduce its emissions. These include replacing fossil fuels with alternative energy sources, increasing the process energy efficiency of the process, replacing clinker components and CO₂ capture [4].

Several alternative fuels can be co-processed in the cement industry [5]. These include: waste oils, solvents, waste plastics, meat and bone, sewage sludge, used tyre, biomass, municipal solid waste, among others. The alternative fuel choice depends on several factors, such as availability, price, transportation and handling, storage, regulations and environmental impacts [5]. Besides contributing to the reduction of CO₂ emission, the use of alternative fuels decreases the volume of waste disposal needed and reduces costs from fossil fuels. This enables greater economic efficiency of the industrial unit [6].

Oxy-fuel combustion is seen as one of the most promising CO₂ capture technologies to reduce greenhouse gas emissions. In this process, the air commonly used as the oxidizer for fuel combustion

is replaced by a mixture of oxygen (O₂) and flue gas (mainly CO₂ and H₂O) [1].

Rahman and co-authors [5, 7, 8] have published a series of studies, in which they analyze the utilization of wastes-derived alternative fuels in the cement industry. Oxy-fuel combustion has been recently studied by Carrasco-Maldonado et al. [1], who have investigated a new burner design for clinker kilns that would be used in oxy-fuel combustion. Granados et al. [9] and Hökfors et al. [10] have analyzed the effect of flue gas recirculation (FGR) in the clinker rotary kiln through computer simulation.

Despite that, to our knowledge no work has been done simulating oxy-fuel combustion and employment of waste-derived alternative fuels in the clinkering process. This study proposes to fill this gap by evaluating the influence of oxy-fuel combustion technology and fossil fuels substitution by waste-derived alternative fuels on CO₂ generation by the cement industry. The analyses were conducted through computational simulation carried out in the commercial software Aspen Plus®.

METHODS

The oxy-fuel combustion and the employment of waste-derived alternative fuels in the clinkering process (Figure 1) was simulated in the steady state simulator Aspen Plus®. The simulated plant was assumed to have a production capacity of 2900 t_{clinker}/d and a thermal consumption of 3200 kJ/kg_{clinker}.

The clinker process model with CO₂ capture by oxy-fuel combustion included a five-stage preheating tower, calciner, clinker kiln, cooler, electrostatic

precipitator, water condensation and flue gas recirculation as shown in Figure 1.

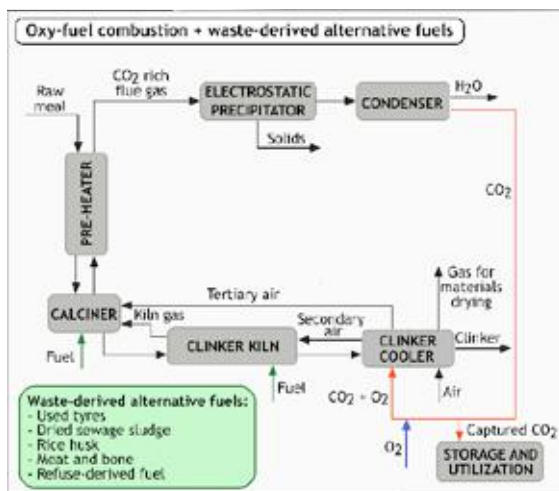


Figure 1. Oxy-fuel combustion and employment of waste-derived alternative fuels in the clinkering process

It was assumed that the process was operated under atmospheric pressure (1.01325 bar), that there was no pressure drop in the equipment and that clinker was composed of components C_2S ($2CaO \cdot SiO_2$), C_3S ($3CaO \cdot SiO_2$), C_3A ($3CaO \cdot Al_2O_3$), and C_4AF ($4CaO \cdot Al_2O_3 \cdot Fe_2O_3$). The SOLIDS calculation method was chosen for thermodynamic and transport properties evaluation [11]. The raw meal composition used in the simulation was selected according to Mastorakos et al. [12].

Each of the five stages of the preheating tower was represented by a heat exchanger (HEATER) and a splitter (SSPLIT). The decomposition of raw meal in the calciner was modeled with a stoichiometric reactor (RSTOIC). Three stoichiometric reactors (RSTOIC) and three solid-gas separators (SSPLIT) were used to simulate the different stages of clinker formation that occur inside the kiln.

Formation that occur inside the kiln. Fuel (coal + waste-derived alternative fuels) combustion in the calciner and in the clinker kiln was simulated using three reactor modules (RYIELD and RGIBBS) and a MIXER module. The fuel mass flow was calculated based on the clinker process thermal consumption and on the fuel heating value. It was assumed that 38% of the available thermal energy was required by the kiln combustion and the remaining 62% by the calciner combustion [13]. Ashes were considered inert during combustion.

In order to analyze the influence of the use of alternative fuels on CO₂ generation by the clinker process, five fuels were chosen: used tyres, dried sewage sludge, rice husk, meat and bone, and refuse-derived fuel. The immediate analysis, the elemental analysis and the calorific value of the evaluated fuels were obtained by Phyllis2 [14]. The mass flow rate of the alternative fuel used during combustion was calculated from the fuel calorific value and the thermal energy demand (Table 1).

Table 1. Parameters used during the simulation

Fuel	Used tyre	Dried sewage sludge	Rice husk	Meat and bone	Refuse derived fuel
Substitution rate (%) [8]	30	5	20	35	30
Feeding site [15]	Kiln	Calciner	Calciner	Kiln	Calciner
Alternative fuel (kg/s) *	0,82	0,47	1,82	1,82	1,72
Coal - Calciner (kg/s) *	2,42	2,22	1,64	2,42	1,25
Coal - Kiln (kg/s) *	0,31	1,48	1,48	0,12	1,48

* Calculated.

The clinker cooler was divided into two stages, each of which was represented by a set of heat exchangers (HEATER), followed by a splitter (FSPLIT). The first stage was operated with the recirculated flue gas and oxygen, which was subsequently used for combustion in the kiln and calciner. The second stage was operated with air, which was then directed to raw materials drying and/or fuel preparation [1, 10].

A separation unit module (SSPLIT) was used to model the electrostatic precipitator. The flue gas water condensation was simulated by a heat exchanger (HEATER) and a flash separator (FLASH2). A fraction of the flue gas (CO_2 -rich) was recirculated and mixed with oxygen. The FGR was fixed in 55% [16]. The mixture was directed for the cooling of clinker and, after that, it was used as the oxidizer in the combustion reactions taking place in both the kiln, as secondary air, and in the calciner, as tertiary air. The other fraction of flue gas was directed to either CO_2 storage or utilization.

The CO₂ molar concentration in flue gas and the CO₂ generated for each alternative fuel was analyzed. The results were compared with the conventional clinker process.

FINDINGS AND ARGUMENT

The simulation for the employment of waste-derived fuels in the clinkering process indicate that the concentration of CO₂ in the flue gas increased from 30.6% - 31.5% in conventional process to 84.0% - 86.9% in the oxy-fuel combustion (Figure 2). The removal of N₂ from the process causes the concentration of CO₂ in the flue gas to increase, which, in turn, is composed predominantly of CO₂ and H₂O.

Oxy-fuel combustion technology, besides enabling CO₂ capture, storage and utilization, thus reducing emissions, also amounted for a lower CO₂ generation when compared to the conventional clinker process, as showed in Figure 3.

In the conventional clinker process, when used tyre was employed, $792.3 \text{ kgCO}_2/\text{t}_{\text{clinker}}$ were generated, whereas in the oxy-fuel combustion process the amount was of $786.4 \text{ kgCO}_2/\text{t}_{\text{clinker}}$. This represents a reduction in CO_2 generation of over $5646 \text{ tCO}_2/\text{year}$, considering that the cement industry produces $2900 \text{ t}_{\text{clinker}}/\text{day}$ and operates 330 days a year. For

dried sewage sludge the reduction in CO₂ generation was 12345 tCO₂/year. For rice husk the reduction was 9857 tCO₂/year and for refuse-derived fuel was 11579,7 tCO₂/year. The largest reduction was found for meat and bone, 13781 tCO₂/year. However, this reduction is only for the CO₂ generation. The CO₂ emissions mitigation through oxy-fuel combustion capture process may be higher than 90% [1].

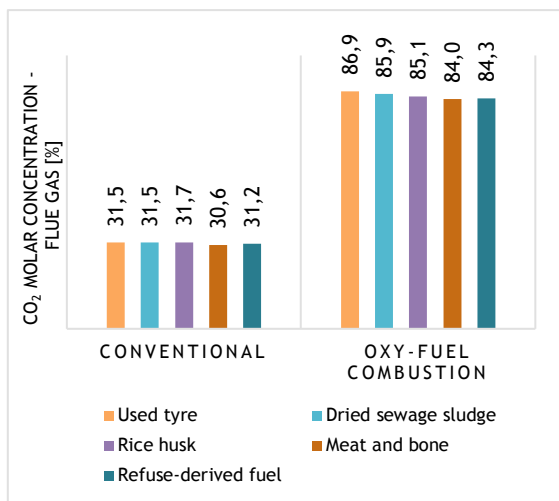


Figure 2. CO₂ molar concentration in the flue gas

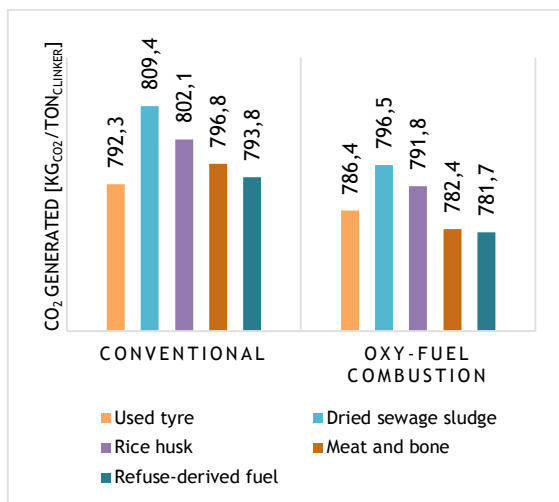


Figure 3. CO₂ generated in the clinkering process

CONCLUSIONS

The analyses showed that the oxy-fuel combustion provides the CO₂ concentration in the flue gas. In this way the CO₂ generated in the clinkering process can be captured, stored and utilized. When waste-derived alternative fuels were employed with oxy-fuel combustion the CO₂ generation was reduced when compared with the conventional process. This emphasizes the environmental importance of oxy-fuel combustion and the employment of waste-derived alternative fuels on the cement industry CO₂ emissions mitigation. Further studies should be

carried out with the objective of analyzing the technical and economic viability of this CO₂ capture process and alternative fuel application.

ACKNOWLEDGMENTS

The authors thank CNPq, Academy of Finland and FAPEMIG for the financial support for this work.

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CHARACTERIZATION OF PARTICLES EMITTED BY PIZZERIAS BURNING WOOD AND BRIQUETTES: CASE STUDY AT SAO PAULO, BRAZIL

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Abstract: The burning of biomass in pizza ovens can be an important source of air pollution in residential areas, at urban and rural sites. Fine particulate matter, PM_{2.5}, represents one of the most aggressive pollutants to human health, besides the potential to interfere with global radiative balance. A study in real-world conditions was performed at three pizzerias in São Paulo city. The quantification and characterization of PM_{2.5} emitted by the burning of biomass in indoor and outdoor areas (exit of the chimney) were done. Two of the pizzerias used eucalyptus timber logs and one used wooden briquettes. The results from the three pizzerias revealed high average concentrations of PM_{2.5}, 6.17 mg/m³ in the exit of the chimney and 68.24 µg/m³ in indoor areas. The burning of briquette revealed lower concentrations of PM_{2.5}. BC, measured by reflectance, represented approximately 20% and 30 % of the PM_{2.5} mass concentration in indoor and exit of the chimney, respectively. Among the trace-elements, potassium, chlorine and sulfur, were the most prevalent in terms of concentration. Although in Brazil there are no air quality standards for PM_{2.5} exposure at indoor areas, when compared with international values, the concentrations obtained within the three pizzerias exceeded those parameters. Concentration of elements dangerous to health such as chromium and zinc were above the recommendation of the WHO. The emission rate of PM_{2.5} and black carbon (BC) due to the burning of logs were 0.38 g/kg and 0.23 g/kg, respectively. The total emissions of PM_{2.5} and BC were 116,73 t/year and 70,65 t/year, respectively, in the burning of timber logs.

Keywords: Air pollution, PM_{2.5}, biomass burning, pizzeria, X-ray fluorescence.

INTRODUCTION

Biomass is one of the main sources of energy in the world. But there are few studies around the world analysing the impact of wood and charcoal use for cooking in metropolitan areas. In Brazil, the biomass represents 25.1% of the energy matrix and is used mainly in residences and in food related commercial establishments (i.e. restaurants, bakeries and pizzerias). In the city of São Paulo the consumption of pizzas is very important, 1.5 million pizzas are produced daily, being the second city in the world in pizza consumption (Brazilian Energy Balance, 2016). Moreover, the biomass burning is also a significant source of air pollutants (Taner et al., 2013; Shen et al., 2014): carbon monoxide (CO), polycyclic aromatic hydrocarbons (PAHs), sulphur dioxide (SO₂), nitrogen oxide (NO_x), black carbon (BC) and particulate matter (PM). PM is one of the most harmful pollutants to human health, and may also contribute to climate change. Particles suspended in the atmosphere can influence the amount of solar radiation that reaches the earth's surface through scattering and absorption processes, causing heating or cooling of the atmosphere, depending on the physico-chemical

and optical properties of the particles (Artaxo et al., 2009). Seinfeld and Pandis (1998), define PM_{2.5} as a group of solid and liquid particles suspended in the atmosphere with aerodynamic diameter less than 2.5 µm. International studies have proven the relationship between exposure to PM_{2.5} and respiratory diseases (Polichetti et al., 2009; Saldiva et al., 2013). The most important anthropic sources of PM are industries, vehicle emissions and biomass burning. Among the diverse elements that compose the mass of PM_{2.5} coming from the burning of biomass, the Black Carbon (BC) is normally present in high concentrations due to its smaller size and its chemical nature. BC is related to adverse effects to human health beyond being an important agent in climatic change. While some aerosol particles possess a cooling effect of the climate, the BC particle is associated with heating (IPCC, 2013). Besides that, the BC particle can be allocated to the body, including the brain, with adverse effects. In Brazil there are no studies concerning the burning of biomass in pizzerias. Studies found in the literature were carried out under controlled conditions of leakage, temperature, use of dilution camera in the obtaining of emission factors (Dash,

1982; Gonçalves et al., 2010; Shen et al., 2014; Calvo et al., 2014). This research studied indoor and outdoor (exit of the chimney) $PM_{2.5}$ and BC concentrations, morphology and particles chemical composition related to the burning of biomass in three pizzerias. This study intended to estimate the emissions of $PM_{2.5}$ and BC coming from the burning of fuelwood and briquettes. The measurements were carried out under real operating conditions of the three pizzerias, on weekdays and weekends, inside the hall and at the exit of the chimney. The estimates of the total emissions were made based on calculated emission factors, and considering the annual consumption of wood/briquettes by pizzerias in the city of São Paulo.

METHODS

Samples were taken in three pizzerias (P1, P2 and P3) situated in the central region of São Paulo City between October and November of 2013. The average daily production during the sampling time was 30, 26 and 38 pizzas in P1, P2 and P3 and the consumption of fuelwood/briquettes was 163.4, 94.2 and 20.4 kg respectively. None of the pizzerias used air conditioning. The chimney diameter was 45 cm and the opening of the indoor oven was 30 cm high and 45 cm wide for all three pizzerias. The main difference between the studied pizzerias was the height of the chimney: 8 m (P1 and P3) and 25 m (P2). The samplings of particulate matter were carried out in real operating conditions of the pizzerias in the year of 2013, on weekdays and weekends, indoor and at the exit of the chimney. Samplings at P1 occurred from October 11th to 14th, while at P2 and P3 occurred from October 18th to 20th and November 02th to 04th, respectively (table 1). The Mini Vol sampler (Airmetrics) was the equipment used in the experimental part of the study to collect $PM_{2.5}$. The Mini Vol operated with a flow of 5 l/min and used filters of polycarbonate, with a diameter of 47 mm and pores of 0.4 μm . After collection, the $PM_{2.5}$ was analysed by different complementary techniques: mass concentration was determined by the gravimetric method, black carbon concentrations were determined by optical reflectance with a smoke stain reflectometer and elemental analysis was performed by EDXRF (Energy Dispersive X-ray Fluorescence).

Table 1. Characteristics of pizzerias: type of biomass used, daily pizza production, sampling period.

	Biomass type	Sales pizza/day	Sampling period	Number of samples
P1	Eucalyptus	30	Oct. 11-14	34
P2	Eucalyptus	26	Oct. 18-20	30
P3	Briquette	38	Nov. 02-04	26

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Considering indoor concentrations, approximately 50% of the mass composition of the particulate

matter at P1 is BC, suggesting that the combustion process is less efficient compared to P2 and P3 (the percentage of BC in the composition of the mass of the particulate matter was approximately 20%) (Figure 1). At P2 a smaller amount of wooden logs, as well as the lower turnover of pizzas, boils down to this, the fact that the chimney is taller (25 m) which makes more suction force possible (high gas flow rate), what can contribute to internal lower concentrations.

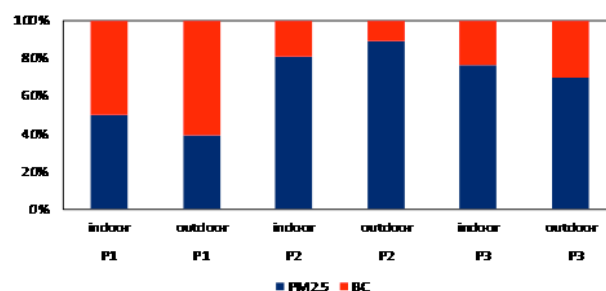


Figure 1. Indoor and exit of the chimney percentage of BC in the mass of the $PM_{2.5}$ in the three pizzerias.

Table 2 presents the measurements and the standard deviations obtained for particulate matter and BC in the three pizzerias at both indoor and at the exit of the chimney. The $PM_{2.5}$ ($\mu g/m^3$) refers to the average of the mass deposited on the filter in each pizzeria; BC ($\mu g/m^3$) refers to the average concentration of BC present in the sample filters. Outdoor concentrations in (mg/m^3) are higher than indoor concentrations ($\mu g/m^3$).

Table 2 $PM_{2.5}$ and BC concentration averages and standard deviations for indoor and outdoor areas

Indoor		
	$PM_{2.5}$ ($\mu g/m^3$) Average	BC ($\mu g/m^3$) Average
P1	111.14±46.94	55.48±72.63
P2	40.89±4.00	7.76±1.93
P3	52.71±21.11	12.51±3.94
Outdoor		
	$PM_{2.5}$ (mg/m^3) Average	BC (mg/m^3) Average
P1	3.42±6.40	2.06±2.96
P2	13.66±9.70	1.50±2.18
P3	1.42±0.98	0.49±0.67

The results from X-ray fluorescence presented a spectrum of chemical elements with differing characteristics. The potassium being found in high concentrations in the processes that involves the burning of biomass, like the burning of fuelwood in pizzeria ovens. The chlorine and the sodium also presented elevated concentrations. Sodium is generally associated with chlorine to form sodium

chloride (NaCl), used as cooking salt (basic ingredient for many fillings used in pizzerias like cheese, smoked sausage, salami and pepperoni). Medium level concentrations were quantified for the elements: aluminium, silicon, iron and calcium. After calculating the EF, it was possible to estimate the total emissions of PM_{2.5} and BC coming from the pizza ovens in the city of São Paulo. 8,000 is the number of pizzerias in the city of São Paulo and 80% (6,400) use wood as fuel in their pizza ovens. The average consumption of wood in each pizzeria is 8 m³ per month (96m³ per year). Gentil (2008) indicated that 1m³ of wood is approximately equal to 500 kg considering 30% humidity of the wood. Therefore, 96m³ of wood (annual consumption) corresponded to 48 t/year of wood consumed in each pizzeria in São Paulo. The amount of particulate matter emitted by pizzerias in São Paulo were 116,736 t of PM_{2.5}/year (319 kg/day) and 70,656 t of BC /year (194kg/day).

CONCLUSIONS

The practice of burning wood in pizzerias represents a potential source of air pollution especially in large urban centres like the city of São Paulo, because the city has an elevated number of pizzerias and the related fuel wood consumption emits elevated quantities of particulate matter. The emissions coming from the burning of fuelwood in pizzerias in the city of São Paulo were 117.73 t/year of PM_{2.5} and 70.65 t/year of BC. These values give the dimension of the polluting potential that pizzerias represent to the air quality of the city, and flag the necessity to think of alternative ways to produce cleaner pizzerias. It is a point of concern that the emissions occur after the sunset when the atmospheric boundary layer starts to become more stable preventing the dispersion of pollutants to high levels of the atmosphere. Moreover, the emissions of PM_{2.5} and BC in pizzerias are significant and should not be excluded from air quality inventories for the city of São Paulo. It is estimated that the pizzerias contribute to 3% of the atmospheric emissions in the city of São Paulo, where the main source of pollution are the vehicles (80%) (Kumar et al., 2016).

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ENVIRONMENTAL ASSESSMENT USING DIESEL SUGAR CANE IN URBAN BUS FLEET

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Abstract: Since the Industrial Revolution, the changes in the climate and its implications have gained the attention of society, initiating discussion movements on the issue. Although Brazil is a developing country and under the terms of the Kyoto Protocol, it has not committed to binding reduction targets, it has committed itself during the 15th Conference of the Parties on Climate (COP 15) to prepare annual inventories of its emissions of greenhouse gases (GHG) and develop national programs for mitigation and adaptation to climate change. Thus, the country ratified the Kyoto Protocol in 2002 and created, through Law No. 12,187/2009, the National Policy on Climate Change (PNMC), formalizing Brazil's voluntary commitment to reduce GHG emissions between 36.1% and 38.9% of the projected emissions by 2020. In Rio de Janeiro State several efforts were made to create a legal regime that would allow the challenges faced for climate change, Decree No. 43,216 in 2011, which regulates the Law on State Policy on Climate Change (State Law No. 5,690/2010), which published sets GHG emission reduction targets for 2030, with a base-line in 2010, including the transportation sector, with a 30% reduction target in 2030. The transportation sector contributes a quarter of global GHG emissions and is the area where carbon emissions have grown most since 2000. In Brazil, the transportation sector is the second largest source of GHG emissions, increasing demand for renewable fuels as an alternative to fossil fuels. In 2009, approximately 87% of passenger travel, performed by collective modes, occurred by buses powered by petroleum diesel oil. In Rio de Janeiro State, in 2015, the transportation sector had the most significant contribution, accounting for 38.1% of Gg CO_{2e} emissions of final energy consumption. In this context, the scientific challenge is to deepen and expand knowledge about biofuels in order to mitigate GHG emissions, especially in the transportation sector. This work aims to evaluate diesel sugar cane in a fleet of urban buses, as a substitute biofuel for fossil fuel (diesel), under the socioeconomic and environmental prisms. For this, the results of the experiments conducted by FETRANSPOR in urban buses that circulated in Rio de Janeiro city from 2012 to 2013 will be adopted. This study proposes to evaluate the autonomy (fuel consumption) of the buses with the use of the proposed diesel, feasibility of commercialization and the environmental impacts related to atmospheric emissions.

Keywords: diesel sugar cane, GHG, transportation sector, mitigation, emissions.

INTRODUCTION

Anthropogenic activities have always been related to the transformation of the environment (SOUZA; SANTIN; ALVIM, 2007). Population growth, economic development, urbanization, increased consumption of energy and inputs, territorial occupation and consequently pollution, cause impacts of different types in different nature cycles (YERGIN, 2014).

Among the effects of pollution, the highlight is exponential increase observed in the last decades of the concentration of local air pollutants and

greenhouse gases (GHG), whose accumulation in the layers closest to the atmosphere and it has amplified the phenomenon of climate change called heating global (GUIMARÃES, 2016).

Since the advent of the Industrial Revolution, global climate change and its implications have achieved little attention from society in general until the end of the 20th century. Although the contribution of carbon to the maintenance of Earth's temperature has been discussed since the XVIII century (YERGIN, 2014).

At the end of the 1970s, a series of political and scientific conferences began, beginning with the first Global Climate Conference in 1979, raising the discussion on the issue of global climate change (GUPTA, 2010).

The National Policy on Climate Change (Federal Law No. 12,187 of 2009) set the voluntary goal of reducing emissions by 38.9% compared to the business as usual scenario in 2020 (base year 2005). The Rio de Janeiro State, through the Decree of Public Targets for Reducing Emissions of Greenhouse Gases and Adapting to Climate Change (Decree 43.216 of 2011), established the voluntary goal of reducing GHG emissions from several sectors, including the energy sector, which includes the transport sector. The reduction target of 30% was set with base year in 2010 and horizon in 2030.

In 2015, the transportation sector accounted for 38.1% of final energy consumption emissions in Rio de Janeiro state, which is the main source of GHG emission in the state (SEA, 2017).

In the transport sector, there is the second largest source of GHG emissions in Brazil (MCTI, 2017), increasing the demand for renewable fuels as an alternative to fossil fuels. In 2009, approximately 87% of passenger travel, carried out by collective modes in Brazil, occurred through the use of buses powered by petroleum diesel oil (ANTP, 2009).

Efforts are being made to establish biodiesel in Brazil that will enable the country to achieve world leadership in agroenergy and protect the environment in a broad way. It can be observed for some decades ago laws were created to encourage biodiesel blending in the diesel oil.

The importance of diesel cycle engines in the Brazilian energy matrix and of biofuels as an alternative to the partial replacement of diesel oil is indisputable, among other purposes, mitigation of greenhouse gas emissions.

In this context, since the publication of law 11.097/2005, the National Program for the Production and Use of Biodiesel (PNPB) in Brazil was prepared through working time, in charge of presenting studies on the feasibility of using vegetable oil for biodiesel production.

The sugarcane sweet cane can already be called ethanol cane, electric energy cane, with the burning of bagasse that generates electricity, cane of *cachaça*, the typical national drink, and now also diesel sugarcane (FAPESP, 2008).

The present experiment aims to evaluate the environmental efficiency of the use of sugarcane

diesel in a fleet of urban buses, based on experiments carried out by the Federation of Passenger Transport Companies of the State of Rio de Janeiro - FETRANSPOR, in order to have a biofuel alternative substitute for fossil fuel (diesel).

METHODS

Data collection was provided by database of the experiments carried out by FETRANSPOR (COPPETEC, 2013) to evaluate the environmental performance of using sugarcane diesel through the indicators of yield and CO₂ equivalent emissions. The yield (km/L) was measured over a period of 12 months, between a fleet of 20 urban buses from lines 125 and 409 that circulated through the Rio de Janeiro city from Feb/2012 to Jan/2013.

Commercial diesel (B5), which contained 5% biodiesel in mineral diesel, was used in 10 buses, and in the other 10 buses was used a mixture containing 70% of the commercial diesel and 30% sugarcane diesel (AMD30), which is a fuel formed by a fermentation process through modified yeast cells that convert glucose or sucrose into a compound called *farnesene*, an unsaturated oil with molecular structure C₁₅H₂₄.

For the determination of the indicator average yield of the buses (Rend), in km/L, data were extracted regarding the daily distance traveled (km) and daily fuel consumption of the buses (L) of the 20 urban buses that participated in the experiment.

In order to calculate the GHG emission indicator (CO₂), it was used Equation 1 following the IPCC bottom-up approach (2007).

$$\text{GHG} = (\text{EF}/1000) \times Y \times C \times \text{FC} \text{ (Equation 1)}$$

Where:

GHG: greenhouse gas emission [kg/month];
EF: GHG emission factor [g/km];
Y: average yield of buses [km /L];
C: monthly fuel consumption [L];
FC: GHG characterization factor [kg CO₂eq/kg].

The emission factors (EF) adopted were those of the PROCONVE P7 phase, according to Table 1.

Table 1: CO₂eq emission factors

Fuel	Emission factor	Unit
Mineral Diesel	2.603	Kg/L
Biodiesel	2.431	Kg/L

Font: Adapted MMA (2013)

Also, regarding the GHG characterization factor was used, as presented in Table 2.

Table 2: Values of the heating potential of greenhouse gases

GHG	GWP
CO ₂	1
CH ₄	25
N ₂ O	298

Font: Adapted IPCC, 2007.

FINDINGS AND ARGUMENT

The approach of this work opted for the comparison and evaluation of two scenarios of urban mobility: the real scenario with the use of commercial fuel (B5) and the sustainable scenario, which uses commercial diesel within 30% of sugarcane diesel (AMD30).

The first results showed that a volume of 599086 L of B5 and 587488 L of AMD30 was used at the end of the experiment. In addition, the total distance traveled was 1,595,178 km when using the B5 fuel and 1,567,418 km when using the AMD30. Table 1 shows the average monthly yields of the two bus lines, adopting the information collected from each of the 20 participating buses of the experiment each month, which part of this fleet supplied with fuel B5 and the other part with AMD30.

Table 3: Average monthly yields (km/L) of bus lines 125 e 409.

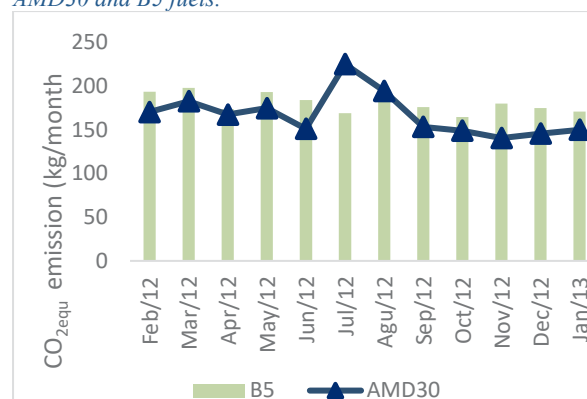
Month	125 bus line		409 bus line	
	AMD30	B5	AMD30	B5
Feb/12	2.74	2.70	2.55	2.58
Mar/12	2.91	2.83	2.60	2.56
Apr/12	2.74	2.74	2.58	2.59
May/12	2.90	2.81	2.53	2.68
Jun/12	2.58	2.87	2.58	2.60
Jul/12	2.78	2.79	2.73	2.55
Agu/12	2.86	2.81	2.54	2.50
Sep/12	2.83	2.84	2.55	2.52
Oct/12	2.86	2.75	2.56	2.55
Nov/12	2.83	2.90	2.57	2.55
Dec/12	2.85	2.90	2.64	2.59
Jan/13	3.00	2.98	2.76	2.65

Font: Authors

It is verified that the yields were very similar in the two bus lines for both fuels during the 12 months of experiment. The monthly efficiency of sugarcane diesel versus commercial diesel ranged from 90% to 107%. However, the average efficiency of all period was 101%, which makes biofuel competitive in terms of efficiency.

Figure 1 shows the average monthly CO₂ equivalent emissions of buses on line 125, which used the AMD30 and B5 fuels.

Figure 1: CO_{2eq} emission results for 125 bus line for AMD30 and B5 fuels.

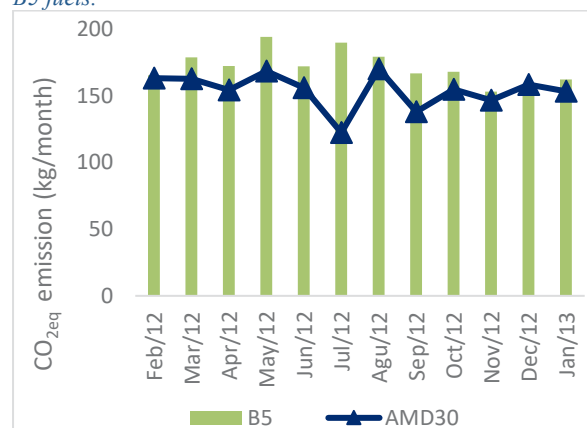


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It can be observed CO_{2eq} emissions reduction during the evaluated months when the AMD30 is used as fuel. However, it is evident in July a peak using that fuel, exceeding in that month the B5 emissions. This was due to the fact that the bus fleet using AMD30 fuel of line 125 had performed around 28.7% more trips, consequently consuming more fuel and emitted more too.

Figure 2 shows the average monthly CO₂ equivalent emissions of 409 bus line, which used AMD30 and B5 fuel.

Figure 2: CO_{2eq} emission for 125 bus line for AMD30 and B5 fuels.



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The same finding in CO_{2eq} emissions reduction over the months can be also observed when the AMD30 was adopted in substitution to B5 fuel in Fig. 2. CO_{2eq} emissions estimated using the AMD30 fuel were 3803 kg/year, while GHG emissions with the use of B5 fuel were 4152 kg/year. Therefore, the adoption of

the AMD30 in the urban bus fleet evaluated brought an 8.4% reduction in GHG emissions in relation to the use of commercial fuel.

Emissions from biodiesel combustion must be reduced from total GHG emissions in transport sector. Therefore, in the real scenario the reduction of CO_{2eq} emissions was 13,718 kg/year, while in the sustainable scenario the reduction was 349,444 kg/year, reducing 8,5 % of GHG emitted, which contributes to meeting government targets for climate change.

CONCLUSIONS

Advancing the development of cleaner and more efficient fuels in terms of yield, coupled with the gradual establishment of public policies to enable them to be implemented, are key tools for governments to achieve their goals for climate change and the creation of sustainable cities.

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ESTIMATING GREENHOUSE GAS EMISSIONS FROM HYDROELECTRIC POWER DAMS IN COLOMBIA AND ITS IMPACT ON THE AGGREGATED POWER GENERATION EMISSION FACTOR

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Abstract: Electricity generation through reservoirs has been considered a renewable and clean process, but studies conducted over the last two decades reveal that hydroelectric reservoirs generate substantial amounts of GHG¹, particularly CH₄ and CO₂, due to the degradation of organic matter in these reservoirs. The ~ 70% of the electric power in Colombia is generated by hydroelectric dams and there are not GHG emissions attributed to this, therefore, the emissions and the EFEG² of the electric power have been associated to thermoelectric generation. The carbon footprint is also attributed to emissions, particularly internal combustion engines, associated with the construction of reservoirs, so, the emission of GHG are underestimated. Our research estimates the CH₄ and CO₂ emissions of some hydroelectric dams in Colombia, and evaluates the impact of these additional emissions that were not previously considered in the EFEG estimated by the UPME³. For this purpose, we use the IPCC methodology 2006, and we also adapt a simple mathematical model that statistically expresses the dependence of the emission factor [tCO₂-eq / MWh] with the ED⁴ [MW / km²]. The estimates with both methods are very similar. In the selected period⁵ (2013-2018), the UPME estimates that the thermoelectric plants emitted 6333x10³ [tCO₂-eq], 12149x10³ [tCO₂-eq], 14364x10³ [tCO₂-eq], 6695x10³ [tCO₂-eq], 5701x10³ [tCO₂-eq] and 5078x10³ [tCO₂-eq]; additionally we estimate that hydroelectric dams emitted 102x10³ tCO₂-eq / month (2013), 118x10³ t CO₂-eq / month (2014) and 139x10³ tCO₂-eq / month (2015 - 2018) in the base period, which would imply an increase of 11, 12, 11, 19, 29 and 22% (for each year selected) of emissions.

Keywords: Emissions, hydroelectric dams, CO₂ and CH₄ emissions, Colombia.

¹ GHG: Green House Gases

² EFEG: Emission Factor of the Electric Generation

³ UPME: Energy Mining Planning Unit, for its acronym in Spanish.

⁴ ED: Energy Density

⁵ Selected period refers to 2013 - 2018 every calculation was made for each of them.

INTRODUCTION

According to the Colombian Mining and Energy Planning Bureau (UPME - *Unidad de Planeación Minero-Energética*), Colombia had an electric power installed capacity of 17,720 MW in 2018. Nearly 70% of this power, i.e. ~4682 GWh/month, is generated by reservoir-based hydroelectricity power systems. The other ~30% is produced by thermopower systems (mostly natural gas combustion based). The Colombian power industry estimates its greenhouse gas (GHG) emissions and calculates its aggregated GHG emission factor (AGEF), which is calculated following a methodology established by UPME in 2014.

The manmade damming of rivers is known to change their biogeochemistry. The extent of this change heavily depends on the damming depth, as previously inexistent, anoxic conditions can appear at depths that depend on the water circulation, the hydraulic residence time and the wind-controlled surface layer oxygenation rates.

The so far the emission factor didn't include the emissions related to hydropower reservoirs.

Our research is about the emissions from hydropower reservoirs in Colombia with the objective to obtain the historical emissions of electricity generation and emission factor by this kind of electricity production.

This document takes as a starting point the research of Fearnside, P.M. 2001-2004 and Demarty, M & Bastien, J. 2011, in which the greenhouse gas emissions from hydroelectric dams are analyzed mainly those located in tropical zones. Demarty, M & Bastien, J. 2011, did a review of 20 years of CH₄ emissions measurements from hydroelectric reservoirs in tropical and equatorial regions, from this we were able to obtain a static mathematical model that would account for the emissions of hydroelectric dams in Colombia taking advantage of the condition of tropical equatorial country.

Also we found information about what is known and what is lacking related to the greenhouse gases from hydroelectric as well as the comparison of emissions with respect to thermoelectric systems; likewise, a detailed review was made of the IPCC guidelines, the country's commitments at COP21 and the possibilities of diversifying the energy matrix with renewable energy projects.

METHODS

To calculate additional emissions in electricity generation (from hydroelectric dams) in Colombia we use the IPCC methodology 2006 (METHOD 1) and we also adapt a simple mathematical model (METHOD 2) that statistically expresses the dependence of the emission factor with power density; this model is support in Demarty, M &

Bastien, J. 2011, in its research it is found information of CO₂ and CH₄ emissions from tropical hydroelectric dams that made it possible to analyze and relate the emission factor of these reservoirs with respect to their energy density, obtaining a non-dynamic mathematical model that allowed to calculate the emission factor of hydroelectric generation in Colombia.

METHOD 1 - IPCC 2006

With IPCC methodology, the calculation is divided into two components: calculation of CO₂ emissions (by diffuse, not by degassing) and calculation of CH₄ emissions (by diffuse and bubble, not degassing).

According to the methodological structure of the IPCC, the equation used to calculate the CO₂ diffuse emissions was as follows:

$$\text{Total diffuse emissions CO}_2 = ((Pf \times Ef|_{\text{diffuse}}(\text{CO}_2) \times (FA \times fa \times 10^{-6}))$$

Pf: Time no ice (in Colombia = 365 days / year)

FA: Flooded area

fa: area fraction flooded in the past 10 years

$Ef|_{\text{diffuse}}(\text{CO}_2) = 44,9 \text{ (kgCO}_2/\text{ha} \cdot \text{day)}$ - (Average of emissions per day diffuse air - water interface in time no ice; according to IPCC data by tropical highly wet climate)

In CH₄ emissions case, the equation used was as follows:

$$\text{Total diffuse emissions CH}_4 = ((Pf \times Ef|_{\text{diffuse}}(\text{CH}_4) \times (FA \times 10^{-6}))$$

Pf: Time no ice (in Colombia = 365 days / year)

FA: Flooded area

$Ef|_{\text{diffuse}}(\text{CH}_4) = 0,63 \text{ (kgCH}_4/\text{ha} \cdot \text{day)}$ - (Average of emissions per day diffuse air - water interface in time no ice; according to IPCC data by tropical highly wet climate)

METHOD 2 - STATIC MATHEMATICAL MODEL

From tropical hydroelectric dams, from Brazil and French Guyana, we obtained an emission factor and power density given by (Table 1, Figure 1):

$$\ln(EF) = -1,174 \ln(ED) + \ln(0,7068)$$

With the model obtained, the corresponding calculations of emission factor of the main hydroelectric dams in Colombia were made.

In Colombia there are 26 hydroelectric dams but the calculation of greenhouse gas emissions (with method 1 and method 2) was made 18 of them (Table 2).

Once the emission factor was obtained, the emissions from each reservoir were calculated, estimating their contribution considering the year in which the operation of each hydroelectric plant began. Even though only six out of the 18 reservoirs studied are less than 10 years old, the calculations were extended to the total of reservoirs, considering that in CO₂ case the emissions can vary from a maximum value that occurs after the flood to reach a stable point in a period of 10 years (Delmas et al., 2005; Abril et al., 2005); when it comes to CH₄, bubble emissions can be high in ancient tropical reservoirs (Duchem et al., 2000; Stallard & Keller, 2004), condition that fits quite well to the Colombian case where there are dams up to 65 years old (Alban dam for example).

Table 1. Haydroelectric dams used to obtain emission factor and power density relate with

Dam / Reservoir	Emission factor [tCO ₂ eq/MWh]	Energy density [MW/km ²]
Três Marias	1,02	0,34
Barra Bonita	3,60	0,42
Tucuruí	0,53	2,91
Samuel	2,08	0,39
Balbina	18,63	0,11
Segredo	0,02	15,37
Xingó	0,01	50,00
Miranda	0,10	5,83
Petit Saut	0,88	0,37

Reference: Demarty, m & Bastien, J. 2011

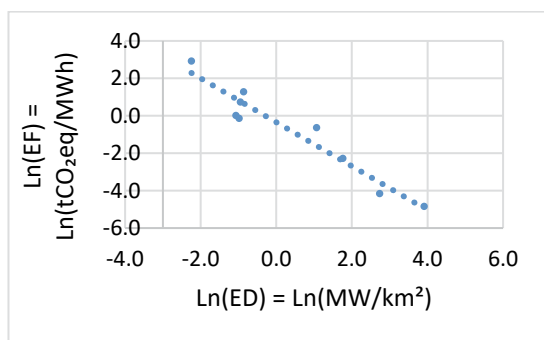


Figure 1. Mathematical model from hydroelectric dams in Brazil

Specifically with method 1, the CO₂ and CH₄ emissions were calculated independently for the hydroelectric dams, identifying the relationship between the emissions of each one of these greenhouse gases and the geometry of the reservoirs.

Finally, the results of emissions obtained from the Calima reservoir with the proposed model were compared with the results of the research carried out by Loaiza, S. (2016), in which the greenhouse gas emissions were quantified through montly monitoring and a methodological adaptation for the quantification of them.

FINDINGS AND ARGUMENT

In Colombia, UPME reports greenhouse gas emissions from electricity generation and its emission factor only for emissions from thermoelectric plants. With the calculations estimated with both method 1 and method 2 it is observed that hydroelectric contributes an additional percentage of emissions compared to what was calculated by the UPME.

Table 2 shows the emission factor obtained by both methods for hydroelectric dams in Colombia.

Table 2. Hydroelectric dams in Colombia for calculation of greenhose gases emissions

Dam / Reservoir	IPCC emission factor [tCO ₂ eq/MWh]	Model emission factor [tCO ₂ eq/MWh]	Power density [MW/km ²]
Urrá	0,11	0,12	4,45
Porce II	0,01	0,01	45,51
Miel I	0,02	0,01	32,65
Porce III	0,003	0,002	143,17
Sogamoso	0,03	0,04	11,88
El Quimbo	0,08	0,11	4,85
Guatapé	0,07	0,05	8,97
Troneras	0,56	1,23	0,63
Jaguas	0,03	0,03	16,04
San Carlos	0,001	0,001	364,71
Chivor	0,008	0,004	76,92
Salvajina	0,04	0,03	14,03
Guavio	0,05	0,04	12,27
Betania	0,08	0,07	7,14
Prado	0,40	0,67	1,05
Calima	0,23	0,08	6,20
Alban	0,001	0,001	326,92
La Tasajera	0,02	0,01	27,55

Figure 2 presents the comparison of the emissions calculated by both method 1 and method 2 with the UPME report.



Figure 2. Comparison of hydroelectric emissions with respect to UPME report

In percentage, comparing with the emissions by UPME report with the estimates of hydroelectric dams, method 1 estimates contributions of 11% (2013 y 2014), 10% (2015), 17% (2016), 27% (2107) and 20% (2018); with method 2 the estimated contributions are 11% (2013 y 2015), 12% (2014), 19% (2016), 29% (2017) and 22% (2018).

The monitoring done in the Calima reservoir (52 years old) yielded an estimate of 19220 [tCO_{2eq}/año]; with method 2 the estimation for this reservoir is 14936 [tCO_{2eq}/año], with an uncertainty of 11% calculated from the error propagation.

CONCLUSIONS

With this first estimate for the country the importance of accounting the emissions from hydroelectric dams is highlighted; although the hydroelectric energy with reservoirs constitutes a form of renewable energy, it does not represent a source of zero emissions (Mendonça et al., 2012).

The proposed model allowed to estimate the emissions coming from the hydroelectric reservoirs in the country; however, this model does not allow an independent estimation of the main greenhouse gases (CO₂ and CH₄) as allowed the IPCC methodology.

The result of the research allows making a correction to the historical estimation of greenhouse gas emissions from the electrical generation and makes a methodological contribution for the calculation of emissions of the country with unpublished results.

It is necessary to establish a national strategy to measure the emissions of these hydroelectric dams and restructure the actions aimed at achieving the commitments proposed for 2030.

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TITLE

PLEATED FILTER TECHNOLOGY IMPROVES PERFORMANCE AND INCREASES EFFICIENCY WHILE CAPTURING PARTICULATE AND EMISSIONS

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Abstract: Air pollution control becomes more and more important, as does energy savings. We aim to demonstrate the effectiveness of pleated filter technology as well as illustrate how this product line actually conserves energy. We will share performance data of different filter types, both traditional filter bags and the pleated filters will be discussed through an in-depth case study following a customer who chose to upgrade their filtration technology.

There is a continued importance for plants to become more energy efficient coupled with the increasingly strict rules and regulations for air pollution control. The pleated product portfolio brings meaningful benefits and advantages, providing a path to achieve the new regulations while also being energy conscious. In this paper, filtration performance will be investigated and analyzed. We will cover the differences between traditional bag and cage filters and the pleated filter element. A case study with Voith Paper in São Paulo, a company with a baghouse using 288 filter bags with just four months of life, will be used to share filtration fundamentals and challenges, observations, the final solution and accompanying results of their recent technology upgrade.

The technology used in pleated filter elements is relevant to most industrial process applications. Often existing baghouse and baghouse components can be utilized when you transform your operation. The paper will uncover how performance improvements are accomplished, energy savings opportunities, reducing downtime, and maintenance costs, plus extending the life of your filter elements. Finally, the details of the fabrics, specifically spunbond or resin stiffened needle felt is selected for an application and how that impacts filtration will be studied.

Following this discussion, you will be able to confirm and measure the performance of overhauling a baghouse.

Keywords: pleated filter bag, spunbond, baghouse, repowering, energy efficiency, upgrade, air pollution control.

INTRODUCTION Competition is a key driver for change among companies in our industries, we have to continue to improve our production, demonstrate energy and cost savings, as well as ensure we are protecting our environment and our employees. This paper intends to share filtration knowledge including that of specific types of filters, fabric considerations, the steps to contemplate before considering an upgrade to a baghouse, componentry that can be reutilized, and most importantly, performance expectations of the new baghouse.

The objective is to propose an efficient methodology of the basic knowledge for upgrading a baghouse, changing to a new filter type, concepts of flow and pressure, filtration fundamentals, types of filter media, and pollution control devices. We will also review the tools and calculations that were used in our analysis.

METHODS

The methodology is driven by the fundamental concepts of filtration and the impacts of a given application.

FINDINGS AND ARGUMENT

A pleated filter element is shorter, more compact, yet includes typically double the filtration area of a standard bag and cage style filter. The pleated filter may reduce or eliminate abrasion and resulting failures, standardizes multiple filter lengths, and reduces housing velocity of grain load. The ease of filter installation is notable, reduces downtime by up to three times, lowers maintenance cost, energy, and compressed air savings will be realized, lower operating DP, lower pulse pressure required, reduced cleaning frequency, provide higher efficiency, increased particulate capture, and increased filter life.



AIR POLLUTION CONFERENCE BRAZIL

CMAS SOUTH AMERICA

COMMUNITY MODELING AND ANALYSIS SYSTEM

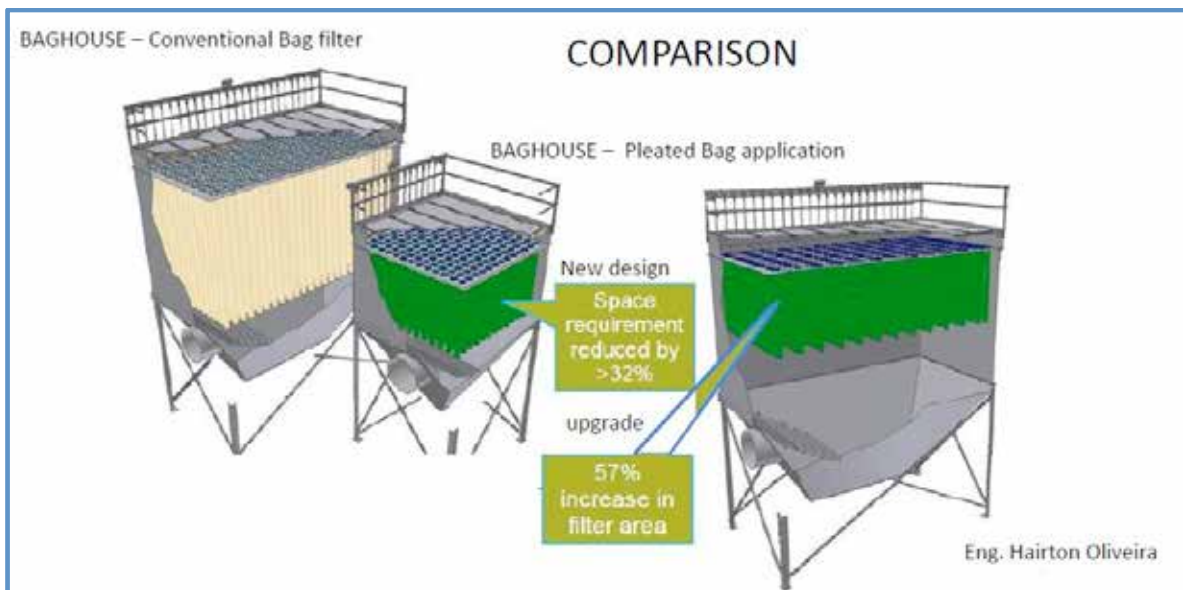


Figure 1. Comparison of conventional bag filter and pleated filter element (source Parker Hannifin)

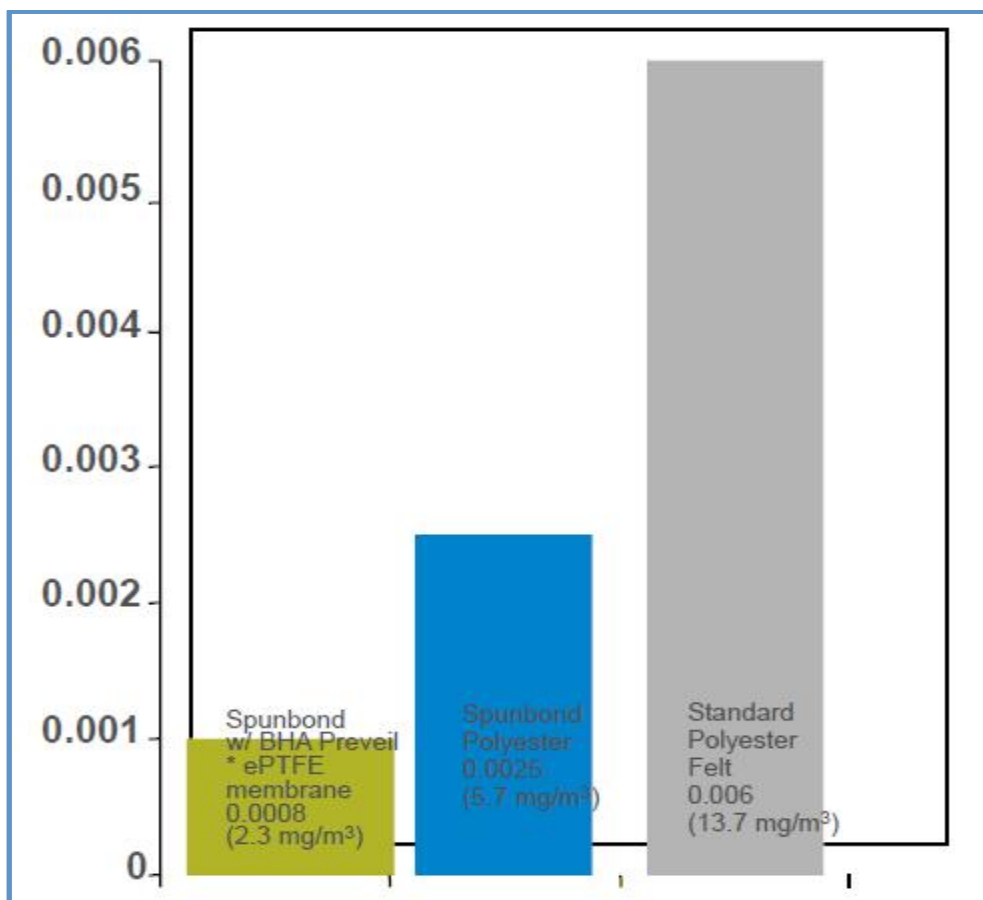


Figure 2. Improved Outlet Emissions (source Parker Hannifin)

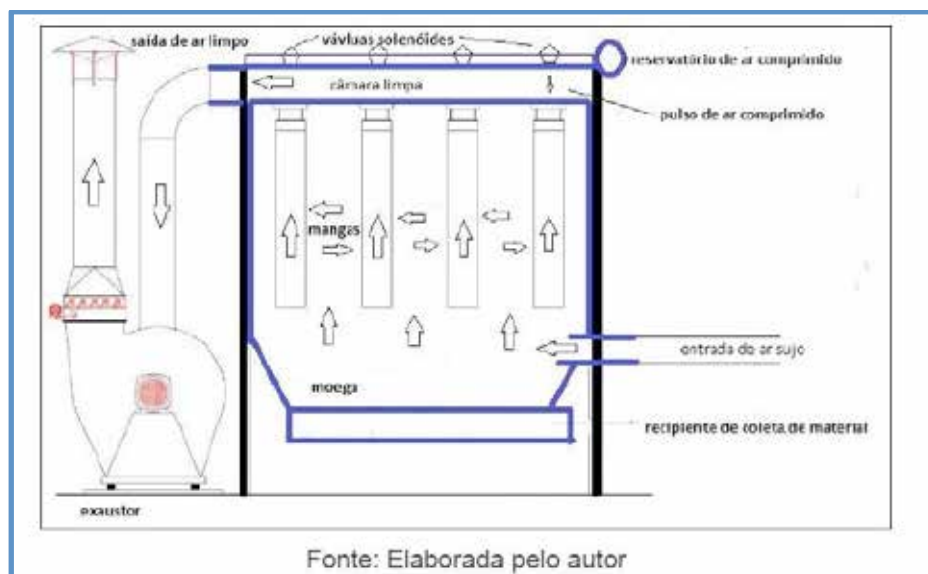


Figure 3. Baghouse

CONCLUSIONS

It is understood that energy efficiency seeks to improve the use of energy sources. This is the challenge of reconciling technologies and revitalizing systems, improving the efficiency of operations and advancing air pollution control while keeping costs low. More and more energy has an important meaning in productive processes, and it is necessary to rethink at what cost, we are generating our energy. It is necessary that the environmental issue is considered and expanded to existing applications where energy demand can be rationalized. Above all, this work allowed Voith Paper in São Paulo to improve efficiency of their filtration processes, improve their environmental impact, that is, allowed pollution indices below the allowed levels of concentration, and indirectly the low loss of load, reduced the use of compressed air, that is spent on energy. The company also wins, with savings in the buying processes and fewer changes of filter elements, no fines, lower compressed air costs, hour/man, equipment stoppage, etc. In this respect, it is concluded that five themes summarize the result of the case study presented: AVAILABILITY, RELIABILITY, PRODUCTIVITY, ENERGY EFFICIENCY, ENVIRONMENTAL PROTECTION

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TITLE

PLEATED FILTER TECHNOLOGY IMPROVES PERFORMANCE AND INCREASES EFFICIENCY WHILE CAPTURING PARTICULATE AND EMISSIONS

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Abstract: Air pollution control becomes more and more important, as does energy savings. We aim to demonstrate the effectiveness of pleated filter technology as well as illustrate how this product line actually conserves energy. We will share performance data of different filter types, both traditional filter bags and the pleated filters will be discussed through an in-depth case study following a customer who chose to upgrade their filtration technology.

There is a continued importance for plants to become more energy efficient coupled with the increasingly strict rules and regulations for air pollution control. The pleated product portfolio brings meaningful benefits and advantages, providing a path to achieve the new regulations while also being energy conscious. In this paper, filtration performance will be investigated and analyzed. We will cover the differences between traditional bag and cage filters and the pleated filter element. A case study with Voith Paper in São Paulo, a company with a baghouse using 288 filter bags with just four months of life, will be used to share filtration fundamentals and challenges, observations, the final solution and accompanying results of their recent technology upgrade.

The technology used in pleated filter elements is relevant to most industrial process applications. Often existing baghouse and baghouse components can be utilized when you transform your operation. The paper will uncover how performance improvements are accomplished, energy savings opportunities, reducing downtime, and maintenance costs, plus extending the life of your filter elements. Finally, the details of the fabrics, specifically spunbond or resin stiffened needle felt is selected for an application and how that impacts filtration will be studied.

Following this discussion, you will be able to confirm and measure the performance of overhauling a baghouse.

Keywords: pleated filter bag, spunbond, baghouse, repowering, energy efficiency, upgrade, air pollution control.

INTRODUCTION Competition is a key driver for change among companies in our industries, we have to continue to improve our production, demonstrate energy and cost savings, as well as ensure we are protecting our environment and our employees. This paper intends to share filtration knowledge including that of specific types of filters, fabric considerations, the steps to contemplate before considering an upgrade to a baghouse, componentry that can be reutilized, and most importantly, performance expectations of the new baghouse.

The objective is to propose an efficient methodology of the basic knowledge for upgrading a baghouse, changing to a new filter type, concepts of flow and pressure, filtration fundamentals, types of filter media, and pollution control devices. We will also review the tools and calculations that were used in our analysis.

METHODS

The methodology is driven by the fundamental concepts of filtration and the impacts of a given application.

FINDINGS AND ARGUMENT

A pleated filter element is shorter, more compact, yet includes typically double the filtration area of a standard bag and cage style filter. The pleated filter may reduce or eliminate abrasion and resulting failures, standardizes multiple filter lengths, and reduces housing velocity of grain load. The ease of filter installation is notable, reduces downtime by up to three times, lowers maintenance cost, energy, and compressed air savings will be realized, lower operating DP, lower pulse pressure required, reduced cleaning frequency, provide higher efficiency, increased particulate capture, and increased filter life.



AIR POLLUTION CONFERENCE BRAZIL

CMAS SOUTH AMERICA

COMMUNITY MODELING AND ANALYSIS SYSTEM

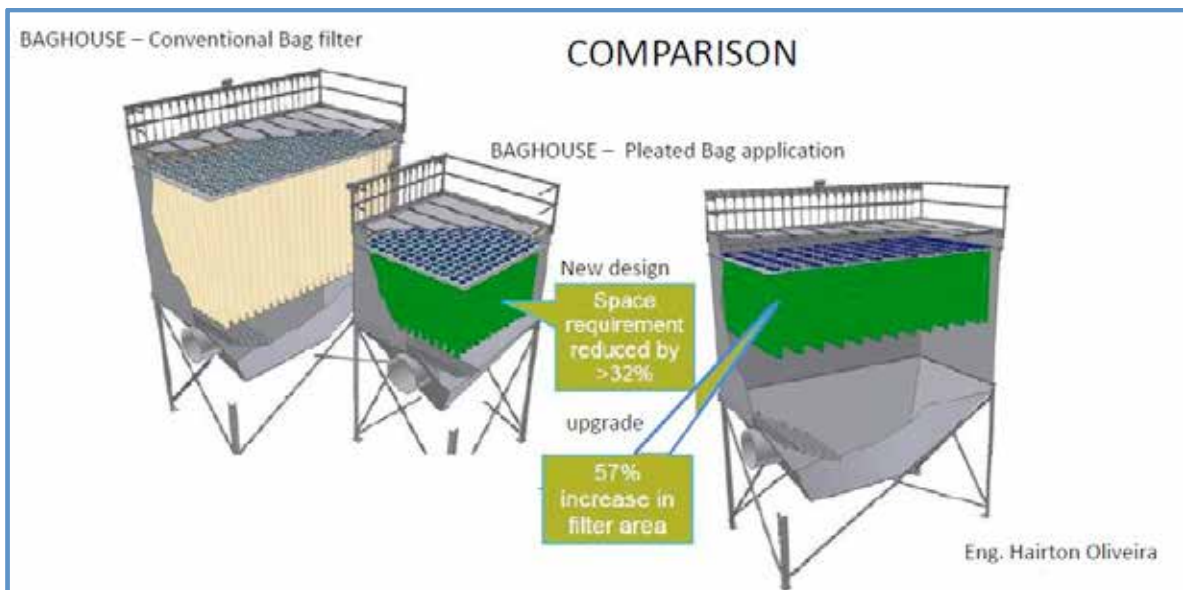


Figure 1. Comparison of conventional bag filter and pleated filter element (source Parker Hannifin)

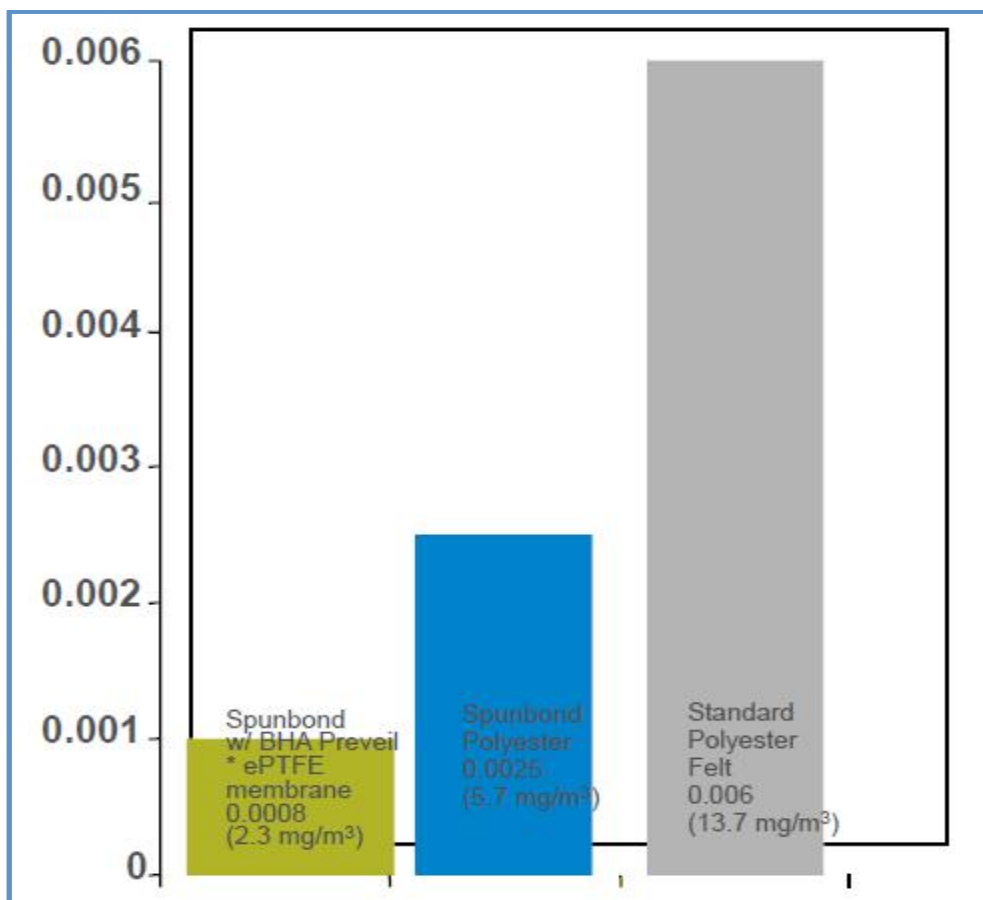


Figure 2. Improved Outlet Emissions (source Parker Hannifin)

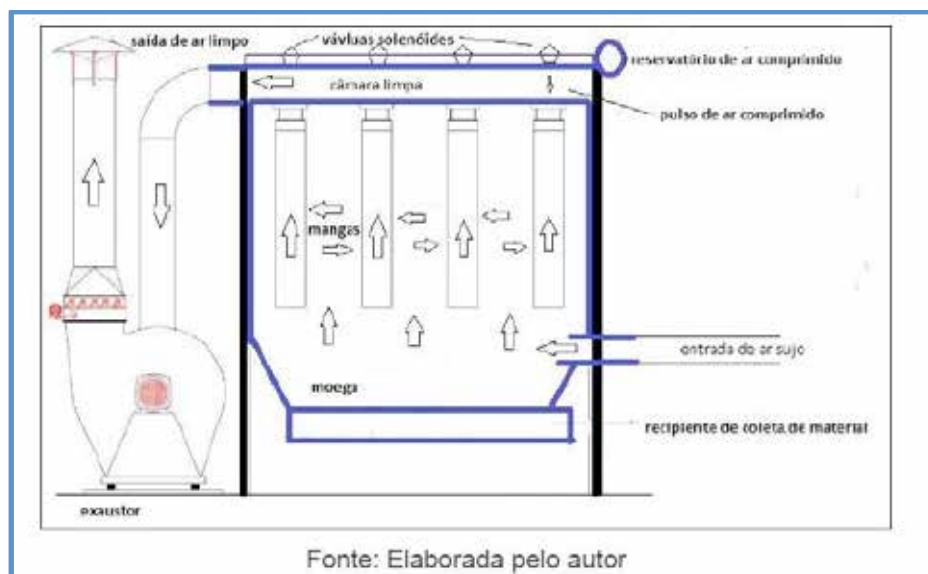


Figure 3. Baghouse

CONCLUSIONS

It is understood that energy efficiency seeks to improve the use of energy sources. This is the challenge of reconciling technologies and revitalizing systems, improving the efficiency of operations and advancing air pollution control while keeping costs low. More and more energy has an important meaning in productive processes, and it is necessary to rethink at what cost, we are generating our energy. It is necessary that the environmental issue is considered and expanded to existing applications where energy demand can be rationalized. Above all, this work allowed Voith Paper in São Paulo to improve efficiency of their filtration processes, improve their environmental impact, that is, allowed pollution indices below the allowed levels of concentration, and indirectly the low loss of load, reduced the use of compressed air, that is spent on energy. The company also wins, with savings in the buying processes and fewer changes of filter elements, no fines, lower compressed air costs, hour/man, equipment stoppage, etc. In this respect, it is concluded that five themes summarize the result of the case study presented: AVAILABILITY, RELIABILITY, PRODUCTIVITY, ENERGY EFFICIENCY, ENVIRONMENTAL PROTECTION

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ANALYSIS OF THE TROPOSPHERIC OZONE SAMPLINGS MADE IN THE CITY OF UBERLÂNDIA/MG IN BRAZIL AND ITS RELATION TO THE CLIMATOLOGICAL PARAMETERS

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Keywords: Ozone, pollution, atmospheric, quality, air

INTRODUCTION

In recent years there has been a great mobilization of the scientific community for a better understanding of the physical and chemical processes of the atmosphere responsible for global warming and degradation of air quality. Both have adverse effects on human health and the biotic environment. Ozone gas (O₃) is an example of pollutant responsible for such impacts in the lower troposphere and it's more intense in large cities and surrounding areas, mainly due to vehicular emissions (Cólón et al, 2001). The ozone concentration has been studied in large cities and it has been found that one of the main sources of emission of its precursors are the vehicles, being volatile organic compounds (VOC's) and nitrogen compounds (NO_x) (Seinfeld & Pandis, 2006). The city of Uberlândia is the second largest city in the state of Minas Gerais in Brazil and one of the largest in the country with a logistics center with intense traffic of all types, besides having a large industrial park. It is located in a cerrado region, where there is dry season (May-September) and rainy season

(October-April), in the dry season atmospheric pollutants are in great concentrations in the troposphere which favors the formation of secondary pollutants. Thus, the proposal of this project is innovative, since there are no air quality monitoring stations maintained by municipal health or environmental agencies and there was no knowledge of tropospheric O₃ concentrations in the city before 2017. The focus of this work is the study of concentrations of O₃ which is a secondary pollutant, that is formed from photochemical reactions of precursor pollutants emitted into the atmosphere (Orlando et al, 2010). O₃ gas is harmful to human health when it is formed in the lower troposphere and affects mainly the most sensitive groups of people such as children, the elderly and people with cardiorespiratory weaknesses. It is also harmful to plants, and can affect agricultural productivity (Orlando et al, 2010). O₃ also destroys agricultural crops (Felzer, Cronin, Reilly, Melillo, & Wang, 2007) because of their ability to attack plant chloroplasts, which are responsible for the respiration of plants.

Therefore, this work aims to study and analyze the data collected from ozone concentration in the year 2017 for a study of seasonality in the city of Uberlândia-MG, Brazil. Also, to observe the behavior of the concentrations according to the hours of the daytime period. Another important point of this project is to verify if the patterns established by CONAMA 491/18 legislation has been exceeded.

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FINDINGS AND ARGUMENT

Since there is no other study on ozone concentrations in the city of Uberlândia, it is very important to have a sampling throughout the day so that you can have data to build a daily profile of the ozone concentrations in µg/m³ (Figure 1) and see how is their behavior at the site of data collection. The O₃ gas presented daily profile for days without cloudiness, with low concentrations in the morning with peak at 13:30 on the first day, at 15:30 in the second and at 16:30 on the last day.

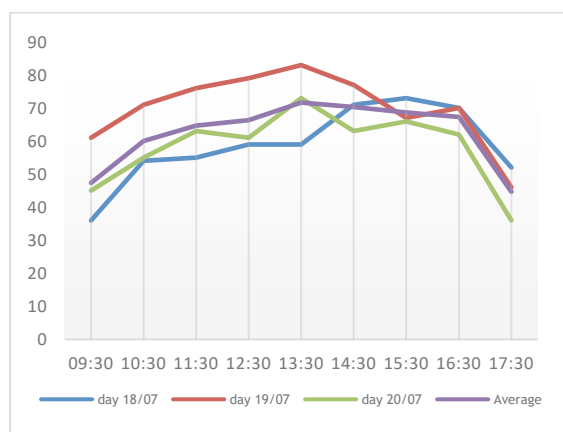


Figure 1. Daily profile of averages over days

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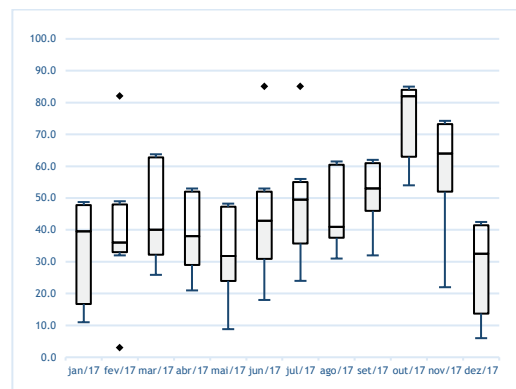


Figure 2. Box-plot of the averages of 2017

With this study during the year, it was observed that the highest mean values of concentration were obtained in the months between September and November (53 - 60 µg/m³), an effect that can be related to spring and the highest amount of VOC's produced by plants at this time of year, in addition, because it is a photochemical pollutant, O₃ has great interaction with solar radiation so for those months we have the combination of these factors: little rainfall and increased solar radiation. And the lowest mean values were identified in the period of highest rainfall in the city, from December to January (30 - 39 µg/m³).

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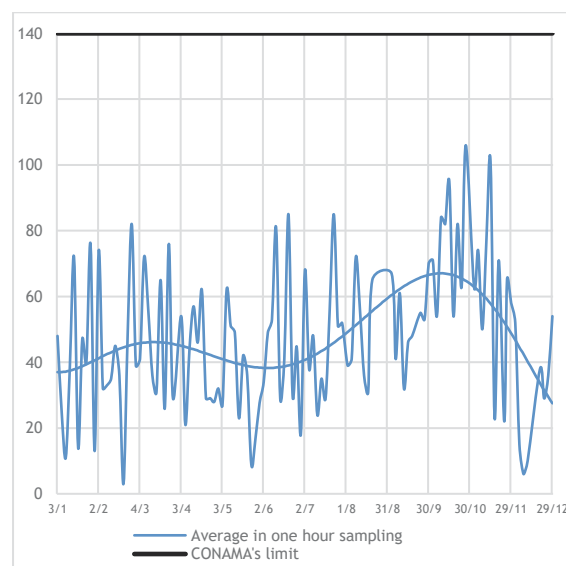


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One of the objectives of this work was to observe the behavior of the concentrations according to the hours of the daytime period, therefore, Figure 4 shows this distribution of the concentrations ($\mu\text{g}/\text{m}^3$) by the sampling schedule, it is worth mentioning that many samples were lost due to faults in the schedule annotations.

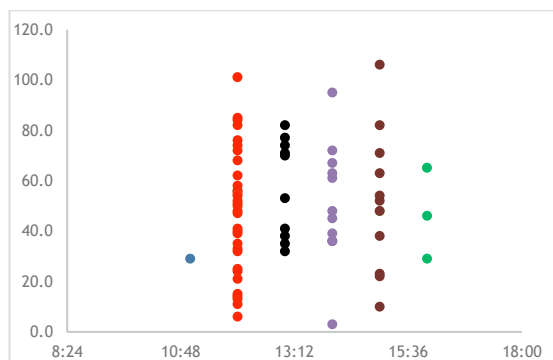


Figure 4. Hourly distribution of averages of ozone concentration

CONCLUSIONS

In the 3 days of study of the daily profile of O_3 , it presented concentration peaks between 13-16h. This variability may be associated with the location of the station, which is very close to the source of emission of the precursor pollutants, and this variability also contributes to the lack of relation between time and concentration collected.

Factors such as radiation incidence, cloudiness, rainfall and emission of VOC's by plants may have contributed to the formation of O_3 .

With the analysis of all the 6,780 concentration data collected during the year, the limit established by CONAMA 491/18 of $140 \mu\text{g}/\text{m}^3$ of air was not exceeded.

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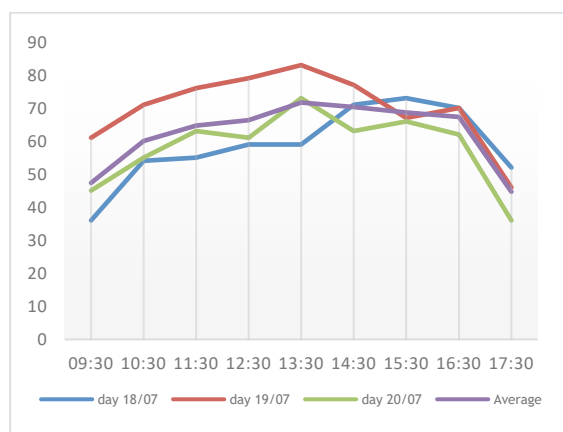


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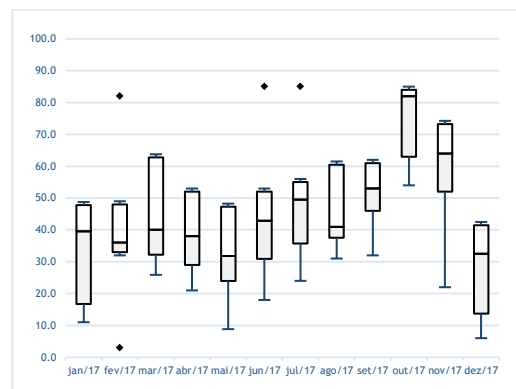


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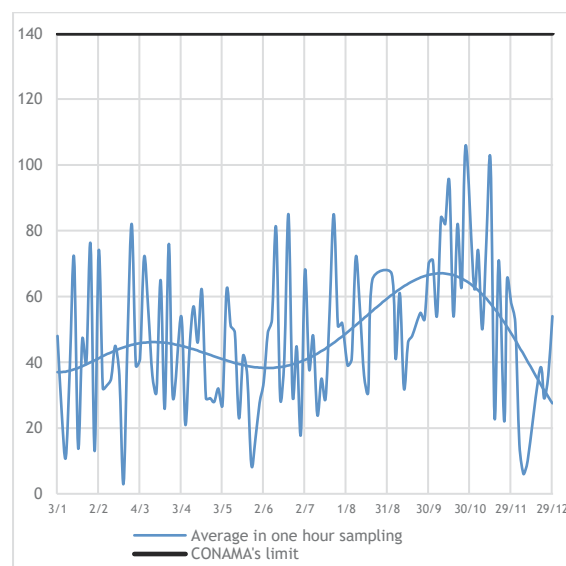


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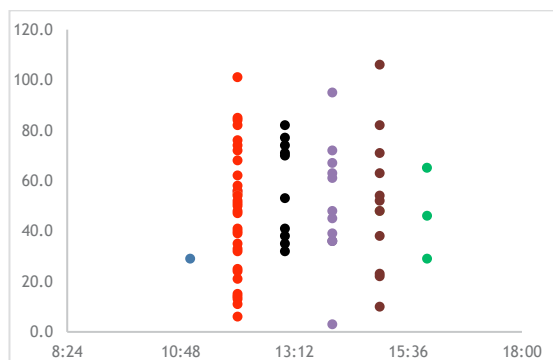


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EVALUATION OF CLIMATE VARIABILITY IN COLOMBIA: OPPORTUNITIES FOR THE OUTLINING OF CLIMATE CHANGE AND HUMAN HEALTH ADAPTIVE STRATEGIES.

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Abstract: Climate change acts as a multiplier of existing human health problems. Therefore, the need arises to improve the population's adaptive capacity to deal with human health risk associated to extreme meteorological events. Colombia already has public policies aiming to develop climate change adaptation plans. However, these policies do not include the need to outline specific adaptive strategies for the public health sector envisioning direct effects of climatic variability. The approach described in this paper, applies a combination of methods to allow the assessment and planning of adaptive measures to diminish the direct health risks associated to extreme thermal sensations in Colombia.

Keywords: Climate variability, Social Vulnerability, Environmental health.

INTRODUCTION

Climate change acts as a multiplier of existing human health problems (McMichael & Wilcox, 2009). During this century a rise of the average global temperature (post-industrialization) over 2°C is expected (Barrett; Charles; Temte, 2015), and important environmental and climatic cycles affectations may occur.

In practical terms, this scenario represents an urgent need for the reduction of vulnerabilities such as poverty and its inequalities of access to health public services and a general improvement in the quality of life of the poor. Although the relationship disease/climate is a complex one, the detection and attribution of changes in the patterns of occurrence of diseases is vital to contribute in the prioritization of public resources allocation and political discussions about climate adaptation (Ebi, 2013).

In those terms, the management of the climate change effects over the population's health requires information from all sectors of the social and health sciences (Costello et al., 2009).

Colombia already has public policies aiming to develop climate change adaptation plans. However, these policies do not include the need to outline specific adaptive strategies for the public health sector envisioning direct effects of climatic variability. The approach described in this paper, applies a combination of methods to allow the assessment and planning of adaptive measures to diminish the direct health risks associated to extreme thermal sensations in Colombia.

Study area

As shown in Figure 1, Colombia is located in the north-west of South America. The mainland borders Venezuela, Brazil, Ecuador, Peru and Panama. The

general forms of the terrain allow establishing a difference between the mountainous zone of the Andes mountain range to the center-west of the country (Andes Region) and the Great Plains in the east. Among the plains, it is accustomed to differentiate between the humid Amazon jungle (Amazon Region), and the open Orinoco basin savana (Orinoco Region). It follows, in size, the Caribbean plains in the north of the country (Caribbean Region), and then the Pacific Plain, a narrow fringe of lowlands located between the ridge and the Pacific Ocean (Pacific region).



Figure 1. Colombia's localization and regions.

METHODS

The methodology followed was developed in two main steps. First, we used the max/min

temperature complex analysis (Lecha and Florido, 1989). This method aims to assist the biometeorological evaluation of tropical climate locations. It involves the construction of a contingency table that combines the simultaneous behavior of the daily maximum and minimum temperatures consistent with a subdivision of 5°C intervals. The classification of the local regime entails the grouping of the temperature data series into categories, types and subtypes depending on the frequency analysis for each interval. The analysis of the complex was aid by data of almost 200 weather stations, representative of the geomorphological diversity of the country, considering a period of 30 years (making a later cut for a 5-year period). To pinpoint the geographical location for each climatic category, the frequencies were mapped applying a multiple linear regression method, using altitude and geographic coordinates (Latitude and Longitude) as independent variables and frequency as the dependent variable.

As a second step, we contrasted the characterization of the thermal regime against the map of social vulnerability to natural hazards index (SoVI®) calculated for the country at the municipality level (1118 municipalities). The data used for constructing this index came from the 2005 official census from the Colombian National Administrative Department of Statistics (DANE) and the 2009 data of the Selection System for Beneficiaries of Social Programs (SISBEN). The vulnerability assessment is based on the original SoVI® by Cutter et al (2003), making the necessary adaptations for the Latin American context (HUMELL, 2016). A final set of 31 variables was defined and standardized according to the original method (Cutter et al 2003). The statistical analysis was made using Principal Components Analysis (PCA), with Varimax rotation and seven as the set number of factors (set after previous analysis of the results of using the Kaiser criterion). The most significant indicators were assumed as drivers of each component and provided the logic for the naming and cardinality of each factor according to their contribution in social vulnerability. To identify the most and least vulnerable cities, SoVI® scores were mapped based on six categories according to the standard deviation from the mean, ranging from -1.5 (low vulnerability) to +2.5 (high vulnerability).

FINDINGS AND ARGUMENT

The first analyses showed the definition of predominant intervals of daytime and nighttime temperatures and the frequency of thermal comfort intervals and extreme thermal sensations, as well as changes of the thermal regime with altitude and seasonal variations in Colombia. As spected for a tropical climate, Figure 1 shows a concentration of very hot days and nights at sea level and on altitudes lower than 500 m. Also a larger temperature

variation between day and night at higher altitudes is observed within the Andes mountain range (higher than 500) home to 80% of the population of the country (DANE, 2005).

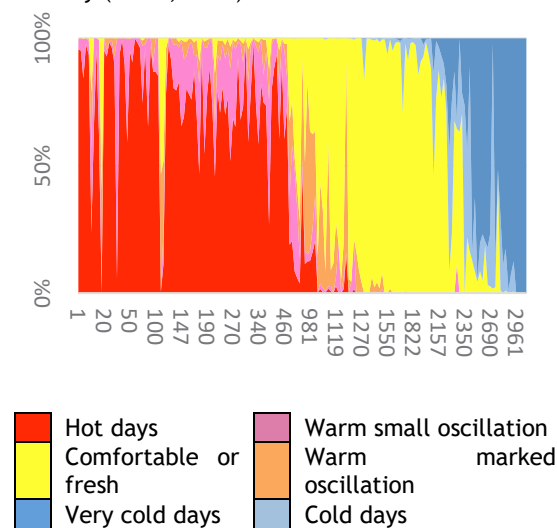


Figure 1. Weather station analyzed. Altitude vs. Frequency of category.

The most important findings describe a definition of thermal regimes in different areas of the country. Although diverse authors (Eslava, 1992; Barón, 2003) have calculated equations to describe the behavior of temperature with altitude in the Colombian territory, the max/min method characterized these differences with more detail, giving opportunity for the analysis of human adaptation to the thermal variations.

In contrast, table 1 shows the seven factors resulting from the statistical analysis of SoVI® Colombia. These components were found to explain 64% of the total variance of the set. Overall, the factors correspond to Colombia's settlement and historical population dynamic's process.

Poverty and Urban educated female population are the factors that combined explain almost 30% of the total variance of the variables' set. However, their influence towards social vulnerability is inverse. Poverty (a factor associated with lack of sanitation services and education access) adds to the overall vulnerability of the municipalities and is found mostly in areas away from urban and administrative centers. In the other hand, urban educated female population acts as a preventing component (observed mostly in capital cities of the national states). It is interesting to note that recent migration due to violence (5 years or less) appears as one of the factors that increase vulnerability and accounts for the population dynamics due to the Colombian internal conflict.

Table 1. Social vulnerability components

Component	Cardinality	Explained variance (%)
Poverty	+	14,214
Urban educated female population	-	13,669
Indian population	+	9,711
Recent migration +recent migration due to violence	+	8,554
Low % of special needs population in extreme poverty.	-	6,686
Age dependency		6,055
Black population and ethnic minorities	+	5,149
Total variance explained		64,036

Table 2 compares the five highest scores found for the social vulnerability index and the thermal regime classification obtained with the max/min complex analysis.

Table 2. Social vulnerability vs. Weather classification

Region	Municipality	SoVI®	Weather Category
Pacific	Bahía Solano	10.65	Hot days
Pacific	Medio Baudó	11.09	Hot days
Pacific	Bagadó	11.5	Hot days
Pacific	Vigía del Fuerte	12.54	Warm small thermal oscillations
Pacific	Argelia	17.87	Hot days

As observed, the highest vulnerability scores are located in small municipalities of the Pacific basin. With the exception of Bagadó, located on a warm area of little thermal oscillation, all areas were classified within the hot days category (maximum temperature higher than 30°C and minimum temperatures higher than 25°C). Although the population in these areas may be more adapted to the high temperatures and the thermal oscillation of the regime, the social vulnerability index shows a lack of adaptation capacity. In case of natural disasters such as heat waves and meteorological extreme events, the population in these areas may not be prepared to respond and recover from these events.

CONCLUSIONS

As such, this paper presents arguments for potential development of climate-change adaptation strategies at the national level, aimed to improve public health care based on peculiarities of the country's thermal regime and population social vulnerability. It constitutes a novel approach in support of national development policies, due to potential improvement of health care strategies, centered on the effects of extreme climate variation and significant social needs. It also promotes nationwide risk management measures based on the climate diversity of the country.

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SHORT-TERM WIND SPEED FORECASTING USING COMPUTATIONAL INTELLIGENCE IN BAHIA, BRAZIL

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Abstract: In this paper the short-term wind speed forecasting in the tropical region of Mucuri, Bahia, Brazil, applying artificial neural network (ANN) technique to the hourly time series representative of the site is presented. To perform the training and validation of this technique, one month of data were collected in a tower with anemometers installed at heights of 100, 120 and 150 m. Different ANN configurations were applied to this site and heights with aimed to define the most efficient ANN configuration, all of Multilayer Perceptrons with Levenberg-Marquardt Backpropagation training algorithm, to predict the wind speed for 1 hour ahead, and then apply it for 3 and 6 hours ahead. Then a quantitative analysis was conducted, and the statistical results (MAE, MSE, RMSE, Pearson Coefficient or Pearson's r , R-square or R^2 , MAPE and Percentage of the data of a factor of two) were evaluated in order to select the one that better predicts the real data. This kind of method has low computational costs when compared with other techniques (like numerical modelling). The mean R-square and Pearson's r for wind speed forecasting for 1 hour ahead was 0.890 and 0.943, respectively. The statistical results showed that the application of the ANN technique to predict the wind speed at Bahia's site and at higher heights presented good accuracy, attesting its ability to be used as a powerful tool in order to help the Brazil's National Electric System Operator (ONS) to improve the usage and integration of the wind energy into the national electrical grid. The innovative aspect of this work is that there is no previous work applying computational intelligence targeting short term wind speed forecasting for such heights (100, 120 and 150 m) in a tropical region, specifically for Brazil and Bahia state, comparing the computational intelligence's results with real data (anemometer's data).

Keywords: Computational Intelligence; Artificial Neural Networks; Wind Energy; Wind Speed Forecasting; Computational Modeling.

INTRODUCTION

Currently, environmental pollution is a global issue that is receiving significant attention, and the development of new forms of renewable resources to reduce pollution is a problem that must be solved (Cheng et al., 2017). As a burgeoning renewable energy, wind energy has been developing fast in the recent decade (Jiang et al., 2016; Li et al., 2018) and Huang, Li, and Jin (2015) states that wind power has the largest market share and is expected to maintain rapid growth in the coming years. Works such as Alencar et al. (2017) and Zucatelli et al. (2019) showed results of mathematical modeling and numerical simulation for short-term prediction with computational intelligence techniques, especially using Multilayer Perceptron Neural Networks with Feed-forward and Backpropagation training algorithm, all with good results achieved and low associated errors. In Zucatelli et al. (2019), the short-term wind speed forecasting for Colonia Eulacio, Soriano Department, Uruguay, is performed by applying an artificial neural network (ANN) technique to the hourly time series representative of the site. The ANN was trained to perform the forecasting of 1 hour ahead and then, using it, the trained network was applied to recursively infer the

forecasting for the next hours of the wind speed, is smaller than if it were necessary to train to predict the next 6 h for each input/sample of anemometric data. The results of the short-term wind speed forecasting showed good accuracy at all the anemometer heights tested, suggesting that this method is a powerful tool. This study is a novel investigation related to the operation of wind power plants for Mucuri. The main contributions of this study are provided as follows: a) Another innovative aspect of this work is that it uses an approach to train the model for the next hour forecasting, then recursively inferring the forecasting for the following hours, in addition to applying this artificial intelligence method targeting short-range wind speed forecasting for this height in a tropical region. b) the proposed model elucidates the behavior of the wind speed and allows accurate wind speed prediction at an important height (100, 120 and 150 m). The model can be used to identify optimal locations of wind turbines and forecast irregular wind energy, for different heights. Short-term wind energy forecasting can be improved using this model to enhance the wind power quality 6 h ahead (nowcasting). c) No previous studies applied computational intelligence for short-range wind

speed forecasting for these heights in such a humid tropical climate region (or humid coastal region). Therefore, the results constitute a significant contribution to the scientific community. d) The short-range wind speed forecasting model is an important contribution for reliable large-scale wind power forecasting and integration in Bahia.

METHODS

To reach the objective of the present work, with respect to the computational procedure to perform this work, was adopted the computational intelligence model applied in Zucatelli et al. (2019). The Mucuri city is located at an altitude of 7 m in relation to the sea level and it has a territorial area of 1,775 km², approximately. The Mucuri's anemometer tower is located in a coastal plain, at a distance of 340 m from the sea, with latitude 18° 1'31.52"S and longitude 39° 30'51.69"W (Figure 1). The time series used in the models consists of 744 data in total, corresponding to hourly mean data for each of the period November 30, 2015, 2:00 p.m. to December 31, 2015, 1:00 p.m.. The training set with 550 data was used for the models' training and validation. The prediction set consisting of 194 data was used to verify their accuracy during the prediction stage. The best ANN configurations for Mucuri are: 100 m: Four layers, nine input nodes (day, month, year, hour, wind speed, wind direction, air pressure, air humidity, air temperature), six hidden neurons (1st hidden layer), three hidden neurons (2nd hidden layer), and one output node (wind speed); 120 m: Four layers, nine input nodes (day, month, year, hour, wind speed, wind direction, air pressure, air humidity, air temperature), six hidden neurons (1st hidden layer), three hidden neurons (2nd hidden layer), and one output node (wind speed); 150 m: Three layers, nine input nodes (day, month, year, hour, wind speed, wind direction, air pressure, air humidity, air temperature), nine hidden neurons, and one output node (wind speed). The aforementioned ANN architectures that were identified as the most efficient for the 1 h forecast for each height were applied in the computational simulation to predict the wind speed for 3, and 6 h in Mucuri at all the heights tested.



Figure 1. Location of the Mucuri tower in Bahia.

FINDINGS AND ARGUMENT

The statistical treatment employed in the results are Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Percentage Error (MAPE), R² coefficient of determination, Pearson's correlation coefficient (r) and percentage of data of factor of two. For these statistical indicators values close to 0.0 (zero) are adequate for the MAE, MSE, RMSE, MAPE errors, and values close to 1.0 (one) are adequate for the R² and Pearson. The Table 1 to Table 2 show the evaluation metrics of the prediction results obtained by the proposed model. The Percentage of the data of a factor of two is a fraction of data [%] for 0.5 ≤ Wind predicted/Wind anemometer ≤ 2.0.

Table 1. Simulation results (Errors): 1, 3 and 6-h wind-speed forecasting for Mucuri using the ANN model.

Anemometer at 100 m				
Prediction horizon	MAE	MSE	RMSE	MAPE
1 h	0.72	0.82	0.91	9.28%
3 h	1.37	3.53	1.88	16.94%
6 h	2.43	13.17	3.63	29.14%
Anemometer at 120 m				
Prediction horizon	MAE	MSE	RMSE	MAPE
1 h	0.73	0.83	0.91	8.95%
3 h	1.18	2.29	1.51	14.30%
6 h	1.67	4.62	2.15	19.45%
Anemometer at 150 m				
Prediction horizon	MAE	MSE	RMSE	MAPE
1 h	0.79	1.02	1.01	9.19%
3 h	1.38	3.22	1.79	15.34%
6 h	2.16	8.58	2.93	22.93%

Table 2. Simulation results (Regression): 1, 3 and 6-h wind-speed forecasting for Mucuri using the ANN model.

Anemometer at 100 m			
Prediction horizon	Pearson	R ²	Percentage of the data of a factor of two
1 h	0.95	0.91	100.0%
3 h	0.81	0.66	98.95%
6 h	0.34	0.12	86.17%
Anemometer at 120 m			
Prediction horizon	Pearson	R ²	
1 h	0.95	0.90	100.0%
3 h	0.86	0.73	100.0%
6 h	0.73	0.53	98.40%
Anemometer at 150 m			
Prediction horizon	Pearson	R ²	
1 h	0.93	0.86	100.0%
3 h	0.79	0.62	100.0%
6 h	0.47	0.22	92.55%

By ascertaining the results recorded in Tables 1 and 2, it is observed that as the wind speed forecasting load increases, there is a reduction in the quality of the output data during ANN prediction so that the higher the forecasting time, the greater the associated error. These results were expected since

the adopted procedure uses the input data from the start of the forecasting, in addition to the wind speed computed in each forecast hour, to predict the n th hour, leading to an increasingly accumulated error. This is in accordance with what the literature describes in Kusiak et al. (2009), Blonbou (2011), Carpinone et al. (2015) and Filik and Filik (2017). The Figure 2 shows: a) The results of six-step predictions of the wind speed series. b) Comparison data of a factor of two (wind predicted/wind anemometer versus time) of the results obtained with the forecast model (six-step predictions) and the real data. c) Comparison data of a factor of two (wind predicted/wind anemometer versus wind anemometer) of the results obtained with the forecast model (six-step predictions) and the real data.

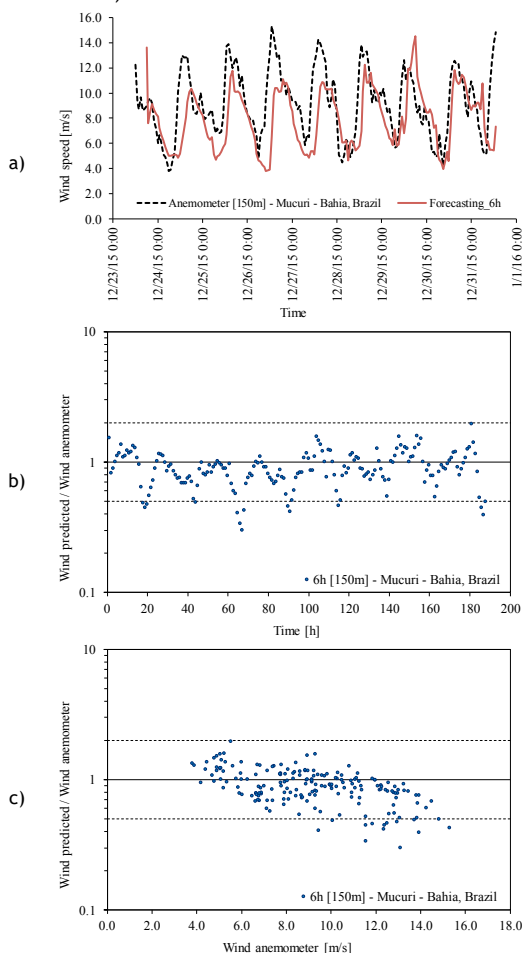


Figure 2. Wind speed forecasting at 6h ahead, 150 m.

CONCLUSIONS

In the light of the statistical results recorded in this work, the application of computational intelligence is a viable alternative for the predictability of wind speed and, in this way, wind power generation, mainly due to the low computational cost, however one must choose the ANN architecture that best

suits the project, as well as quantitatively and qualitatively analyze the available data that will feed the network, since these variables directly impact the results of the forecast. These results are presented as a novelty, since other works that used this computational model to predict wind speed for 1, 3, and 6 hours (nowcasting) in Brazil, especially in the Bahia state, were not found in the literature, particularly for very high positions of the anemometers, where wind turbines are usually positioned. The application of the technique of Artificial Neural Networks to predict the wind speed at different heights was adequate when interpreting the statistical results. Specially, it can be pointed out that the 6 hours forecast presented good results, and, as the forecast time increases, the produced results degrade, as expected. Nevertheless, this degradation did not characterize the results of the forecasting of more hours forward useless, making it possible to use this technique to produce satisfactory forecasts of wind speed for short term applications with low computational costs, in order to help wind farm operators in decision making processes.

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**AIR POLLUTION
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Session 02

**Emissions Inventories,
Models, and Processes**

REAL-WORLD VEHICULAR EMISSION FACTORS OF CARBONYL COMPOUNDS MEASURED IN A RIO DE JANEIRO TUNNEL, BRAZIL

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Abstract: On urban areas on the world, vehicles emissions are a major source of atmospheric impact. In Brazil, the vehicular fleet is fueled with gasohol (gasoline with 27% v/v of ethyl alcohol), ethanol, diesel and natural gas. Rio de Janeiro, the second largest urban center in Brazil, represents the third largest running fleet: 7 million vehicles (light duty, heavy duty, motorcycles and others). According the official emissions inventory local (Rio de Janeiro), roughly 76% of the primary emissions of criteria pollutants are due to mobile sources, for example, 98% of total CO are vehicles emissions. Vehicle emissions are a major source of carbonyls compounds, an important pollutant in atmospheric chemistry and urban air quality. This study summarizes the main results of the campaigns on Rebouças Tunnel, to build a more accurate assessment of the “real world” vehicular emissions factor (carbonyls compounds) coming from the local fleet. The choice of this tunnel as the monitoring spot in Rio de Janeiro is justified by its relevance as a transportation artery linking the South and North portions of the city. Rebouças is an urban tunnel with 2840 m length split into two bores, with three lanes per bore, in which typically traffic density is relatively flat with time and roughly 190000 vehicles pass on a per day basis. The local fleet is predominantly composed of light duty vehicles (LDV), 94%. To calculate the emission factors of carbonyl compounds by method Pierson, one pair of samples was collected simultaneously at the tunnel entrance and exit during each sampling run. The vehicular emission factor is the mass of specific pollutants produced in a unit kilometer. The results, in this study, for vehicular emission factor showed for formaldehyde, acetaldehyde, respectively 8.23 mg km⁻¹ and 14.85 mg km⁻¹.

Keywords: vehicular emission factor, tunnel, carbonyls compounds, Brazil.

INTRODUCTION

Vehicular emission factor is the mass of specific pollutants produced by specific fleet (light duty, heavy duty, motorcycles and others) in a unit kilometre. We have different techniques to measure the vehicular emission factor: chassis dynamometer tests, remote sensing, road tunnel studies and portable emission measurements systems (on board emissions). For example, chassis dynamometer is the test with controlled conditions: temperature, maintenance, driving conditions (speed and acceleration), type of fuel and route. Differently, tunnel studies can measure an “real world” of vehicular emission factor, where in-use vehicles are measured. This study report the main results of the campaigns on Rebouças, an urban tunnel in Rio de Janeiro, to measure vehicle emission factor.

METHODS

To calculate the emission factors of carbonyl compounds pairs of samples were collected simultaneously at the tunnel entrance and exit during each sampling run. The first sampling station was located 500 m inside the entrance of the south bore and the second sampling station was located 1500 m inside the entrance, so the distance of two point was 1000m. The emission factors from tunnel measurements were calculated according to the method of Pierson. The vehicular emission factor is

the mass of specific pollutants produced in a unit kilometer.

$$EF = ((C_{out} - C_{in})A \times U \times t) / (N \times L) \quad \text{Eq. (1)}$$

Where, EF is the average vehicular emission factor in mg km⁻¹ traveled, C_{out} and C_{in} represent the mass concentrations of specific pollutants at the two sampling stations in mgm⁻³, A is the area of tunnel cross-section in m², U is the wind speed in ms⁻¹, t is the sampling duration, N is the number of vehicles and L is the distance between sampling points (km). To measure speciated atmospheric carbonyls, nine campaigns and two samples per campaign were collected. The sampling system consist a pump with battery. Cartridges with C18 resin impregnated with 2,4-dinitrophenylhydrazine (DNPH) were used. The sampling system runned at the flow rate of 1.0 lmin⁻¹. A total of 18 samples were collected from Setember 2018 to March 2019.

The samples were analysed by Agilent Technologies 1100 Series high performance liquid chromatography with an binary pump (G1379A), auto-sampler (G1313A), degasser (G1379A) and a UV-DAD detector (λ = 360 nm). The method followed the U.S. EPA guideline TO-11A (US EPA, 1997).

Information regarding total traffic flow and vehicle speed were provided by a data acquisition and management package called TESC, Model Flexcode IV, run by the Tunnel Administration, and made available for this study. The whole system included primary sensors for counting vehicles and calculating speed; additionally classification into main categories (regarding only vehicle size and speed) was provided on regular basis.

FINDINGS AND ARGUMENT

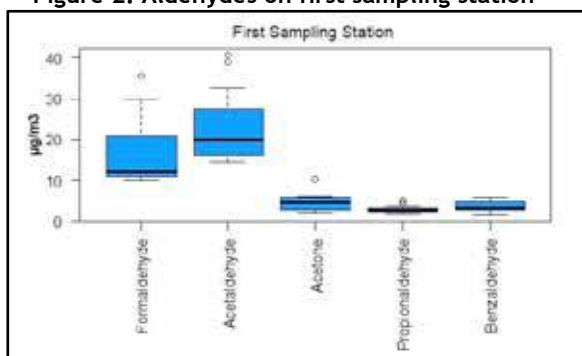
The vehicle counting included all vehicle categories, without distinguishing types of fuels or vehicle types and sizes. As shown in Figure 1 the fleet profile is practically constant with time, and the LDV fleet represents roughly 94% of the local traffic.

Figure 1. Vehicle Counting



Were identified five aldehydes on first sampling station, the most abundant carbonyls emitted by vehicles at the tunnel was acetaldehyde.

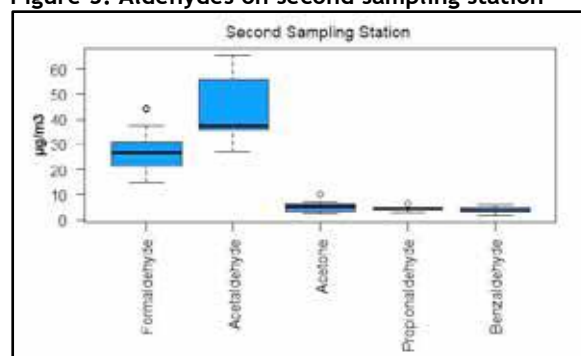
Figure 2. Aldehydes on first sampling station



The measured concentration levels are also a reflex of the location of the monitoring station (about 1.5 km inside the uphill tunnel gallery, thus potentially maximizing the emissions).

Figure 3 shows the results of all aldehydes identified on second sampling station

Figure 3. Aldehydes on second sampling station



The emission factors of aldehydes from the vehicles in Rebouças tunnel were calculated by the following Eq. (1). The total measured carbonyls emission factors ranged from 0.83 to 13.82 mg km⁻¹. The acetaldehyde and formaldehyde emission factors in tunnel contributed more than 97% of the total measured carbonyl emission.

Table 1. Emission factors calculated from Rebouças tunnel

Carbonyl	Emission Factor(mg km ⁻¹)
Formaldehyde	7.46 ± 2.6
Acetaldehyde	13.82 ± 5.7
Acetone	0.41 ± 0,41
Propionaldehyde	1.12 ± 1,12
Benzaldehyde	0.86 ± 0,81

CONCLUSIONS

The most abundant emission factor calculated was acetaldehyde, this value can be linked to the Brazilian composition of fuels used by the vehicular fleet of Brazil, where 88% of the vehicles sold in 2018 were Flex-fuel and alcohol consume increase 16,3% in 2018 when compared with 2017.

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VEHICULAR EMISSION FACTOR BASED ON BURNED FUEL - TUNNEL REBOUÇAS CASE, RIO DE JANEIRO

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Abstract: On urban areas on the world, vehicles emissions are a major source of atmospheric impact. In Brazil, the vehicular fleet is fueled with gasohol (gasoline with 27% v/v of ethyl alcohol), ethanol, diesel and natural gas. Rio de Janeiro, the second largest urban center in Brazil, represents the third largest running fleet: 7 million vehicles (light duty, heavy duty, motorcycles and others). According to the official emissions inventory local (Rio de Janeiro), roughly 76% of the primary emissions of criteria pollutants are due to mobile sources, for example, 98% of total CO are vehicles emissions. Vehicle emissions are a major source of carbonyls compounds, an important pollutant in atmospheric chemistry and urban air quality. This study summarizes the main results of the campaigns on Rebouças Tunnel, to build a more accurate assessment of the “real world” vehicular emissions factor (carbonyls compounds) coming from the local fleet. The choice of this tunnel as the monitoring spot in Rio de Janeiro is justified by its relevance as a transportation artery linking the South and North portions of the city. Rebouças is an urban tunnel with 2840 m length split into two bores, with three lanes per bore, in which typically traffic density is relatively flat with time and roughly 190000 vehicles pass on a per day basis. The local fleet is predominantly composed of light duty vehicles (LDV), 94%. To calculate the emission factor based on burned fuel, two measuring sites were used; the first placed at a distance of about 500 m from the entrance of the tunnel, and the second at a distance of about 1500 m from the entrance. Fuel-based emission factor can be defined as the grams of pollutant emitted for every kilogram of fuel burned, using the following equation. The vehicular emission factor is the mass of specific pollutants produced in a unit kilometer. The results, in this study, for vehicular emission factor showed for formaldehyde, acetaldehyde, respectively 1,91 mg km⁻¹ and 3,61 mg km⁻¹.

Keywords: vehicular emission factor, tunnel, carbonyls compounds, Brazil.

INTRODUCTION

Vehicular emission factor is the mass of specific pollutants produced by specific fleet (light duty, heavy duty, motorcycles and others) in a unit kilometre. We have different techniques to measure the vehicular emission factor: chassis dynamometer tests, remote sensing, road tunnel studies and portable emission measurements systems (on board emissions). For example, chassis dynamometer is the test with controlled conditions: temperature, maintenance, driving conditions (speed and acceleration), type of fuel and route. Differently, tunnel studies can measure a “real world” of vehicular emission factor, where in-use vehicles are measured. This study report the main results of the campaigns on Rebouças, an urban tunnel in Rio de Janeiro, to measure vehicle emission factor.

METHODS

To calculate the emission factor pairs of samples were collected simultaneously at the tunnel entrance and exit during each sampling run. The first sampling station was located 500 m inside the entrance of the south bore and the second sampling station was located 500 m upwind of the exit. The emission factors to this study were calculated based on burned fuel. The vehicular emission factor is the

mass of specific pollutants produced in a unit kilometer.

$$EF = \Delta[P] / (\Delta[CO_2] + \Delta[CO]) \times w_c \quad \text{Eq. (1)}$$

Where: $\Delta[P]$ (pollutant), $\Delta[CO_2]$ and $\Delta[CO]$ are the concentration on second station (about 1500 m from the entrance of the tunnel) subtracted concentration of a certain pollutant on first station (distance of about 500 m from the entrance), given in $\mu\text{g m}^{-3}$. w_c is the carbon weight fraction of the fuel (0.85 for gasoline or 0.87 for diesel). To measure speciated atmospheric carbonyls, nine campaigns and two samples per campaign were collected. The sampling system consist a pump with battery. Cartridges with C18 resin impregnated with 2,4-dinitrophenylhydrazine (DNPH) were used. The sampling system runned at the flow rate of 1.0 lmin⁻¹. A total of 18 samples were collected from September 2018 to March 2019. A continuous analyser measured CO using an electrochemical cell, and CO₂ using Non-Dispersive Infrared (NDIR) method.

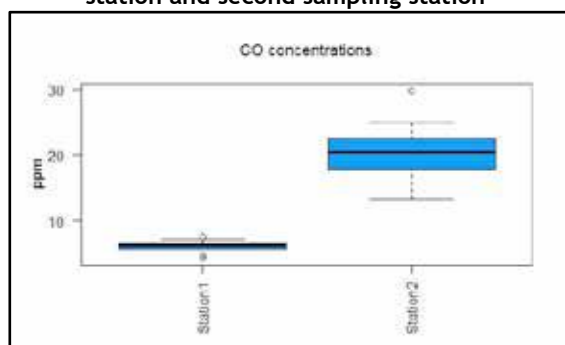
The samples were analysed by Agilent Technologies 1100 Series high performance liquid chromatography with an binary pump (G1379A),

auto-sampler (G1313A), degasser (G1379A) and a UV-DAD detector ($\lambda = 360$ nm). The method followed the U.S. EPA guideline TO-11A (US EPA, 1997).

FINDINGS AND ARGUMENT

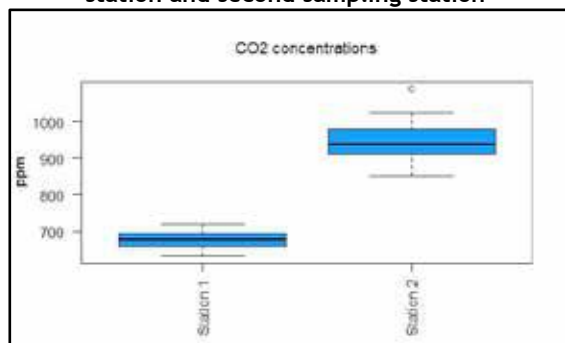
To measured CO concentrations was used a continuous analyser using an electrochemical cell. The first station was installed at a distance of about 500 m from the entrance of the tunnel, and the second at a distance of about 1500 m from the entrance. Figure 1 shows the results of CO on first and second sampling stations.

Figure 1. CO concentrations on first sampling station and second sampling station



To measured CO₂ concentrations was used a continuous analyser Non-Dispersive Infrared (NDIR) method. The first station was installed at a distance of about 500 m from the entrance of the tunnel, and the second at a distance of about 1500 m from the entrance. Figure 2 shows the results of CO₂ on first and second sampling stations.

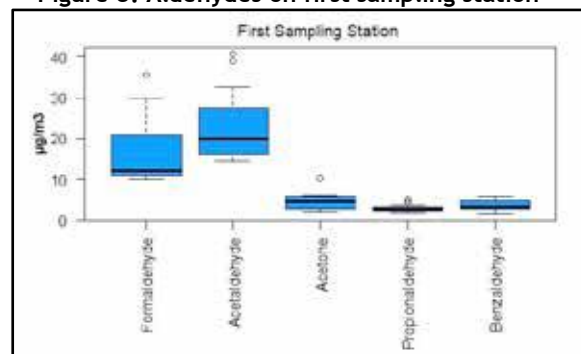
Figure 2. CO₂ concentrations on first sampling station and second sampling station



Were identified five aldehydes on first and second sampling stations, the most abundant carbonyls emitted by vehicles at the tunnel was acetaldehyde.

Figure 3 shows the results of all aldehydes identified on first sampling station

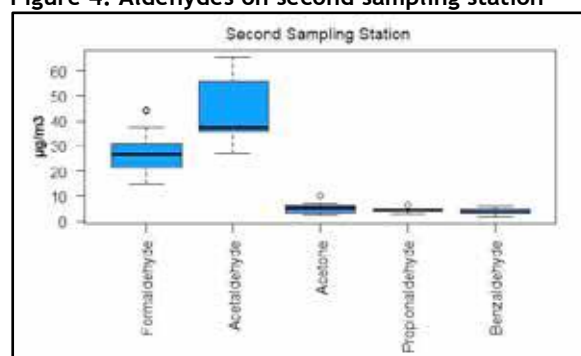
Figure 3. Aldehydes on first sampling station



The measured concentration levels are also a reflex of the location of the monitoring stations (inside the uphill tunnel gallery, thus potentially maximizing the emissions).

Figure 4 shows the results of all aldehydes identified on second sampling station

Figure 4. Aldehydes on second sampling station



The emission factors of aldehydes from the vehicles in Rebouças tunnel were calculated by the following Eq. (1). The total measured carbonyls emission factors ranged from 0.07 to 3.61 mg km⁻¹. The acetaldehyde emission factors in tunnel contributed more than 63% of the total measured carbonyl emission.

**Table 1. Emission factors calculated from
Reboucas tunnel**

Carbonyl	Emission Factor(mg km ⁻¹)
Formaldehyde	1,91
Acetaldehyde	3,61
Acetone	0,09
Benzaldehyde	0,07

CONCLUSIONS

The most abundant emission factor calculated was acetaldehyde, this value can be linked to the Brazilian composition of fuels used by the vehicular fleet of Brazil, where 88% of the vehicles sold in 2018 were Flex-fuel and alcohol consume increase 16,3% in 2018 when compared with 2017.

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STUDIES OF AIR QUALITY IN THE METROPOLITAN REGION OF PORTO ALEGRE USING NUMERICAL MODELING

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Abstract: The Metropolitan Region of Porto Alegre (MRPA) consists of 34 municipalities, the greater Porto Alegre (GPA - capital of Rio Grande do Sul state - south of Brazil), has a territorial area of 10,345.45 Km², concentrating more than 4 million inhabitants. However, the MRPA has insufficient coverage of air quality monitoring and poor information from emission inventories. The strategy adopted by the Atmospheric Pollution Group (GEPA-UFPEL) is to analyze the air quality with the use of the numerical modeling, specifically with the Brazilian Developments of Regional Atmospheric Modeling System (BRAMS). In this step, it was decided to evaluate the impact of vehicular emissions on the dispersion of pollutants for the base year 2016 and the ozone formation in future scenarios. The first study aims to study of the dispersion of pollutants in MRPA, was simulated two periods - January 2009 and January 2016 - using emission information from the precursor gases inventories developed by FEPAM for the base years of 2009 and 2011, respectively. The emissions were distributed in the traffic streets and merged with the inventory prepared exclusively for the BR 116 highway, that crosses the GPA, using the PREP-CHEM-SRC emissions preprocessor. In general, the simulations consistently represented the data observed by the monitoring network. The results also revealed that concentration of GPA was influenced by approximately 60/40% (2009) and 55/65% (2016) by local sources and regional transport, respectively. In the second study, considering mainly the ozone precursor species and carbon monoxide and using the year 2001 as a base year, scenarios are obtained for vehicular emissions of pollutant gases in the MRPA until the year 2030. In addition, scenarios related to the evolution of the study region's vehicle fleet were estimated. The statistical tool LEAP (Long Range Energy Alternatives Planning System) was used. The scenario analysis shows that the vehicle fleet will grow exponentially until 2030, considering that the Light Flex vehicles category will mainly contribute to this increase. It is also noted that vehicle emissions of CO, NO_x, and THC decrease in the region. This decrease was caused mainly by the renewal of technology fleet and the implementation of emission control programs created by the government. In addition, was performed ozone formation/destruction simulations using BRAMS. The reduction in the emissions caused a decreasing in the NO_x average concentrations estimated for 2030 and an increasing in the ozone average concentrations of at night and morning and decline of this species in afternoon and early evening. It was also possible to observe the influence of reduced emissions in MRPA on levels of O₃ and NO_x in the neighboring areas, demonstrating the strong impact of major urban centers in the towns and surrounding areas.

Keywords: Vehicular inventory, BRAMS, MRPA, emission scenarios.

INTRODUCTION

In the environmental pollution, the air pollution has an important role, it affects considerably and in different ways the life of organisms. In polluted environments, such as large urban areas, human health can be severely damaged in medium and long terms, because of poor air quality. Several studies have been showing the strict relation between the air quality, the respiratory and cardiovascular diseases (Arbex et al. 2012, Santos et al. 2008). Particularly, in the Metropolitan Region of Porto Alegre (MRPA), that concentrate more than 4 million inhabitants, the insufficient coverage of air quality monitoring and poor information from emission inventories encourages studies of dispersion and chemistry of pollutants using numerical models and more accurate inventories. The strategy adopted by the Atmospheric Pollution Group (GEPA-UFPEL) is to analyze the air quality with the use of Brazilian Developments of Regional Atmospheric Modeling

System (BRAMS). For MRPA, it was decided to evaluate the impact of vehicular emissions on the dispersion of pollutants for the base year 2016 and the ozone formation in future scenarios. The first work aims to study of the dispersion of pollutants in MRPA, was simulated two periods - January 2009 and January 2016 - using emission information from the precursor gases inventories developed by FEPAM for the base years of 2009 and 2011, respectively (Silva, 2018). The Second one, considering mainly the ozone precursor species and carbon monoxide and using the year 2001 as a base year, scenarios are obtained for vehicular emissions of pollutant gases in the MRPA until the year 2030 (Chovert and Alonso, 2017).

METHODS

The CCATT-BRAMS (Coupled Aerosol and Tracer Transport model to the Brazilian developments in the Regional Atmospheric Modeling System), is an Eulerian model of atmospheric chemical transport

coupled in line with a limited atmospheric area model. The system is designed for local and regional studies of atmospheric and low-stratospheric chemistry for both operational and research purposes (Longo et al., 2013). Currently the model is in version 5.2 (BRAMS 5.2 - Freitas et al., 2017).

The modeling system has three pre-processors: a) Simplified Preprocessor for Atmospheric Chemical Kinetics (SPACK) tool that allows the choice of chemical mechanism; b) PREP-CHEM-SRC (Freitas et al., 2011) which has the function of compiling pollutant emission data into the atmosphere and c) DPREP-CHEM that generates the initial and boundary conditions for the chemical species to be used in the simulation of the model.

More specifically, the PREP-CHEM-SRC preprocessor is a tool developed to provide information on trace gas and aerosol emissions at any spatial resolution making it suitable for use in both global and regional models for dispersion and chemistry of pollutants. Currently the tool covers emissions from urban / industrial, biogenic, biomass burning and volcanic sources.

To elaborate the emission scenarios, was used the LEAP (Long range Energy Alternatives Planning System) that is an integrated modeling tool that can be used to conduct a study about the energy consumption, production and the extraction of resources in all the sectors of an economy. It is also applicable to determine the greenhouse gases emissions in the energetic and non-energetic sectors. The LEAP has the capacity to operate in two different conceptual levels, in the first level the calculations incorporated in the LEAP take charge of measuring and working with all the non-conventional energy, the emissions and the effective cost accounting. In the second level, the users introduce information that can be used to specify the temporal variation to be applied in the first level (<http://www.energycommunity.org>).

Dispersion Study of Carbon Monoxide (CO)

To elaborate more accurate inventory, was used information from two inventories developed by FEPAM environmental agency. The methodology proposed in the reports follows the US Environmental Protection Agency (EPA) and the data collection was of the Bottom-Up type.

Was elaborated an estimate of CO emission from vehicular sources circulating on the BR 116 highway, crossing the urban zone, not inventoried by FEPAM. The "Bottom-Up" methodology proposed by the North American Environmental Protection Agency (EPA) was also applied for the elaboration of this inventory, applying the appropriate adaptations proposed by Silva et al. 2016.

The emission factors used were obtained in CETESB and later corrected by a deterioration factor (Silva et al., 2016). The vehicular density was provided by

the National Traffic Contingency Plan (PNCT - DNIT) for the toll booth located in the municipality of São Leopoldo.

With aim to obtain a spatial distribution, it was considered that the largest vehicular emission is found in the central region of these municipalities (central and surrounding neighborhoods), with a contribution of 60 percent of the total emission estimated by the FEPAM inventory, and the remainder distributed among other peripheral urban areas. For the greater Porto Alegre (capital city), it was considered that 60% of the total emission estimated by the FEPAM inventory is concentrated in the primary runways and the remainder in other categories (figure 1).

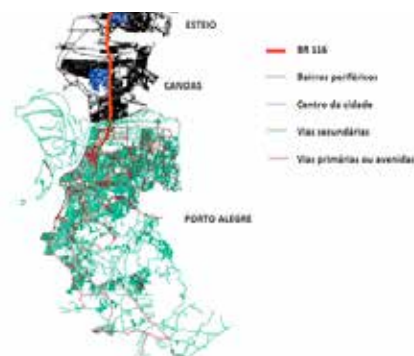


Figure 1 - Route map showing the layout used for the emissions distribution.

The simulations are conducted in BRAMS 5.2, to January 2009 and January 2016, using a domain with 20km over Rio Grande do Sul state and 2km over MRPA. Some experiments are conducted to analyze regional transport contribution over Greater Porto Alegre. The simulated CO mixing ratio was validated with observational data from air quality stations of Esteio, Porto Alegre and Canoas municipalities (FEPAM).

Emissions Scenarios and ozone simulations

A big set of data has been recompiled from several sources; these ones have been analyzed and inserted in the LEAP statistic tool. The selected basis year, or start year, for the creation of the scenarios was 2001, and this is because in this year precisely is that it has the first detailed information about the vehicles license by Brazilian municipalities. The scenario hypothesis was constructed follow table 1.

To separate by type of fuel for the period between 2016 and 2030, it was applied the same percentage utilized in 2014 in the licenses of this period.

Table 1. Raise Percentage of the new vehicles licenses by categories between the years 2016 and 2030.

Vehicle category	Pessimistic growth	Optimistic growth
Light Vehicles	6.6%	3.8%
Light Commercial	6.6%	3.8%
Trucks	5%	3% (2016-2025) 1.5% (2026-2030)
Motorcycles	4.4%	3.8%
Bus	1.7%	1.7%

Source data available in Chovert and Alonso, 2017.

The simulations were conducted with BRAMS 5.2. The 2009 was the base year for analysis and the 2030, the study year. The coarse grid cover Rio Grande do Sul state with 50km of spatial resolution. The finer grid cover MRPA and has 10 km of spatial resolution.

FINDINGS AND ARGUMENT

Dispersion Study of Carbon Monoxide (CO)

Using the proposed inventory, it can be concluded that the highest carbon monoxide emissions are found in the cities of Greater Porto Alegre and the central region of the satellite cities of MRPA. When comparing the time series and diurnal cycle of the stations analyzed in the year 2009, we can see a good representation of the model for the stations located in the municipalities of Porto Alegre, Esteio and Canoas.

Another important point is the regional transport of carbon monoxide in the Greater Porto Alegre. Comparing the proposed simulations, it was possible to verify that the cities to the north of the capital influenced significantly their local concentration, being responsible for 40% of the local carbon monoxide simulated by the model. In fact, the emission of the great Porto Alegre is responsible for only 60% of the CO local concentration and the predominant average wind is also from east - southeast (figure 2). This is a counterpoint to the premise that only the Greater Porto Alegre influences concentrations of pollutants in the neighboring cities of the MRPA.

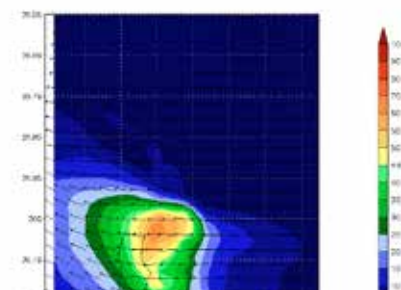


Figure 2 - Percentage of contribution (%) of the Greater Porto Alegre (GPA), between 01/01/2016 (21:00 local time) to 25/01/2016 (00:00 local time)-> [CO (All cities) - CO (without GPA) / CO (All cities) x 100].

Emissions Scenarios and ozone simulations

It was obtained scenarios of quantity of vehicles for each one of the seven categories of studies in the period between 2002 and 2030, having as basis year 2001. It was created the pessimistic scenario (with the biggest quantity of licensing in the period) and the optimistic one (with the least quantity of license in the period).

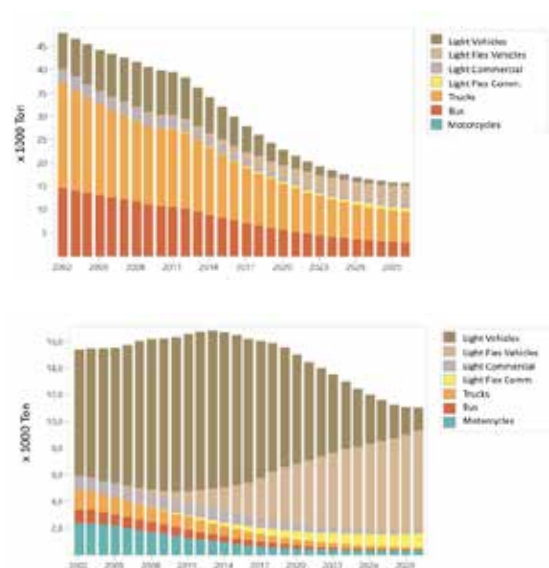


Figure 3 - Emission scenarios of NOx (up) and NMHC (Bottom) in the MRPA (associated with the pessimistic estimation of the fleet) for the period between 2002 and 2030.

With relation to Ozone (O_3), variations in the emissions of the main precursors (NO_x and NMHC) caused an increase in the average concentrations in the evening and in the morning as well as a decrease for this pollutant in the afternoon and early evening (figure 4). In general, when analyzing daily averages, there is an increase in concentrations of O_3 in the municipalities with the greatest circulation of vehicles and surroundings. This is due to the fact that there is not enough nitrogen in the absence or minimum photolysis period for the ozone depletion reactions in this interval. The spatial analysis of the concentrations of pollutant gases showed the influence of the emissions in the MRPA on the concentrations recorded in the surrounding areas, evidencing the strong impact of large urban centers in neighboring municipalities and rural areas (figure 5).

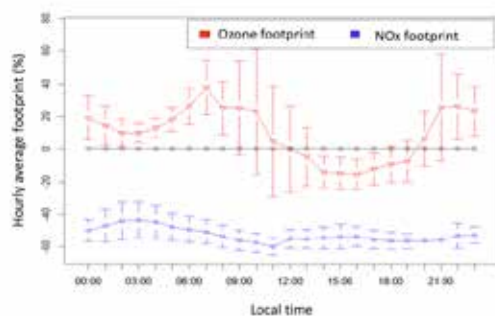


Figure 4 - Ozone and NO $_x$ footprint of difference between 2030 and 2009 simulations.

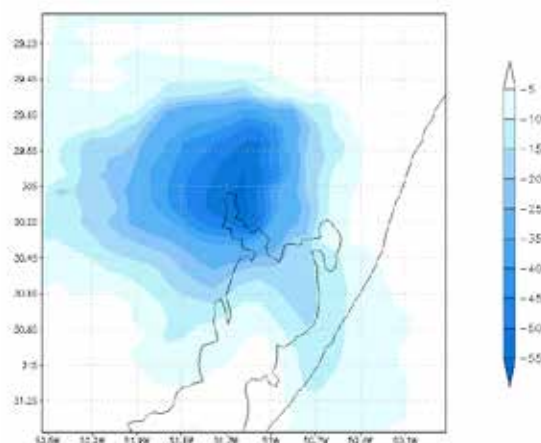


Figure 5 -Difference between 2030 and 2009 NO $_x$ simulations (%).

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SPATIAL DISTRIBUTION OF THE BRAZILIAN OFFICIAL VEHICULAR EMISSION INVENTORY FOR AIR QUALITY MODELING

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Abstract: Vehicles are usually responsible for the largest emissions of CO and NO_x, besides significant emissions of PM, and the use of a vehicle emission inventory (VEI) in an urban area is an important tool for air quality purposes. This work evaluates the emission spatial distribution of the national VEI of 2013. The Brazilian total emission of PM, CO, and NO_x from vehicular sources were distributed into the urban areas of 5557 municipalities, with 1 km² grid resolution, considering two approaches: population and fleet. A comparison with some local inventories is discussed. Additionally, the inventory was compiled in PREP-CHEM-SRC and a 2-day modeling was performed with BRAMS model for the Metropolitan Area of Belo Horizonte (MG), Brazil. Comparing to the local emissions inventory, PM was better represented by fleet distribution, while CO and NO_x were better represented by population segregation. The air quality modeling showed the importance of the distributed emissions carried out in this work.

Keywords: Vehicular inventory, emission, population, fleet, Brazil.

INTRODUCTION

Emissions inventories of atmospheric pollutants are strategic environmental management tools and its development is the starting point for the successful implementation and reorientation of any program that aim to improve air quality. This work evaluates the spatial distribution of the Brazilian official vehicular emission inventory based on population and fleet for air quality modeling purposes, since limited number of local inventories is found in Brazil.

METHODS

The total annual PM (63,000 t), CO (1,300,000 t) and NO_x (1,163,000 t) emission estimated for 2013 by Brazilian Ministry of the Environment - MMA (2014) were distributed among the cities considering two approaches: population and fleet. In 2015, the Brazilian population was estimated in around 204 million inhabitants, and the fleet was 90.6 million vehicles. PM emissions considered exhaust and wear from tire, break, and road surface.

After distribution, the emissions for each city (in t year⁻¹) were recalculated considering its correspondent urban area (in t year⁻¹ km⁻²). The polygons that represents each urban area containing the emissions was converted in raster format with 1 km grid spacing. After, each raster grid cell was converted into point, and PM, CO and NO_x emission values for each point were summarized in a .txt file and compiled in PREP-CHEM-SRC v.1.5 (Freitas et al., 2011). Based on Santos (2018), it was considering that 63.1% of the total PM is PM_{2.5} and 86.3% is PM₁₀.

A 2-day modeling (1-day as spin-up) was performed with BRAMS v.5.2 (Freitas et al, 2017). The air quality modeling considered only the pollutants dispersion. Two nested domains were used covering the metropolitan area of Belo Horizonte (MG), Brazil. The domain D01 has a grid spacing of 25 km with 32 grid-cells in both longitudinal and latitudinal extensions. The domain D02 has a grid spacing of 5 km with 40 grid cells in both longitudinal and latitudinal extensions, forming a domain of 200 × 200 km, centered in -19.90° S and -43.95° W. The vertical structure was represented by 32 vertical levels, starting in 80 m and increased at a rate of 1.09 to the level of 9,930 m, wherein the height increases at a constant rate of 950 m until around 12,780 m. The initial and boundary conditions were obtained from the National Center for Environmental Prediction (NCEP) Global Forecast System (GFS) final (FNL) with a six-hour time resolution, 26 vertical levels, and a horizontal resolution of 0.25 × 0.25 degrees (ds083.3).

FINDINGS AND ARGUMENT

Figure 1 shows the raster output containing PM emission (population distribution) allocated in the urban areas. A zoom was made highlighting emissions from Brazilian southeast capitals. As emissions are depended on population (or fleet), the capitals presented higher values, but small cities, with limited urban area, may present higher emissions when it is normalized by 1 km resolution.

Tables 1, 2, and 3 summarizes PM, CO and NO_x emissions, respectively, for Belo Horizonte (BH), and Metropolitan Areas of Rio de Janeiro (MARJ),

São Paulo (MASP), Vitória (MAV), and Fortaleza (MAF), comparing the estimated emission with a local reference.

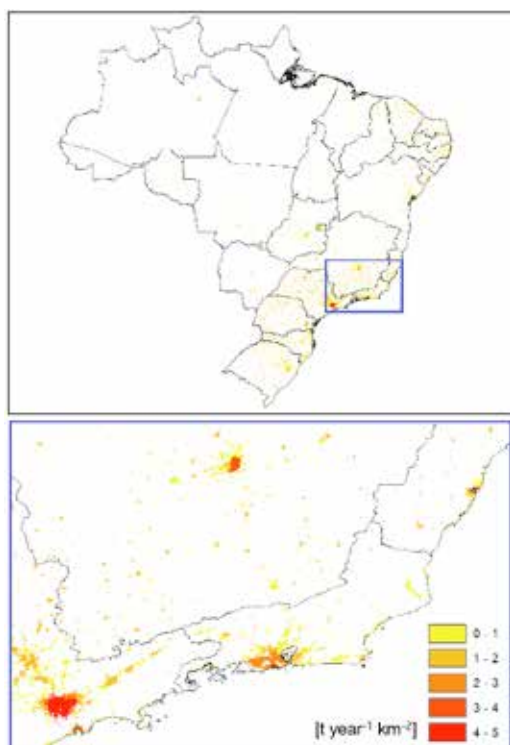


Figure 1 - PM emission [$\text{t year}^{-1} \text{ km}^{-2}$].

Table 1: PM emission [ton year^{-1}].

	Reference	Pop.	Fleet
BH ¹	1220	772	1192
MARJ ²	351	3779	3063
MASP ³	1529	6508	8523
MAV ⁴	490	546	523
MAF ⁵	604	1052	844

Table 2: CO emission [ton year^{-1}].

	Reference	Pop.	Fleet
BH ¹	16574	15934	24598
MARJ ²	25334	77976	63212
MASP ³	127157	134288	175879
MAV ⁴	11237	11272	10787
MAF ⁵	72863	21715	17416

Table 3: NO_x emission [ton year^{-1}].

	Reference	Pop.	Fleet
BH ¹	13992	14255	22006
MARJ ²	14912	69758	56550
MASP ³	54355	120136	157344
MAV ⁴	8942	10084	9651
MAF ⁵	15036	19426	15581

¹Santos (2018); ²INEA (2016); ³CETESB et al. (2016); ⁴IEMA et al. (2019); ⁵Policarpo et al. (2018).

A better agreement of the estimated emission was obtained for BH, MAV and MAF, when comparing to

the local emissions inventories. Depending of the region/city, the emissions estimated using population segregation may be higher or smaller than when fleet distribution is used.

For PM, the fleet segregation presented smaller but closer emission value for BH. Although higher than the references, this distribution was also the best for MAV and MAF. It is highlighted that for MARJ, INEA (2016) considered only the exhaust emissions, and for MASP, the MP estimated by CETESB (2016) considered just flex-fuel vehicles using Gasoline C. Therefore, the total PM for MARJ and MASP may be underestimated in the references. For CO, the population basis obtained better results. For example, for MAV the estimated emission was just 0.3% higher. For NO_x, population distribution was better for BH, while fleet distribution better represented the emissions of MAV and MAF.

The PM_{2.5} emission (population distribution) generated by PREP-CHEM-SRC for domain D02 is shown in Figure 2 (5 km grid spacing). The maximum emission occurs in Belo Horizonte (4.76 kg km⁻²). The metropolitan region is highlighted in white boundaries.

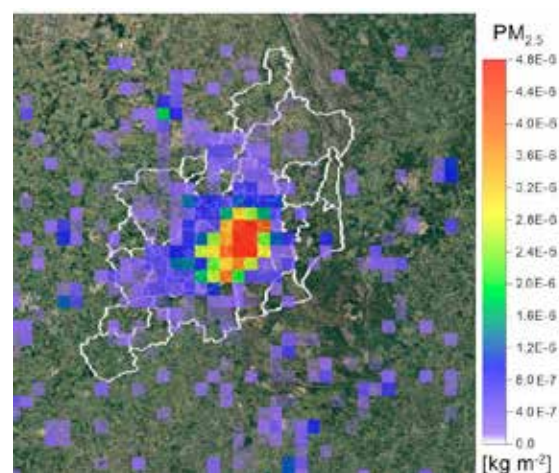


Figure 2 - PM_{2.5} emission [kg km^{-2}] for D02.

Figures 3 and 4 shows the CO and PM_{2.5} daily average (Aug. 02nd) concentration, respectively, considering (a) population and (b) fleet emission segregation. The daily maximum concentration was higher for fleet distribution: PM_{2.5 pop} = 3.86 $\mu\text{g m}^{-3}$; PM_{2.5 fleet} = 5.66 $\mu\text{g m}^{-3}$; CO_{pop} = 92.6 ppb; and CO_{fleet} = 107.9 ppb. These concentrations occurred in the western part of Belo Horizonte and in the cities of Contagem and Betim, demonstrating the east wind action, characteristic of the region. If the role of aqueous chemistry, point source emission, and biomass burning is considered, for example, the concentration results may be higher than those presented here. However, the importance of the vehicular emission is well demonstrated.

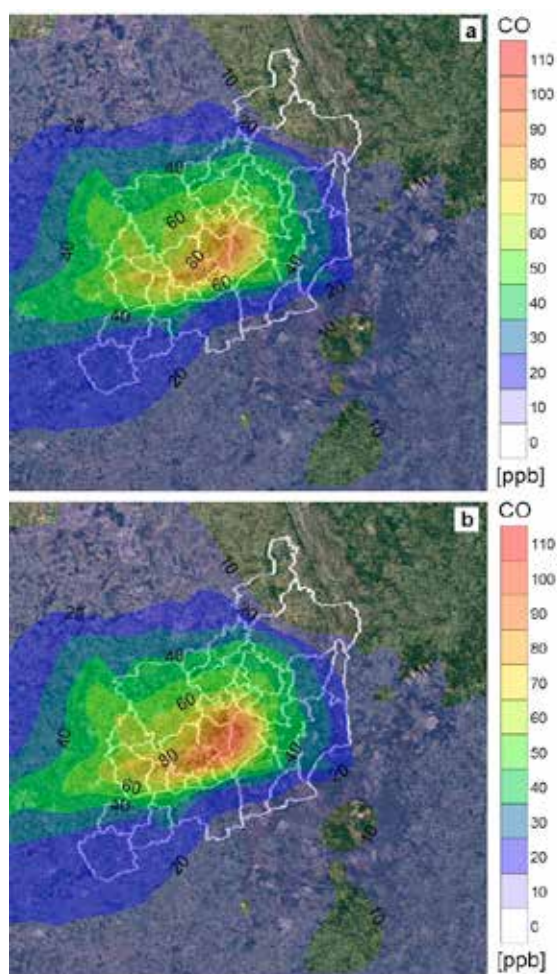


Figure 3 - CO concentration [ppb] for a) population and b) fleet.

CONCLUSIONS

The vehicle emission inventory proposed in this work showed as a reasonable tool for air quality modeling, especially for region that do not have any information of pollutants emission. Additionally, other emissions/inventories may be merged in PREP-CHEM-SRC, as for example, EDGAR, MEGAN and 3BEM. The fleet distribution showed be more adequate in the total PM emission estimated, while CO and NO_x was better estimated considering population distribution.

ACKNOWLEDGEMENTS

Authors acknowledge CAPES.

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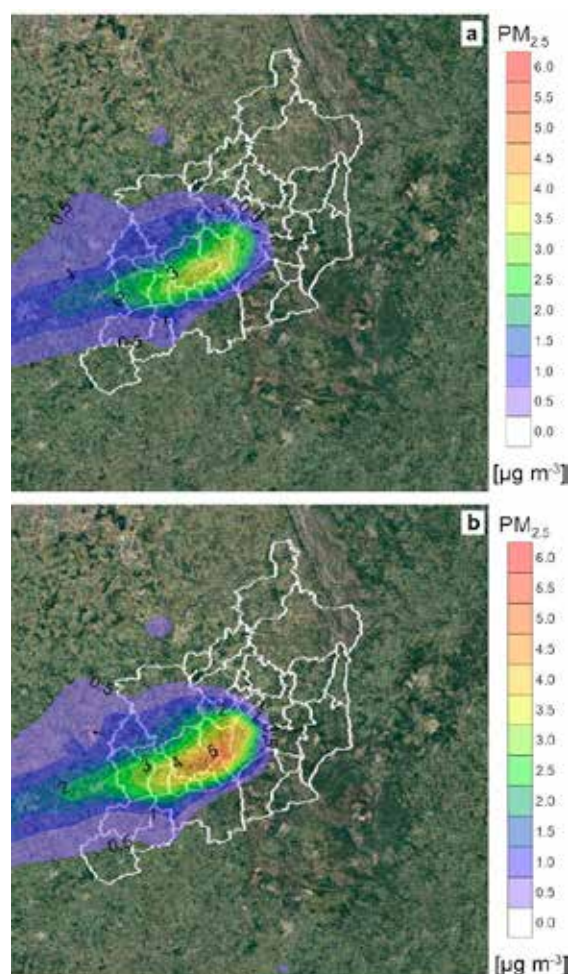


Figure 4 - PM_{2.5} concentration [µg m⁻³] for a) population and b) fleet.

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INVENTORY OF ATMOSPHERIC EMISSIONS STATIONARY SOURCES MONITORED FROM RIO DE JANEIRO STATE - YEAR BASE 2017

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Abstract: Air pollution is a growing threat to human well-being and ecological welfare, since the pollutants emissions and the fast urban and industrial increase rates seen in Brazil in the last few decades are directly related, the local air quality decreases. In this context, the dynamic of the atmosphere degradation is better understood when the main emission sources are acknowledge, as well as their variability over time. Through this better understanding of the processes responsible for the emissions, it is easier to establish qualified interventions to avert or minimize the formation, emission and exposure of the pollutants. Furthermore, it's developed an essential environmental management mechanism with strategies that reduce air contaminants effects, which is called emissions inventory. This mechanism assemble information regarding the type, amount, location, and level of distribution about the emissions, therefore, it is possible to identify ascendant spots and analyse the divisions and specific pollutants that are discharged into the atmosphere and deteriorate air quality in certain locations. In the sight of public politics, inventories helps in the elaboration of programs that assist, prevent and control air pollution, also annual trends of reduction or increase of certain pollutants and emission reduction monitoring progress. In advance, the main proposal of this research was to inventory Rio de Janeiro's atmospheric emissions from stationary sources. At the beginning, all industrial processes around the state, from enterprises associated with Stationary Sources Atmospheric Emissions Monitoring Program (PROMON AR) were quantified. The program is part of Air Quality Management from an Institute, called Environment Institute of Rio de Janeiro State (INEA), as well as these companies monitored data for the pollutants: particulate matter (PM), sulfur dioxide (SO₂), carbon monoxide (CO), volatile organic compounds (VOC) and nitrogen oxides (NO_x). Thenceforth, industrial emissions sources were georeferenced in order to assemble the result by sectors, such as city and/or state locality, and at the end, the full concentration emitted by each pollutant monitored in 2017 was quantified. As initial results, 564 sources (for Rio de Janeiro's stationary sources) allocated in 112 companies. The pollutants rates emitted from the mentioned sources are: 32060, 4379, 8967, 27060 and 186 tons per year for NO_x, CO, PM, SO₂ and VOC, respectively. Diagnosis, modelling and air quality management can contribute to the results obtained in this inventory at Rio de Janeiro.

Keywords: atmospheric emission, emissions inventory, stationary sources, atmospheric pollution, Rio de Janeiro.

INTRODUCTION

Air pollution is a growing threat to the ecosystem and it's directly affecting human health, with a direct relation to several health complications. Its generation and control includes a complex relation with human activities, along with urban and industrial growth, which degrades air quality. Thinking about depollution includes an important financial cost and hard to be estimated, since present and future consequences are not accurately known. (BRILHANTE, 1999)

Thus, CONAMA (1989) founded the Air Quality Control National Program - PRONAR, in order to protect health and well-being through environmental management. Furthermore, this Council suggests the assembling of a national inventory about sources and air pollutants as a subsidy to PRONAR, with the purpose of developing

methodologies that enable emissions registration and estimation, just like air pollution sources data processing.

In order to continue the PRONAR, in 2003, the inventory of the cities of Rio de Janeiro's metropolitan zone was elaborated based on 2001 datas, and its results were used at this paper. Then, the environmental agency established the range, the methodology, the types of sources, large and medium-sized companies priorities, such as the referenced base year used (PIRES,2005).

Aiming to inventory again the state's stationary sources using the Stationary Sources Monitoring Program - PROMON AR, the activities of companies industrial sources were classified, if they attended the Program under the responsibility of Air Quality Management of State Environmental Institute (INEA) in 2017. This self-monitoring program establishes

general procedures to stationary sources association responsible for a higher level of polluting potential, which is defined by its environmental permits.

This paper's main purpose is to present the total emission of the chosen pollutants in the year of 2017, derived from monitored stationary sources through PROMON AR, as a first step towards a future implementation of a new stationary source state inventory.

METHODS

The developing procedure of stationary sources inventory at 2001, took place from 500 priority companies selected according to the overall pollutant potential, defined by the Environmental Agency simultaneously with Classification of Pollutants Activities - CAP, classification system implemented by FEEMA. Afterwards, some companies were rejected from this selection as consequence of deactivation, insignificant atmospheric emission or absence of documentation. Accordingly, in this study was used a supplementary list of the companies which were added and at the end, amounted 425 with significant results (PIRES, 2005).

The main information used at this inventory was obtained from licences, prioritizing industrial registrations and the environmental technicians' inspection reports. Subsequently, in order to calculate the emissions, each source was assigned to one of the methods of emissions estimation, according to EPA methodology (1997b), which are: continuous emission monitoring system, source monitoring, mass balance, emissions factors, fuel analysis, emission estimation models and engineering judgement.

The priority methods would be the continuous emission and sources monitoring, due to the best quality of data produced. However, at the time, there was no applications of any source to continuous monitoring, and beyond that, source monitoring would be infeasible economically and timewise. This methodology is restrict to companies associated with Emissions Self-control Program - PROCON-AR, how it was called at the time. Thus, only 35 companies had their results mentioned in the samples obtained in the second semester of 2001 used at the inventory (FEEMA, 1990).

Similarly to the referenced inventory, the approach model used to develop this article was Bottom-Up, where the emissions were calculated individually to each source and the information collected was enough to characterize it, as:

activity level, operating hours and flow rate. Accordingly, emission rate calculations were made to each of them, and subsequently, were added to obtain the annual state estimation.

The evaluated compounds at this inventory were:

- Particulate Matter;
- Sulfur oxides;
- Nitrogen oxides;
- Carbon monoxide;
- Volatile organic compounds.

To obtain results about each pollutant emission sampled from the respective source, information was collected from the companies' reports, sent according to the PROMON AR. The pollutants concentrations (in mg/Nm³), emission rate (kg/h) and gas flow rate (Nm³/h) were used from those reports, information which is essential for the final evaluation. Considering that the sampling took place within load range from 90% to nominal capacity projected for the processing unit, assuming that the results for the PROMON AR must contemplate the worst emission scenario of the unit, under normal processing conditions.

For that reason, the industries were requested to send the amount of operating hours of each equipment linked to stationary sources in 2017. Thus, calculations made through this information produced an emission rate considered regular, where companies would be operating at all time with the referred load range of 90%.

$$E(t/y) = C \text{ (mg/Nm}^3\text{)} * Q \text{ (Nm}^3\text{/h)} * \frac{f \text{ (h/y)}}{10^9}$$

The enterprises used at this study were added accordingly to their industrial typology and administrative region in which they are located. Finally, chimneys and industrial ducts were georeferenced in order to establish results to administrative regions of Rio de Janeiro State.

FINDINGS AND ARGUMENT

In the referenced year, 112 companies that submitted their results to PROMON AR were analysed. From that number, 100 companies had their campaign approved according to the program, 2 of them exclusively by continuous monitoring. The other 12 companies were not approved as a consequence of not following the standard procedure, not providing enough data, for being deactivated or because the source was not operating at the year of the study. These 100

companies totaled 564 different sources and 823 sampling campaigns, considering campaigns in different semesters.

It was considered the concentration of each pollutant, each chimney gas flow rate and the annual operating hours of each equipment, all to calculate the annual emission. Since some sources were sampled more than once at the year, in that case, were considered the results with higher emission rate. Accordingly, the result of emission rate to each source was presented in tons per year and, subsequently, all the sources emission rates were added, to acquire the total values listed below:

Table 1: Summary of the results obtained in emissions calculation

PM (tons/year)	8900,4
SO2 (tons/year)	29113,2
NOx (tons/year)	32680,2
CO (tons/year)	4715,6
VOC (tons/year)	172,2

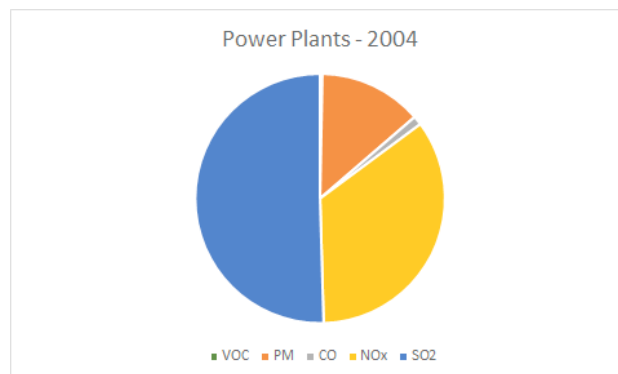
Reference: Personal elaboration, based on the results of PROMON AR (2017)

According to table 1, the results of total emissions indicates that the main monitored pollutant is nitrogen oxide (NOx), which corresponds to more than 42% of total emitted, following, the pollutant sulfur dioxide (SO2) representing 39% of emissions. In that context, it is noticeable a significant difference comparing to 2004's results, of which 40% of total emissions where of SO2 and in second place, representing NOx, 22% of emissions. (FEEMA, 2004)

This comparison can only be evaluated by means of its percentage, that represents the pollutants associated to its respective sample space.

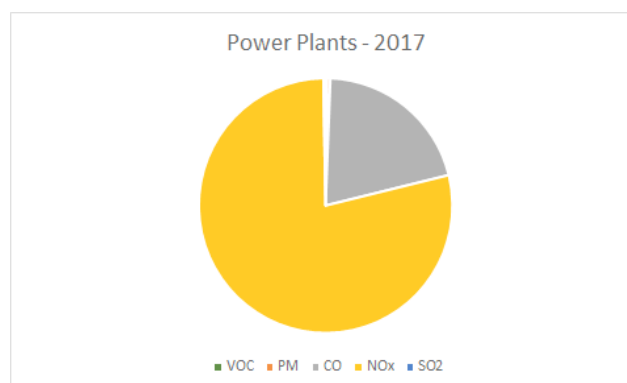
Among the scenarium changes in the past years, the most relevant fact to the comparison above, it's because power plants changed the main fuel used in external combustion, that previously was mostly residual oil (FEEMA, 2004) and in the past few years it was replaced with natural gas, generally (INEA, 2017).

Figure 1: Emission rate in 2004



Reference: Personal elaboration, based on FEEMA (2004)

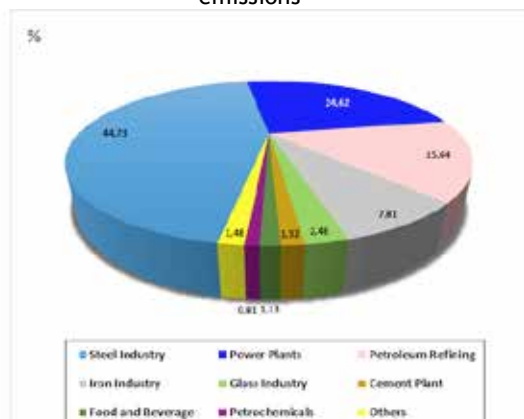
Figure 2: Emission rate in 2017



Reference: Personal elaboration, based on the results of PROMON AR (2017)

Furthermore, among the selected industrial typologies, the more representative ones that were contained in the inventory, considering emission rates, were: steel industry, petroleum refining and power plants, which were responsible for 85% of total emissions.

Figure 3: Typologies participation on Total emissions



Reference: Personal elaboration, based on the results of PROMON AR (2017)

* Others correspond to the sectors: automobilistic, ceramics, asphalt industry, pharmaceutical, laundry, paper, plaster production, chemical, textile, Waste management and others.

An important trait of this sectoral distribution is that in 2004, steel industries were not considered on the study and in 2017, this sector is the biggest in terms of total emission. This happens due to the installation of a steel industry center at metropolitan region of Rio de Janeiro.

However, counting the total amount by typology, chemistry and food and beverage types had a considerable higher number of enterprises, followed by iron and power plants.

Table 2: Number of companies and sources by typology

Typologies	Number of companies	Number of sources
Chemistry and Petrochemicals	18	94
Steel industry	6	74
Iron Industry	7	46
Automobilistic	3	43
Power plants	7	40
Cement Plant	4	32

Food and Beverage	10	31
Ceramic	5	22
Waste management	5	18
Petroleum refining	2	15
Paper	4	7
Asphalt Industry	5	6
Glass	4	4
Others	20	130

Reference: Personal elaboration, based on the results of PROMON AR (2017)

The reason for the “others” designation of those companies is the fact that they don’t fit in the dominant groups and, beyond that, represents less than 1% of the total contribution of total pollutants emitted.

Separating by administrative region, the amount of enterprises by area are defined below:

Table 3: Number of companies by administrative region

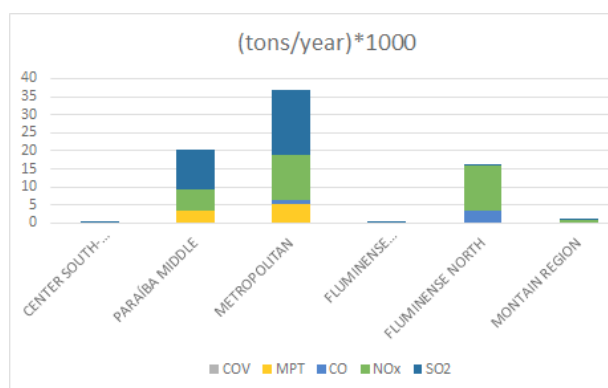
Centro Sul-Fluminense	1
Metropolitan	64
Noroeste Fluminense	3
Norte Fluminense	5
Serrana	9
Médio Paraíba	18

Reference: Personal elaboration, based on the results of PROMON AR (2017)

Among companies located in the metropolitan region, 34 are at Rio de Janeiro city. The table below presents a total emission result summary according to area allocation by administrative regions.

Besides that, it is important to highlight that the administrative regions not mentioned do not have monitored sources, and that is why they are not presented previously. The table below shows emission results summary to each pollutant accordingly to spatial distribution by administrative region, in which can be observed the high relevance of the metropolitan region at the state's monitored emissions:

Table 4: Emission rate by administrative region



Reference: Personal elaboration, based on the results of PROMON AR (2017)

CONCLUSIONS

The current paper demonstrated emission results derived from stationary sources monitored at Rio de Janeiro State and how was carried out its inventory procedure, based on the United States Environmental Protection Agency (EPA) methodology, the same approach that was used in 2001's Metropolitan Region inventory.

It is evident that the number of companies attending to the monitoring program is increasing, and, as a consequence, information necessary to this study's elaboration is more available. Furthermore, data quality is even more accurate, since sampling results get even closer to the real numbers, when well executed, comparatively to estimations.

Also, it can be observed changes in the state's scenarium with additional industries installations relevant to total emissions, such as fuel alteration that became significant to the final result. Furthermore, this study raises questions that must be deeply evaluated, in order to validate the benefits of the public policies applied over the years.

As expected, this study can't replace a complete state inventory since only stationary sources were monitored. Nonetheless, it helps the decision making process in the next steps towards developing a complete state inventory, as well as it can be the foundation to the execution of more precise environmental policies and capable of bringing benefits to air quality at the regions mentioned.

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A NEW METHOD FOR RUNNING MEGAN MODEL FOR BIOGENIC EMISSIONS ESTIMATE USING TERRAIN DATA FROM WRF MODEL

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Abstract: Sources of atmospheric pollution are often classified as anthropogenic or biogenic, being the latter mainly composed by vegetation, soils, volcanos, lightning and sea salt. Plants and trees are of significant relevance and emit a variety of pollutants, with emphasis on the biogenic volatile organic compounds (BVOCs), once they contribute expressively to secondary pollutants formation, such as Ozone (O₃) and fine particles (PM_{2.5}). Considering the important role of BVOCs on the atmosphere chemistry, estimates of emissions of these pollutants need to be considered when running photochemical air quality models. Therefore, tools to provide BVOCs emission fluxes are required, considering that it is not practical to provide such information only with field measurements. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) is one of the existing models that calculates BVOCs emission rates by using meteorological data, vegetation emission factors and land cover data, specifically Plant Functional Types (PFTs) according to Community Land Model 4 (CLM4), and Leaf Area Index (LAI). Meteorology can be obtained by running a separate model, such as Weather Research and Forecasting Model (WRF). The emission factors are available in the literature. PFTs and LAI, on the other hand, are not readily available, needing an extra step to obtain this information, except for North America. To overcome this matter and allow one to easily run the model for all the regions, this paper aims to present a tool developed in order generate MEGAN input files, by extracting and treating data from post-processing files from WRF. To calculate meteorological fields, WRF model uses global and observational data, besides land use/land cover data from the Moderate Resolution Imaging Spectro-Radiometer (MODIS) sensor aboard the Terra and Aqua satellites. MODIS Land Cover Type product uses different classification systems to map five main layers, including 17-class International Geosphere-Biosphere Programme classification (IGBP) and LAI algorithm. After running WRF, the post-processing is carried out by the Meteorology Chemistry Interface Processor (MCIP), which, among other functions, defines gridding parameters and prepares the meteorological fields in a form required by a chemical transport model. MODIS data is included in this post-processing, and then part of MCIP files contains land cover information. Since MODIS and MEGAN use different PFTs classifications, a Correlation Table was developed based on literature to cross IGBP (used by MODIS) and CLM4 (used by MEGAN) classes. In sequence, an algorithm was developed to organize the tasks that are required in order to process MCIP files to obtain PFTs (converted using the Correlation Table) and LAI. Next steps: to develop a code to execute the algorithm. By using this tool, researchers and users will be able to use WRF terrain data, ensuring greater consistency with the inputs used in meteorological modeling, and it will allow the use of even more up-to-date data. Additionally, it will be possible to run MEGAN model for any studied domain, providing BVOCs emission rates, important compounds for the atmospheric chemistry and environmental air quality.

Keywords: biogenic volatile organic compounds, MEGAN, MCIP, WRF, land cover.

INTRODUCTION

The chemical composition of the atmosphere has a high degree of complexity due to its diversity of physical processes and chemical reactions. All atmospheric pollutants will suffer, eventually, the effects of some of these processes. These compounds can be primary pollutants, which are those emitted directly by the sources (e.g. Sulphur dioxide), or secondary pollutants, which are those formed in the atmosphere (e.g. Ozone) when existing compounds are transformed into new air pollutants.

Sources of atmospheric emissions may be classified as anthropogenic or natural. Among the latter, vegetation, specifically, is responsible for the emission of various types of pollutants, with emphasis on Biogenic Volatile Organic Compounds

(BVOCs). BVOCs have a significant contribution for secondary pollutants formation, especially Ozone and Secondary Aerosol, mostly fine particulate matter, also called PM_{2.5} (particulate matter with aerodynamic diameter less than 2.5 µm). (SEINFELD and PANDIS, 2006)

Considering the important role of BVOCs on the atmospheric chemistry, several studies on literature have investigated their influence on local and regional air quality. In general, it was concluded that BVOCs can impact significantly on atmospheric pollutants concentrations, depending on other parameters, such as local weather and anthropogenic emissions (CURCI et al., 2009; PAOLETTI, 2009; MARTIN et al., 2010; SARTELET et al., 2012; KIM et al., 2018; CARLTON et al., 2018). Some of these studies have used modeling tools in order to calculate the contribution of BVOCs on

secondary pollutants formation. This evaluation requires an estimate of BVOCs emissions as an input data, and MEGAN (Model of Emissions of Gases and Aerosols from Nature) is being widely for this purpose. This model has algorithms that describe the main mechanisms that control the emissions of BVOCs by vegetation, which are related to: weather conditions, soil coverage (Plant Functional Types - PFTs, and Leaf Area Index - LAI) and emission factors specific for each PFT (GUENTHER et al., 2012). PFTs are categories of plants that are functionally similar (BOX, 1996) and LAI is defined as the leaf surface area within a grid cell per vegetation fraction of the grid area (KNOTE et al., 2009).

The meteorological data can be obtained from meteorological models, such as WRF (Weather Research and Forecasting Model). The emission factors of each PFT for standard conditions of temperature and radiation (foliar temperature of 30°C and photosynthetic photon flux density of 1000 $\mu\text{mol.m}^{-2}.\text{s}^{-1}$) used by MEGAN can be found in the literature (GUENTHER et al., 2012; HENROT et al., 2017; JIANG et al., 2019). PFTs and LAI maps, however, are not promptly available for regions other than within North America.

Thereby, the present work aims to develop a computational tool to provide all the required input data to run MEGAN model by using WRF terrain data.

METHODS

MEGAN considers vegetation classes based on the Community Land Model (CLM4.0) PFT classification, which is composed by 15 categories of plants (Table 1). This is an important parameter as the emission factors available on literature consider these categories described in CLM4.0. Therefore, the land use input for MEGAN must be coherent with these classes.

Table 1. CLM4.0 PFTs categories.

1	Needleleaf evergreen tree - temperate
2	Needleleaf evergreen tree - boreal
3	Needleleaf deciduous tree - boreal
4	Broadleaf evergreen tree - tropical
5	Broadleaf evergreen tree - temperate
6	Broadleaf deciduous tree - tropical
7	Broadleaf deciduous tree - temperate
8	Broadleaf deciduous tree - boreal
9	Broadleaf evergreen shrub - temperate
10	Broadleaf deciduous shrub - temperate
11	Broadleaf deciduous shrub - boreal
12	C3 arctic grass
13	C3 grass
14	C4 grass
15	Crop

Reference: OLESON et al., 2010.

Similarly, to run WRF model, it is necessary to use input information of land use. However, differently

from MEGAN, in the current version of WRF, the default land use and leaf area index information is derived from the 2001 MODIS-based data developed by Boston University (FRIEDL et al., 2002; YANG et al., 2018). The land use data consider 20 categories based on International Geosphere-Biosphere Programme Data and Information System (IGBP) classification (Table 2), in which 15 classes are vegetation types.

Table 2. IGBP land use classification.

1	Evergreen Needleleaf Forest
2	Evergreen Broadleaf Forest
3	Deciduous Needleleaf Forest
4	Deciduous Broadleaf Forest
5	Mixed Forests
6	Closed Shrublands
7	Open Shrublands
8	Woody Savannas
9	Savannas
10	Grasslands
11	Permanent wetlands
12	Croplands
13	Urban and Build-Up
14	Cropland/Natural Vegetation Mosaic
15	Snow and Ice
16	Barren or Sparsely Vegetated
17	Water
18	Wooded Tundra
19	Mixed Tundra
20	Barren Tundra

Fonte: NATIONAL CENTER FOR ATMOSPHERIC RESEARCH, 2017.

As described above, WRF and MEGAN use the same type of input data (land use information). However, comparing Tables 1 and 2, it can be concluded that the models do not use the same basis of classification, preventing the direct correlation between both. To overcome this matter, it is necessary to evaluate each individual category in order to match one classification with the other. This was accomplished by reviewing the existing literature and defining premises to do the correlation, as show in Annex A.

In sequence, an algorithm was developed in order to extract the data from WRF output to use as MEGAN input. It is important to highlight that the WRF outputs were not directly used; they were preliminarily processed by Meteorology-Chemistry Interface Processor (MCIP), an intermediate pre-processor that prepares the meteorological fields in the way required by Community Multiscale Air Quality model (CMAQ), among other functions. After running MCIP, several files are generated with different type of records. The ones that contain the data for MEGAN input are GRIDCRO2D, for PFT information, and METCRO2D, for LAI data. These files contain, respectively, 2-D time invariant fields and 2-D time varying fields (OTTE e

PLEIM, 2010. The steps to perform the data extraction from MCIP files are shown in Figure 1.

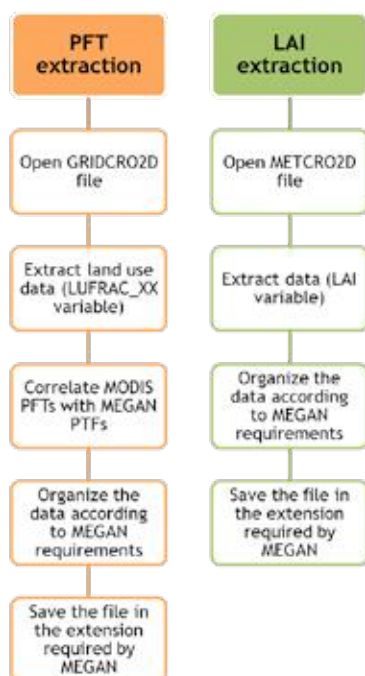


Figure 1. Steps for data extraction.

NEXT STEPS

The next steps of the present work are to develop a code in Python language to run the algorithm and to use the generated input data to run MEGAN model.

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ANNEX A

Table A. Correlation between MEGAN (CLM4.0) and MODIS (IGBP) vegetation classes.

MEGAN classes (CLM 4.0)	MODIS classes (IGBP)	Reference	Premises
Needleleaf evergreen tree - temperate (1)	Evergreen Needleleaf Forest (1)	WEST et al., 2014	Temperate climate ^(a)
Needleleaf evergreen tree - boreal (2)	Evergreen Needleleaf Forest (1)	WEST et al., 2014	Boreal climate ^(b)
Needleleaf deciduous tree - boreal (3)	Deciduous Needleleaf Forest (3)	WEST et al., 2014	Boreal climate ^(b)
Broadleaf evergreen tree - tropical (4)	Evergreen Broadleaf Forest (2)	WEST et al., 2014	Tropical climate ^(c)
Broadleaf evergreen tree - temperate (5)	Evergreen Broadleaf Forest (2)	WEST et al., 2014	Temperate climate ^(a)
Broadleaf deciduous tree - tropical (6)	Deciduous Broadleaf Forest (4)	WEST et al., 2014	Tropical climate ^(c)
Broadleaf deciduous tree - temperate (7)	Deciduous Broadleaf Forest (4)	WEST et al., 2014	Temperate climate ^(a)
Broadleaf deciduous tree - boreal (8)	Deciduous Broadleaf Forest (4)	WEST et al., 2014	Boreal climate ^(b)
Broadleaf evergreen shrub - temperate (9)	Closed Shrublands (6)	BONAN et al., 2002; LOVELAND et al., 2000	-
Broadleaf deciduous shrub - temperate (10)	Open Shrublands (7)	BONAN et al., 2002; LOVELAND et al., 2000	Temperate climate ^(a)
Broadleaf deciduous shrub - boreal (11)	Open Shrublands (7) + Wooded Tundra (18) + Mixed Tundra (19) + Barren Tundra (20)	BOX, 1996; BONAN et al., 2002; LOVELAND et al., 2000	Boreal climate ^(b)
C3 arctic grass (12)	Grasslands (10)	-	Arctic Circle ^(d)
C3 grass (13)	Grasslands (10)	STILL et al., 2003; NIU; LIU; WAN, 2008	Temperate climate ^(a) / Others: Winter / Autumn / Spring
C4 grass (14)	Grasslands (10) + Savannas (8)	BOX, 1996; STILL et al., 2003; NIU; LIU; WAN, 2008	Tropical climate ^(c) / Temperate climate: Summer
Crop (15)	Croplands (12) + Cropland/Natural Vegetation Mosaic (14)	-	-

Reference: prepared by the authors.

a - 23,27°N to 66,5°N and 23,27°S to 66,5°S;

b - 50°N to 70°N;

c - 23,27°N to 23,27°S;

d - 66,5°N to 90°N.

Note: Mixed Forest class (IGBP n°. 5) is not included in Table A, but it will be evaluated according to the surrounding pixels.

TRENDS IN ANTROPOGENIC EMISSIONS IN THE ANDEAN CITY OF MANIZALES, COLOMBIA, BETWEEN 2014-2017

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Abstract: The anthropogenic emissions inventory of the medium-sized Andean city of Manizales, Colombia, was estimated and updated for the base year 2017. The new update included two additional sources of pollution: re-suspended particulate material and stationary area sources (from fuel distribution stations), and covering the two main emission sources: on-road mobile (exhaust and evaporative) and stationary point-source industrial activities.

Total annual fluxes of criteria pollutants, non-methane volatile hydrocarbons, and greenhouse gases were estimated. In terms of on-road mobile emission fluxes, a bottom-up approach was applied using the International Vehicle Emissions (IVE) methodology and IVE emissions model, which were employed for the previous emission estimation. IVE input information were updated for the five vehicular categories evaluated: passenger cars, motorcycles, taxi, bus and truck. Furthermore, vehicular activity in terms of daily vehicle kilometer traveled (VKT) and start-ups per day were re-estimated. In terms of re-suspended particulate material, a top-down approximation was employed evaluating two methodologies applied previously in the city of Bogotá, Colombia. On the other hand, stationary point and area source activities were estimated following a bottom-up approach and using primary information from stack sampling measurements and the emission factor methodology.

Trends and changes in anthropogenic emissions between 2014 and 2017 were analyzed. In the case of on-road vehicular emissions - the most important source of pollution in the city, there was a variation in technology distribution and activity data when comparing 2017 and 2014 vehicular fleet. For example, in the case of motorcycles there was a reduction in 2strokes engine percentage in the fleet (varying from 54% in 2014 to 20% in 2017), result that contributed with a reduction of 36% in total CO emission between 2014 and 2017, in spite of the growth of motorcycle fleet during these period (32% more). These results suggest the importance of a complete technology distribution characterization in order to obtain accurate estimation of emissions. On the other hand, estimation of new sources of pollution in the city, such as re-suspended particulate material from vehicular activity, suggested a small contribution (below 10%) of this source to total vehicular emissions in Manizales.

This emission inventory estimation is the base for future studies which are focused in the disaggregation of total emission fluxes, in order to perform high-resolution air quality simulations in Manizales using the eulerian chemical transport model, WRF-Chem. This exercise will be essential for studding dispersion patterns and dynamics of pollutants such as CO and PM₁₀, also is a useful tool to evaluate and validate the accuracy of emission inventories estimated in the city.

Keywords: Emissions inventory, on-road sources, stationary sources, Andean cities.

INTRODUCTION

Air pollutants derived from urban emissions have become a big concern to human health, environmental sustainability and global climate (Seinfeld and Pandis, 2006; Londoño et al., 2011). In Latin American context, the majority of cities have been characterized by its fast growth and urbanization, enhancing emissions of air pollutants to the atmosphere. This phenomenon is especially severe in medium-sized cities; however, majority of these cities have deficiencies integrating tools such as emission inventories (EI).

Quantification of pollutant fluxes from the estimation of EIs is crucial to identify significant sources of air pollutants (US EPA, n.d.). Furthermore, periodical updates of EIs allows not only the analysis of emissions trends but also the evaluation of regulatory actions, improving methods from previous estimations and including new emission sources in the EI.

The anthropogenic emissions inventory of the medium-sized Andean city of Manizales, Colombia, was estimated and updated for the base year 2017. The main objective of the study was to update the previous emission inventory estimated in the city (2014 as base year). The new update included two additional sources of pollution: re-suspended particulate material and stationary area sources (from fuel distribution stations), and covering the two main emission sources: on-road mobile (exhaust and evaporative) and stationary point-source industrial activities.

METHODS

Total annual fluxes of criteria pollutants (CO, NO_x, SO₂, PM₁₀), non-methane volatile hydrocarbons (NMVOC), and greenhouse gases, GHG (CO₂, CH₄, N₂O) were estimated in the urban area of Manizales city (urban population 390000 inhabitants) with a spatial domain of 54 km². Manizales is characterized by a high urban population density (~6800 inhabitants per km²), a relatively high motorization rate (425 vehicles per 1000 population [Manizales

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On-road mobile source estimation approaches

Estimation of on-road mobile emissions (exhaust and evaporative) followed a bottom-up approach and was performed using the International Vehicle Emissions (IVE) methodology and IVE emissions model (Davis et al., 2005). This model differs from other known and commonly used models, since it assigns an emission level according to the vehicle specific power (VSP), and not according only to the average speed. Detailed description of IVE methodology and its implementation in Manizales is described by González et al. (2017). Main changes on IVE input information were focused on updating the vehicle fleet composition, vehicle technology distribution, engine start/stop patterns and activity data (daily vehicle kilometer traveled, VKT, and start-ups per day) for the five vehicular categories evaluated: passenger cars (PC), motorcycles (2w), taxi, bus and truck.

On the other hand, the estimation of re-suspended particulate material followed a top-down approach and was based on the use of sedimentation load and precipitation correction as main information for the emission estimation. The estimation followed the methodologies described in Amato et al. (2011); Espitia et al. (2017); and EPA (2011).

Stationary source estimation approaches

Stationary point sources covered main large and medium-sized industrial facilities located in Manizales and surrounding zones. Emissions estimation of these sources followed a bottom-up approach and used primary information from stack sampling measurements and the emissions factor methodology. Detailed description of sources of data and emission factors method is described in detail by González et al. (2017). A total number of 43 facilities (130 point sources) were included from diverse sectors such as facilities in diverse sectors such as food and beverage processing, coal-fired metal foundry recycling, plastic processing, metallurgy and solid waste incineration.

In terms of stationary area sources, NMVOC emissions were estimated followed a top-down approach taking into account 30 fuel distribution stations distributed in the whole urban area and using official information about buy and sell of fuel in the city. Methodology reported by the Environmental European Agency was applied using emission factors reported by EPA (2008). Detailed description of methodology applied in Manizales and sources of data is described in detail by Valencia (2019).

FINDINGS AND ARGUMENT

Comparing all emission sources evaluated on the EI, on-road vehicular activity released more than 90% of majority of air pollutants estimated in Manizales

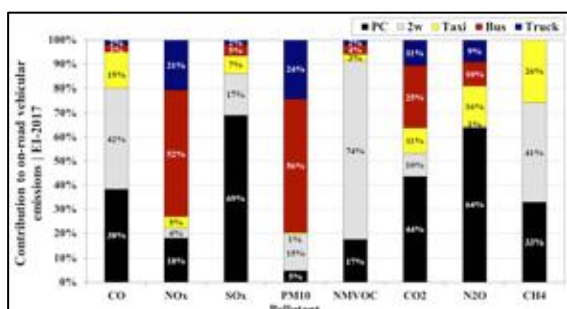
(Table 1 shows results for criteria pollutants and NMVOC). Only stationary point-source emissions of SO_x (214 ton/yr) were higher than that obtained from on-road vehicular sources reaching 88% of the total emission; result attributed to the use of coal and diesel in some industrial processes.

Table 1. Summary of EI-2017 annual fluxes of criteria pollutants and NMVOC

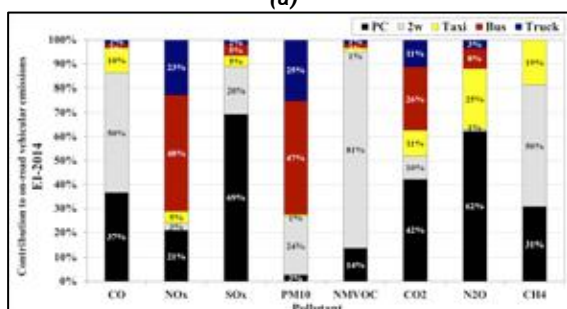
Source type	Emission (ton/yr)				
	CO	NO _x	SO _x	PM ₁₀	NM-VOC
Stationary (point-source)	478	155	214	58	6
Stationary (area-source)					204
On-road vehicular (exhaust and evaporative)	27815	4646	28	631	4992
On-road vehicular (RPM)				49	
Total	28295	4801	243	738	5202
Contribution of each source to total emissions (%)					
Stationary (point-source)	1.7	3.2	88.3	7.8	0.1
Stationary (area-source)					3.9
On-road vehicular (exhaust and evaporative)	98.3	96.8	11.7	85.5	96.0
On-road vehicular (RPM)				6.7	

Among on-road vehicular sources, CO dominated the emission fluxes with 27815 ton/year. As it is shown in Figure 1a, PC and 2w dominated the emission of this pollutant (42% and 38% respectively). The use of petrol as fuel contributed to this pattern (Figure 2). This fuel is used in the total 2w fleet and 85% of PC. On the other hand, emission of PM₁₀ was dominated by buses, with 56% of emissions, and trucks (24%). Bus fleet emitted the highest amount of PM₁₀ (351 ton/yr), in spite of its small percentage in vehicular fleet (1.5% comprising 2604 vehicles).

Results suggest an equivalent behavior in terms of pollutant contribution by each category for both years, being emissions of CO, SO_x and NMVOC dominated by gasoline fueled vehicles (2w and PC); while NO_x and PM₁₀ emissions were dominated by diesel fueled vehicles (Bus and Truck). This results was obtained when comparing trends in emissions of main source of pollution in Manizales (on-road vehicular) between 2014 and 2017 (Figure 1). However, there was a reduction in the total annual emission flux for majority of pollutants (only SO_x and the group of GHG reported increments), in spite of the growth in the total number of vehicles when comparing 2014 with 2017 (132012 veh. in 2014 and 169142 veh. in 2017). Table 2 shows percentages of increment (positive) and reduction (negative) of emissions obtained from 2014 to 2017.



(a)



(b)

Figure 1. Emission distribution by vehicular type in Manizales, Colombia. a) EI-2017. b) EI-2014

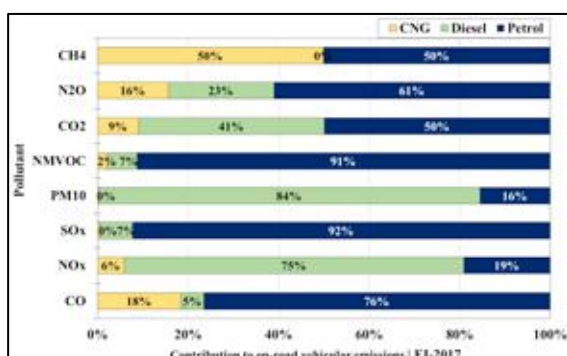


Figure 2. Emission distribution by fuel type from on-road vehicular sources for the EI-2017

Reduction in emissions (mainly associated with PC and 2w contribution), could be attributed to changes in vehicle technology distribution between 2014 and 2017. For example, 2-stroke engines reported a considerable percentage in the motorcycle fleet (54%), being this value lower in 2017 with only 20%. With respect to PC vehicles, 22% of PC fleet used carburetor as, air/fuel control while only 9% reported this technology in 2017. As well as, PC fleet exhaust emission control technology was dominated in 2014 by none control systems (33%) and 3-way catalyst (42%), while in 2017 none control systems reported 14%, 3-way catalyst (42%) and EuroIII systems 20%. Another example about the effect of changes in technology was associated with diesel engines, where higher percentages of better air/fuel and emission control technology in trucks (such as forward injection Euro IV), contributed with reduction of PM₁₀ emissions (around 17% from 2014 and 2017).

Table 2. Differences (%) of total annual fluxes for on-road vehicular sources from 2014 to 2017

Vehicular type	CO	NOx	SOx	PM ₁₀	NM-VOC
PC	-33% ↓	-19% ↓	9% ↑	41% ↑	-35% ↓
2w	-46% ↓	41% ↑	-5% ↓	-49% ↓	-53% ↓
Taxi	-7% ↓	-12% ↓	77% ↑	-20% ↓	3% ↑
Bus	8% ↑	3% ↑	9% ↑	-3% ↓	8% ↑
Truck	-21% ↓	-13% ↓	10% ↑	-21% ↓	-26% ↓
Total	-36% ↓	-5% ↓	10% ↑	-17% ↓	-48% ↓

CONCLUSIONS

Updated anthropogenic emissions inventory of the medium-sized Andean city of Manizales, Colombia, were dominated by vehicular activity, with more than 90% of total emissions for the majority of air pollutants estimated. Only the emission of SOx was higher from stationary point sources.

Analysis of trends in predominant anthropogenic emissions (on-road vehicular) between 2014 and 2017, suggested that variation in technology distribution and activity data contributed with a reduction of majority of pollutants from 2014 to 2017, especially CO (36%) and NMVOC (48%). This results emphasize the importance of vehicular technology distribution profiles and its sensitivity to changes in EI results.

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Stationary source estimation approaches

Stationary point sources covered main large and medium-sized industrial facilities located in Manizales and surrounding zones. Emissions estimation of these sources followed a bottom-up approach and used primary information from stack sampling measurements and the emissions factor methodology. Detailed description of sources of data and emission factors method is described in detail by González et al. (2017). A total number of 43 facilities (130 point sources) were included from diverse sectors such as facilities in diverse sectors such as food and beverage processing, coal-fired metal foundry recycling, plastic processing, metallurgy and solid waste incineration.

In terms of stationary area sources, NMVOC emissions were estimated followed a top-down approach taking into account 30 fuel distribution stations distributed in the whole urban area and using official information about buy and sell of fuel in the city. Methodology reported by the Environmental European Agency was applied using emission factors reported by EPA (2008). Detailed description of methodology applied in Manizales and sources of data is described in detail by Valencia (2019).

FINDINGS AND ARGUMENT

Comparing all emission sources evaluated on the EI, on-road vehicular activity released more than 90% of majority of air pollutants estimated in Manizales

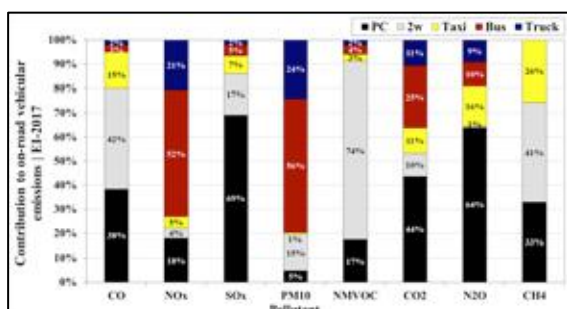
(Table 1 shows results for criteria pollutants and NMVOC). Only stationary point-source emissions of SO_x (214 ton/yr) were higher than that obtained from on-road vehicular sources reaching 88% of the total emission; result attributed to the use of coal and diesel in some industrial processes.

Table 1. Summary of EI-2017 annual fluxes of criteria pollutants and NMVOC

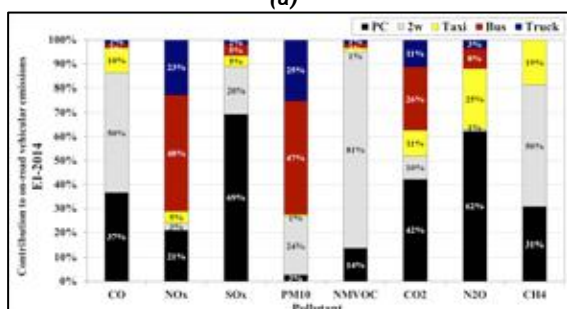
Source type	Emission (ton/yr)				
	CO	NO _x	SO _x	PM ₁₀	NM-VOC
Stationary (point-source)	478	155	214	58	6
Stationary (area-source)					204
On-road vehicular (exhaust and evaporative)	27815	4646	28	631	4992
On-road vehicular (RPM)				49	
Total	28295	4801	243	738	5202
Contribution of each source to total emissions (%)					
Stationary (point-source)	1.7	3.2	88.3	7.8	0.1
Stationary (area-source)					3.9
On-road vehicular (exhaust and evaporative)	98.3	96.8	11.7	85.5	96.0
On-road vehicular (RPM)				6.7	

Among on-road vehicular sources, CO dominated the emission fluxes with 27815 ton/year. As it is shown in Figure 1a, PC and 2w dominated the emission of this pollutant (42% and 38% respectively). The use of petrol as fuel contributed to this pattern (Figure 2). This fuel is used in the total 2w fleet and 85% of PC. On the other hand, emission of PM₁₀ was dominated by buses, with 56% of emissions, and trucks (24%). Bus fleet emitted the highest amount of PM₁₀ (351 ton/yr), in spite of its small percentage in vehicular fleet (1.5% comprising 2604 vehicles).

Results suggest an equivalent behavior in terms of pollutant contribution by each category for both years, being emissions of CO, SO_x and NMVOC dominated by gasoline fueled vehicles (2w and PC); while NO_x and PM₁₀ emissions were dominated by diesel fueled vehicles (Bus and Truck). This results was obtained when comparing trends in emissions of main source of pollution in Manizales (on-road vehicular) between 2014 and 2017 (Figure 1). However, there was a reduction in the total annual emission flux for majority of pollutants (only SO_x and the group of GHG reported increments), in spite of the growth in the total number of vehicles when comparing 2014 with 2017 (132012 veh. in 2014 and 169142 veh. in 2017). Table 2 shows percentages of increment (positive) and reduction (negative) of emissions obtained from 2014 to 2017.



(a)



(b)

Figure 1. Emission distribution by vehicular type in Manizales, Colombia. a) EI-2017. b) EI-2014

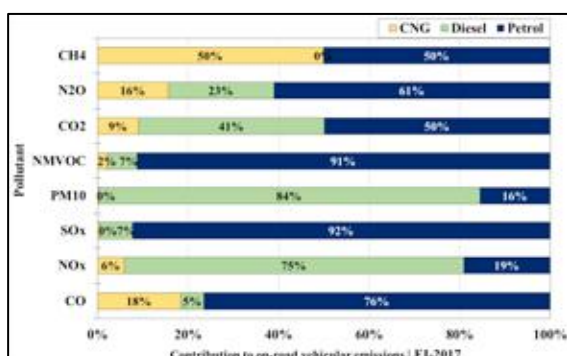


Figure 2. Emission distribution by fuel type from on-road vehicular sources for the EI-2017

Reduction in emissions (mainly associated with PC and 2w contribution), could be attributed to changes in vehicle technology distribution between 2014 and 2017. For example, 2-stroke engines reported a considerable percentage in the motorcycle fleet (54%), being this value lower in 2017 with only 20%. With respect to PC vehicles, 22% of PC fleet used carburetor as, air/fuel control while only 9% reported this technology in 2017. As well as, PC fleet exhaust emission control technology was dominated in 2014 by none control systems (33%) and 3-way catalyst (42%), while in 2017 none control systems reported 14%, 3-way catalyst (42%) and EuroIII systems 20%. Another example about the effect of changes in technology was associated with diesel engines, where higher percentages of better air/fuel and emission control technology in trucks (such as forward injection Euro IV), contributed with reduction of PM₁₀ emissions (around 17% from 2014 and 2017).

Table 2. Differences (%) of total annual fluxes for on-road vehicular sources from 2014 to 2017

Vehicular type	CO	NOx	SOx	PM ₁₀	NM-VOC
PC	-33% ↓	-19% ↓	9% ↑	41% ↑	-35% ↓
2w	-46% ↓	41% ↑	-5% ↓	-49% ↓	-53% ↓
Taxi	-7% ↓	-12% ↓	77% ↑	-20% ↓	3% ↑
Bus	8% ↑	3% ↑	9% ↑	-3% ↓	8% ↑
Truck	-21% ↓	-13% ↓	10% ↑	-21% ↓	-26% ↓
Total	-36% ↓	-5% ↓	10% ↑	-17% ↓	-48% ↓

CONCLUSIONS

Updated anthropogenic emissions inventory of the medium-sized Andean city of Manizales, Colombia, were dominated by vehicular activity, with more than 90% of total emissions for the majority of air pollutants estimated. Only the emission of SOx was higher from stationary point sources.

Analysis of trends in predominant anthropogenic emissions (on-road vehicular) between 2014 and 2017, suggested that variation in technology distribution and activity data contributed with a reduction of majority of pollutants from 2014 to 2017, especially CO (36%) and NMVOC (48%). This results emphasize the importance of vehicular technology distribution profiles and its sensitivity to changes in EI results.

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ESTIMATION OF VEHICULAR EMISSIONS IN BRAZIL FROM 1956 TO 2056

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Abstract: Vehicular emissions are among the main sources emissions of atmospheric pollutants in the world. Road transport, for example is estimate to contribute with around 50% of particulate emissions (PM) in OECD countries, which is mainly due to diesel power vehicles. Therefore, the on-road vehicular emissions in Brazil, from 1956 to 2056 was estimated using emissions factors by age of use and the vehicular emissions inventory (VEIN) model. The traffic dataset was obtained from the national association of motor vehicle manufacture (ANFAVEA), in which was applied survival functions and Autoregressive integrated moving average (ARIMA) methods for projection to 2019. The emissions of CO, HC, NO_x, PM and CO₂ changed from 0.033 Mt, 0.01 Mt, 0.155 Mt, 0.009 Mt and 11.149, in 1956 to 1.188 Mt, 0.179 Mt, 0.998 Mt, 0.032 Mt and 355.158 Mt in 2056, respectively. The state with most emissions is São Paulo, followed by Minas Gerais and Paraná. These results are worrisome indicating that application of more restrictive emissions factors should be applied in order to decrease the emissions.

Keywords: emissions, VEIN, Brazil, 100 years

INTRODUCTION

Air pollutants affects air quality, human health and ecosystems. It has become clear that transportation emissions play an important role on air pollution (Landrigan et al. 2018), especially in urban centers. Several studies show that transportation sector is one the biggest responsible for air pollution (Andrade et al. 2012; Nogueira et al. 2015). Given the implications and effects on environment, climate and economy, it is very important to develop vehicular emissions inventory. There are international efforts to characterize transportation emissions globally. In this way, the EDGAR emissions inventory (Crippa et al., 2018) has covered Brazil from year 1970 to 2012. The Brazilian vehicle fleet has been increasing in the last 50 years, associated with the economic development. Therefore, at country level some emissions inventories have been made. For instance, the Ministry for Environment published an inventory between years 1980 and 2020 showing that the peak of emissions was in 1992 for CO, HC and CH₄, 1998 for NO_x and PM_{2.5}, and 2020 for CO₂ (MMA, 2011). At regional and city level, vehicular studies have shown that solely transportation produce high levels of air pollution (Andrade, 2017). Also, it has been reported the importance of the transportation emissions in several Brazilian cities such as Brasília (Réquia et al. 2015) and Rio de Janeiro (Duarte et al. 2013). These studies help to understand the impact of vehicular emissions on air pollution; however, they cover limited years, it has not been characterized a fully historical inventory or cover cities. Therefore, this

study aims to fill these gaps with a transportation emissions inventory for Brazil from 1956 to 2056.

METHODS

We built the vehicular emissions inventory using the vehicular emissions inventory (VEIN) model (Ibarra-Espinosa et al, 2018), and compiling the emission factors from 1980 to 2017 (CETESB, 2017) and fleet number from national association of motor vehicle manufacture (*Associação nacional dos fabricantes de veículos automotores* -ANFAVEA (2019)). The emission factors for the fleet older than 1980 and newer than 2017 were kept at the same level those of 1980 and 2017, respectively. Hence, our results represent the conditions a business as usual. Mileage comes from Bruni and Bales (2013), which regressed mileage by age of use from millions of odometer readings. We recognize the limitations in this approach, concerning the use of counting with trends on mileage, and the lack of real-word emission factors. However, our methods still provide valid information for environmental policies.

FINDINGS AND ARGUMENT

Vehicle population

The fleet was analyzed using Autoregressive integrated moving average (ARIMA) methods and the R software. The fleet data is shown on Figure 1, and includes already the projection. The ARIMA regressions require the series to be stationary, hence we applied the augmented Dickey-Fuller (ADF) to our data, resulting stationary. Then we applied the automatic ARIMA regression (Hyndman

and Khandakar 2008). The yearly variation of vehicles is related to the Gross Domestic Product per capita (GDPpp), which has a correlation of 0.9 for Passenger Cars (PC), as shown on Fig 1. Therefore, the global economic crisis explains the stagnation of fleet growth during the 80's, 97 and 2013.

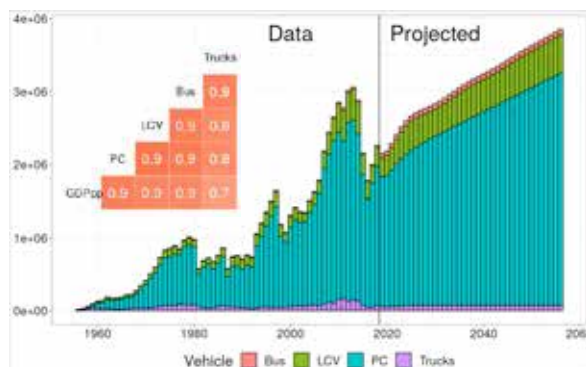


Figure 1. Vehicular fleet in Brazil from 1956 to 2018, the projections from 2019 to 2056, and the correlations with GDPpp.

We applied the survival function of Gompertz, as suggested by other authors (Huo and Wang, 2012), with the coefficient used by MMA (2011). This process is done with VEIN model.

Historical emissions trends

During the 100 years inventory, the transportation sector in Brazil would emit 81 [Mt] of CO, 12.1 [Mt] of HC, 75.1 [Mt] of NO_x, 3.1 [Mt] of PM_{2.5} and 16,909.4 [Mt]. Figure 2 shows the historical trend of vehicular emissions. The emissions of CO, HC, NO_x, PM and CO₂ changed from 0.033 Mt, 0.01 [Mt], 0.155 [Mt], 0.009 [Mt] and 11.2 in 1956 to 1.2 [Mt], 0.179 [Mt], 0.998 [Mt], 0.032 [Mt] and 355.2 [Mt] in 2056, respectively. These results are worrisome indicating that the application of emissions factors more restrictive should be applied in order to decrease the emissions.

Comparison between original and projected data

The average emissions for the period with traffic data are 36.706, 5.407, 32.548, 1.759 and 4221.886 [kt] for CO, HC, NO_x, PM_{2.5} and CO₂, respectively. However, the same calculation for the projected period shows 32.700, 5.016, 31.727, 1.349 and 10245.032 [kt] for CO, HC, NO_x, PM_{2.5} and CO₂, respectively. This indicate the effect of newer emissions standards would limit the emissions despite growth of the fleet. However, the apparent decrease of emissions is marginal and the application of strict emission standards would decrease the emissions.

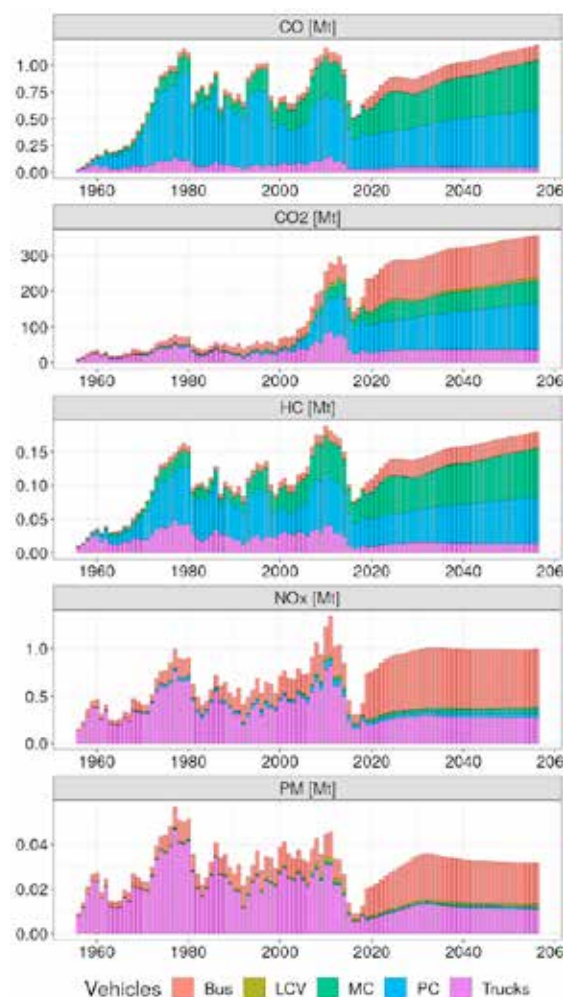


Figure 2. Historical trend of transportation emissions [Mt] in Brazil from 1956 to 2056.

Contribution from type of vehicles

The main contributors for CO and HC are PC and Motorcycles (MC), while for NO_x and PM_{2.5} are Trucks and Buses, as expected (see Fig 2 and Fig. 3). For the projection period, the participation of Trucks on CO and CO₂ emissions decreased from 14% and 50%, to 4% and 11%, respectively. On the other hand, MC increase the participation on CO, CO₂ and HC, from 18%, 3% and 43% to 32%, 16% and 37%, respectively.

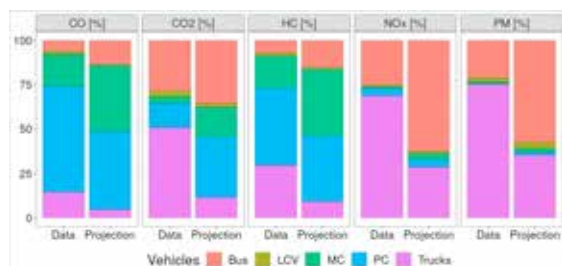


Figure 3. Contribution fraction [%] per vehicle type in the periods from 1956 to 2018 (data), and from 2019 to 2056 (projection).

Spatial analyses

The spatial distribution of emissions was related to the vehicular fleet number on each state. The state with highest emissions is São Paulo, followed by Minas Gerais and Paraná states.

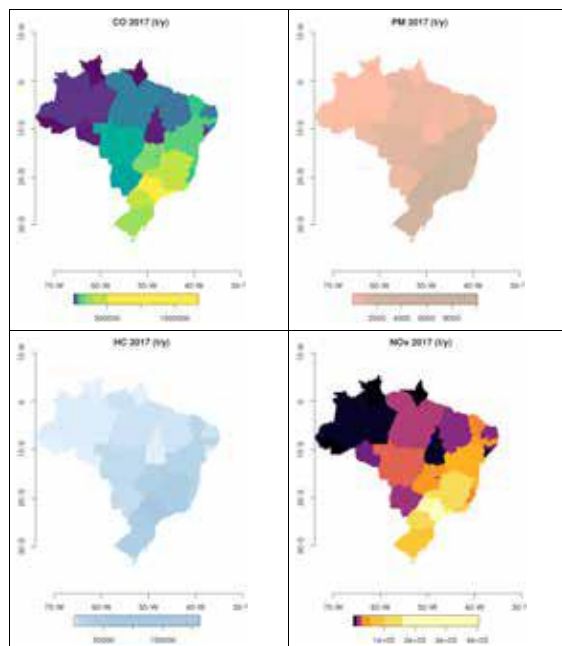


Figure 4. Vehicular emissions from CO, NOx, HC and PM (t/y).

CONCLUSIONS

Traffic fleet will increase, but the associated emissions will not increment linearly. These results are worrisome, indicating that the application of restrictive emissions factors must continue in order to effectively decrease the emissions. Attention must be given to PC and MC to control emissions in future.

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ESTIMATION OF THE EMISSION OF PARTICULATE MATTER BY FIXED SOURCES IN THE CITY OF BRAGANÇA-PA

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Abstract: Air pollution by particulate matter (PM) is also present in small and medium-sized Brazilian cities, such as Bragança-Pa. The city of Bragança is the oldest in the state and concentrates a large amount of fixed sources of air pollution, such as pottery (brick production) and flour houses (cassava flour production), both of which use the burning of biomass in their processes. In addition to mobile sources, such as vehicles and motorcycles, whose fleet increases each year, mainly due to inefficient public transportation of the city. The objective is to estimate PM emissions from fixed sources located in the city of Bragança-Pa. This information will be used to draw up an inventory of atmospheric emissions for the city. The methodology is based on field visits, interviews with local producers to raise biomass consumption plus annual activity in pottery and flour houses. The estimation of the PM emissions has been carried out based on the emission factors available in the literature and air quality reports of CETESB. This is the equation ($E = FE \cdot A$) that was used to estimate the total emissions from fixed sources, where E (represents PM emissions, FE is emission factor and A is activity throughout the year). These methodologies are used in several studies around the world to estimate air pollutant emissions. Preliminary results showed that pottery and flour houses do not use any type of air pollution control technology, are numerous enterprises (18 and 1950, respectively) and with high annual consumption of biomass (10.4 and 1.6 tons, respectively), especially during the summer, when production is more intense. Was estimated at 3.99 and 60 tons of particulate matter emitted by pottery and flour houses in the city of Bragança-Pa. Added to this is the lack of monitoring of activities in pottery and flour houses. Besides the problems of the fires that happen every year in the state of Pará, including in Bragança, contributing to the air pollution.

Keywords: Air Pollution, Fixed Sources, Flour Houses, Potteries, Particulate Matter.

INTRODUCTION

Air pollution is one of the main environmental problems of today, including in medium and small cities, as is the case of the city of Bragança-Pa. However, it is still little studied when compared with studies in the area of water resources or in the area of soil. Air pollution is related to the degradation of air quality and potential effects on the environment and human health (SALDIVA, 2008). In large cities or large urban centers, there are a large number of sources of pollution, but there is also greater control over these emissions (BAIRD, 2011). In smaller cities the number of sources of air

pollution is lower when compared to large urban centers, but there is less control over these emissions, making it necessary to identify the sources, characterize and estimate the emissions and generate data for the elaboration of an emission inventory, with the purpose of proposing strategies for the reduction / control of pollution in the city of Bragança. The city of Bragança has significant stationary sources of air pollution, such as: bakeries, pizzerias and, above all, potteries and flour houses. Pottery and flour houses play an important economic and cultural role in the city. Should be noted that in the production process in flour houses and pottery, we have the burning of biomass as an energy source. The burning of the biomass emits several gaseous pollutants into the atmosphere, such as: carbon dioxide, nitrogen oxides, sulfur oxides and, in particular, particulate matter. Particulate matter or atmospheric aerosol is understood to mean solid and liquid particles with a size ranging from 0.1 to 50 μm in suspension in the atmosphere (SEINFELD AND PANDIS, 1998). Particulate matter is associated with climate change, in the process of cooling and warming the climate, in addition to the potential deleterious effect on human health. The lower the particle size, the greater the ability to penetrate the human body and cause more severe damage to human health, especially in the respiratory and circulatory system (SALDIVA, 2008). Therefore, biomass burning in these production processes constitutes a potential impact on the environment, even at the local level. It also represents a potential deleterious effect on human health, especially for workers in these activities, often children and the elderly. Always be family enterprises. Just those who constitute the so-called risk group and more susceptible to the effect of pollution. It is worth noting that the city is located in the so-called "Deforestation Arc" with increasing vegetation losses due to the burning process, which further aggravates the degradation of the air quality in Bragança. Therefore, the objective of this research was to estimate the atmospheric emissions of MP provenientes from fixed sources and the emissions of MP and NOX from mobile sources in the city of Bragança-PA.

Houses of flour

There are approximately 100 flour houses in Bragança-PA, none of which use a chimney or any kind of technology to treat emissions. The practice of cassava flour production is one of the oldest activities in the Amazon and northeastern Brazil. This is because it is a practice that refers to the natives, who are the forerunners of this activity and that was passed down from generation to generation until today. In the production of flour, rustic means and very old and traditional equipment are still used (CHISTÉ and COHEN, 2006). This means of production preserves the culture of many indigenous, quilombola and traditional peoples, but

it is also a way of emitting particulate matter into the atmosphere. The burning of the firewood is typical among the Producers. In some places, wood burning is no longer used as a plow, but still, firewood is used extensively in flour houses, due to the lower economic value and ease of processing (OLIVEIRA, 2002, BORGES, 2017). Figure 1 illustrates two flour houses located in the city of Bragança-Pa



Figure 1. Flour houses located in the city of Bragança-Pa

Potteries

The activities in pottery are mainly focused on the production of raw materials for the construction industry, generally in the process of extraction of the clay, the vegetal cover is totally withdrawn and stored, for later use in the recovery of the own area after the end of the extraction. In the manufacture of bricks, potters deforest, consume firewood as a source of energy, contribute to pollution of the atmosphere, water and groundwater, damaging the natural cycle of sediment (sand, clay, site) flow to rivers, between others. In the city of Bragança pottery plays an important socioeconomic function, generating job and income in the municipality. More than 20,000 pieces are produced every month in the 18 potteries of the city. On the other hand, the burning of the biomass in the potteries, release the smoke resulting from this burning that produces indirect adverse effects on health. Since the population affected by the products generated by biomass combustion corresponds to those individuals with less access to health services. Added to this is possible changes in the local climate as well as the degradation of air quality. Figure 2, firewood being burned in the kiln of a pottery in the city of Bragança-Pa.



Figure 2. Wood burning in pottery

Emissions by motorcycle and vehicles

The vehicular and motorcycle fleet in Brazil has increased over the years, even in the smaller cities. In Bragança the motorcycle fleet is estimated at 9,045 and the fleet of vehicles is 19,128 (DENATRAN, 2016), almost 100% of the fleet of motorcycles and vehicles in the city use gasoline as fuel. In Bragança the increase of the fleet of motorcycles and vehicles is approximately 10% in relation to the previous year. This situation points to the need to implement environmental management instruments that adequately control and monitor the sources of pollution, seeking mitigating measures for the impacts caused by these emissions. In the national context, CONAMA RESOLUTION N°. 1, of May 6, 1986, was created on the creation of the Air Pollution Control Program for Automotive Vehicles - PROCONVE. In this context, PROMOT (Air Pollution Control Program for motorcycles and similar vehicles) was created in 2002 to complement PROCONVE (Air Pollution Control Program for Automotive Vehicles). Both PROCONVE and PROMOT work to reduce the emission of pollutants.

METHODS

The methodology is based on 3 phases: 1st stage: survey of the literature, national and international on the theme. Consultations to the air quality reports published by CETESB, the main environmental agency in Brazil, which served as a basis for the estimation of emissions in the city of Bragança, through the Emission Factors (FE) already calculated and available in the literature. Visits to DEMUTRAN (Municipal Department of Transit), flour houses and potteries for initial conversations; Elaboration of questionnaires and interview script that were applied to determine the amount of biomass and gasoline used; 2nd stage: on-site visits, visits to DEMUTRAN to obtain the average age of the vehicle fleet, type of fuel used; visits to olarias to obtain the estimated amount of biomass used in the

production process; visits to the flour houses to obtain the estimated amount of biomass used in the production. The calculation to estimate the emissions was done using methodologies already used in the national and international literature, for example in the CETESB air quality reports of 2017, especially in the elaboration of emission inventories, since measurements are not performed directly in the source, but by estimates of activity, represented by the formula:

$$E = FE \times \text{Activity}$$

At where:

E: annual pollutant emissions. Value normally expressed in ton/year;

FE: emission factor, that is, amount of pollutant emitted by the burning of 1kg of firewood, 1 L of gasoline among other fuels. In this study we considered only the burning of gasoline to the mobile sources, considering that almost 100% of the fleet of motorcycles and vehicles use the gasoline as fuel. The value of the emission factor is available from the literature, for the biomass burning was used the emission factor 0.38 g / kg calculated by (LIMA, 2015).

FINDINGS AND ARGUMENT

Brazil's small and medium-sized cities also have potential sources of air pollution, especially because of poor enforcement in these areas. In Bragança-Pa, there are potential sources of air pollution, such as flour houses and pottery, as well as emissions from motorcycles and vehicles. The motorcycle fleet is crescent, mainly due to the almost nonexistence of public transport in the city. The average amount of biomass used in the 18 potteries of the city of Bragança is 864,000 kg per month, per year corresponding to a total of 10,368,000 kg or 10.36 tons, generating an annual estimate of 3,939 tons of PM emitted by the potteries launched annually in the air. Particulate matter emissions per flour houses were estimated at 60 tons per year, considering the existence of 100 enterprises in the city, according to information obtained empirically through interviews with local residents and producers. High emissions give the dimension of the potential impact on good air quality, and the need to think about alternatives for the production of this important food but with significant potential for air degradation.

CONCLUSIONS

Particulate matter emissions from flour houses were estimated at 60 tons per year. High emissions give the dimension of the potential impact on good air quality, and the need to think about alternatives for the production of this important food but with significant potential for air degradation. The estimate of PM emissions in potteries was 3,939 MT

of MP. These values reveal how much these emissions can impact air quality and need to be better studied and considered in emissions inventories.

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ESTIMATION OF THE EMISSION OF PARTICULATE MATTER BY FIXED SOURCES IN THE CITY OF BRAGANÇA-PA

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Abstract: Air pollution by particulate matter (PM) is also present in small and medium-sized Brazilian cities, such as Bragança-Pa. The city of Bragança is the oldest in the state and concentrates a large amount of fixed sources of air pollution, such as pottery (brick production) and flour houses (cassava flour production), both of which use the burning of biomass in their processes. In addition to mobile sources, such as vehicles and motorcycles, whose fleet increases each year, mainly due to inefficient public transportation of the city. The objective is to estimate PM emissions from fixed sources located in the city of Bragança-Pa. This information will be used to draw up an inventory of atmospheric emissions for the city. The methodology is based on field visits, interviews with local producers to raise biomass consumption plus annual activity in pottery and flour houses. The estimation of the PM emissions has been carried out based on the emission factors available in the literature and air quality reports of CETESB. This is the equation ($E = FE \cdot A$) that was used to estimate the total emissions from fixed sources, where E (represents PM emissions, FE is emission factor and A is activity throughout the year). These methodologies are used in several studies around the world to estimate air pollutant emissions. Preliminary results showed that pottery and flour houses do not use any type of air pollution control technology, are numerous enterprises (18 and 1950, respectively) and with high annual consumption of biomass (10.4 and 1.6 tons, respectively), especially during the summer, when production is more intense. Was estimated at 3.99 and 60 tons of particulate matter emitted by pottery and flour houses in the city of Bragança-Pa. Added to this is the lack of monitoring of activities in pottery and flour houses. Besides the problems of the fires that happen every year in the state of Pará, including in Bragança, contributing to the air pollution.

Keywords: Air Pollution, Fixed Sources, Flour Houses, Potteries, Particulate Matter.

INTRODUCTION

Air pollution is one of the main environmental problems of today, including in medium and small cities, as is the case of the city of Bragança-Pa. However, it is still little studied when compared with studies in the area of water resources or in the area of soil. Air pollution is related to the degradation of air quality and potential effects on the environment and human health (SALDIVA, 2008). In large cities or large urban centers, there are a large number of sources of pollution, but there is also greater control over these emissions (BAIRD, 2011). In smaller cities the number of sources of air

pollution is lower when compared to large urban centers, but there is less control over these emissions, making it necessary to identify the sources, characterize and estimate the emissions and generate data for the elaboration of an emission inventory, with the purpose of proposing strategies for the reduction / control of pollution in the city of Bragança. The city of Bragança has significant stationary sources of air pollution, such as: bakeries, pizzerias and, above all, potteries and flour houses. Pottery and flour houses play an important economic and cultural role in the city. Should be noted that in the production process in flour houses and pottery, we have the burning of biomass as an energy source. The burning of the biomass emits several gaseous pollutants into the atmosphere, such as: carbon dioxide, nitrogen oxides, sulfur oxides and, in particular, particulate matter. Particulate matter or atmospheric aerosol is understood to mean solid and liquid particles with a size ranging from 0.1 to 50 μm in suspension in the atmosphere (SEINFELD AND PANDIS, 1998). Particulate matter is associated with climate change, in the process of cooling and warming the climate, in addition to the potential deleterious effect on human health. The lower the particle size, the greater the ability to penetrate the human body and cause more severe damage to human health, especially in the respiratory and circulatory system (SALDIVA, 2008). Therefore, biomass burning in these production processes constitutes a potential impact on the environment, even at the local level. It also represents a potential deleterious effect on human health, especially for workers in these activities, often children and the elderly. Always be family enterprises. Just those who constitute the so-called risk group and more susceptible to the effect of pollution. It is worth noting that the city is located in the so-called "Deforestation Arc" with increasing vegetation losses due to the burning process, which further aggravates the degradation of the air quality in Bragança. Therefore, the objective of this research was to estimate the atmospheric emissions of MP provenientes from fixed sources and the emissions of MP and NOX from mobile sources in the city of Bragança-PA.

Houses of flour

There are approximately 100 flour houses in Bragança-PA, none of which use a chimney or any kind of technology to treat emissions. The practice of cassava flour production is one of the oldest activities in the Amazon and northeastern Brazil. This is because it is a practice that refers to the natives, who are the forerunners of this activity and that was passed down from generation to generation until today. In the production of flour, rustic means and very old and traditional equipment are still used (CHISTÉ and COHEN, 2006). This means of production preserves the culture of many indigenous, quilombola and traditional peoples, but

it is also a way of emitting particulate matter into the atmosphere. The burning of the firewood is typical among the Producers. In some places, wood burning is no longer used as a plow, but still, firewood is used extensively in flour houses, due to the lower economic value and ease of processing (OLIVEIRA, 2002, BORGES, 2017). Figure 1 illustrates two flour houses located in the city of Bragança-Pa



Figure 1. Flour houses located in the city of Bragança-Pa

Potteries

The activities in pottery are mainly focused on the production of raw materials for the construction industry, generally in the process of extraction of the clay, the vegetal cover is totally withdrawn and stored, for later use in the recovery of the own area after the end of the extraction. In the manufacture of bricks, potters deforest, consume firewood as a source of energy, contribute to pollution of the atmosphere, water and groundwater, damaging the natural cycle of sediment (sand, clay, site) flow to rivers, between others. In the city of Bragança pottery plays an important socioeconomic function, generating job and income in the municipality. More than 20,000 pieces are produced every month in the 18 potteries of the city. On the other hand, the burning of the biomass in the potteries, release the smoke resulting from this burning that produces indirect adverse effects on health. Since the population affected by the products generated by biomass combustion corresponds to those individuals with less access to health services. Added to this is possible changes in the local climate as well as the degradation of air quality. Figure 2, firewood being burned in the kiln of a pottery in the city of Bragança-Pa.



Figure 2. Wood burning in pottery

Emissions by motorcycle and vehicles

The vehicular and motorcycle fleet in Brazil has increased over the years, even in the smaller cities. In Bragança the motorcycle fleet is estimated at 9,045 and the fleet of vehicles is 19,128 (DENATRAN, 2016), almost 100% of the fleet of motorcycles and vehicles in the city use gasoline as fuel. In Bragança the increase of the fleet of motorcycles and vehicles is approximately 10% in relation to the previous year. This situation points to the need to implement environmental management instruments that adequately control and monitor the sources of pollution, seeking mitigating measures for the impacts caused by these emissions. In the national context, CONAMA RESOLUTION N°. 1, of May 6, 1986, was created on the creation of the Air Pollution Control Program for Automotive Vehicles - PROCONVE. In this context, PROMOT (Air Pollution Control Program for motorcycles and similar vehicles) was created in 2002 to complement PROCONVE (Air Pollution Control Program for Automotive Vehicles). Both PROCONVE and PROMOT work to reduce the emission of pollutants.

METHODS

The methodology is based on 3 phases: 1st stage: survey of the literature, national and international on the theme. Consultations to the air quality reports published by CETESB, the main environmental agency in Brazil, which served as a basis for the estimation of emissions in the city of Bragança, through the Emission Factors (FE) already calculated and available in the literature. Visits to DEMUTRAN (Municipal Department of Transit), flour houses and potteries for initial conversations; Elaboration of questionnaires and interview script that were applied to determine the amount of biomass and gasoline used; 2nd stage: on-site visits, visits to DEMUTRAN to obtain the average age of the vehicle fleet, type of fuel used; visits to olarias to obtain the estimated amount of biomass used in the

production process; visits to the flour houses to obtain the estimated amount of biomass used in the production. The calculation to estimate the emissions was done using methodologies already used in the national and international literature, for example in the CETESB air quality reports of 2017, especially in the elaboration of emission inventories, since measurements are not performed directly in the source, but by estimates of activity, represented by the formula:

$$E = FE \times \text{Activity}$$

At where:

E: annual pollutant emissions. Value normally expressed in ton/year;

FE: emission factor, that is, amount of pollutant emitted by the burning of 1kg of firewood, 1 L of gasoline among other fuels. In this study we considered only the burning of gasoline to the mobile sources, considering that almost 100% of the fleet of motorcycles and vehicles use the gasoline as fuel. The value of the emission factor is available from the literature, for the biomass burning was used the emission factor 0.38 g / kg calculated by (LIMA, 2015).

FINDINGS AND ARGUMENT

Brazil's small and medium-sized cities also have potential sources of air pollution, especially because of poor enforcement in these areas. In Bragança-Pa, there are potential sources of air pollution, such as flour houses and pottery, as well as emissions from motorcycles and vehicles. The motorcycle fleet is crescent, mainly due to the almost nonexistence of public transport in the city. The average amount of biomass used in the 18 potteries of the city of Bragança is 864,000 kg per month, per year corresponding to a total of 10,368,000 kg or 10.36 tons, generating an annual estimate of 3,939 tons of PM emitted by the potteries launched annually in the air. Particulate matter emissions per flour houses were estimated at 60 tons per year, considering the existence of 100 enterprises in the city, according to information obtained empirically through interviews with local residents and producers. High emissions give the dimension of the potential impact on good air quality, and the need to think about alternatives for the production of this important food but with significant potential for air degradation.

CONCLUSIONS

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of MP. These values reveal how much these emissions can impact air quality and need to be better studied and considered in emissions inventories.

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VARIABILITY OF EMISSIONS FROM SOIL RESUSPENSION: A STUDY CASE IN FLORIANÓPOLIS, BRAZIL

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Abstract: Among all sorts of pollutants found in the local atmosphere, particulate matter (PM) is pointed as one of the most threatening to human well-being. In urban centers, resuspended material from paved roads can be a significant source of PM, being influenced by meteorological conditions and vehicular activity. Therefore, the emissions from resuspended PM can vary significantly along days, week, month and year. This influence factors could add some difficulties on understanding air pollution in urban areas. The present study aimed to analyze the influence of vehicular flow and precipitation on PM resuspension. The USEPA's equation described by the AP-42 for estimating soil resuspension was applied to a road in the city of Florianópolis, South of Brazil. To disaggregate emissions temporarily, a two terms Gaussian curve was fitted to modeled data on vehicular flow. Based on a Monte Carlo simulation, uncertainties on emission levels were found to be the highest in between peak hours of vehicular flow. Concerning the influence of the meteorological input, it was observed that PM emissions reduced as the probability of rain increased. Another influencing factor on estimation of PM emissions from soil resuspension is associated to the averaging time employed.

Keywords: emissions inventory, Monte Carlo, particulate matter, vehicular flow, soil resuspension.

INTRODUCTION

Particulate Matter (PM) exposure on the local atmosphere has been associated to several adverse effects on human health, from respiratory diseases to cardiopulmonary mortality (Amato et al, 2010 and Anderson et al, 2012). In urban centers, literature points that the majority of particles with diameter smaller than 10µm are attributed to resuspended material from vehicular activities (Van der Gon, 2013).

The United States Environmental Protection Agency (US EPA) provides methods to quantify traffic related emissions, including dust/soil resuspension from paved roads. According to the agency, inventories of resuspended material from paved roads should consider meteorological conditions, vehicle weight and the silt load.

To analyze the importance of specific inputs on emissions estimation, and to study hypothetical pollutant emissions scenarios, a sensitivity analyses can be performed. It consists in randomly fluctuate inputs of an equation allowing for many possible outcomes (Garcia-Días e Gonzalez-Zafrilla, 2012). The Monte Carlo simulation approach is an example of sensitivity analyses applied to emissions inventories.

In that context, the objective of the present study is to calculate the variability of resuspended particulate matter emitted by vehicles, and to assess the influence of vehicular flow and meteorological conditions on emission levels. The Monte Carlo simulation approach will be applied to vehicular flow and precipitation inputs to analyze uncertainties and possible scenarios. The study area is a road in the City of Florianópolis, South of Brazil. As PM emissions from resuspension have

never been estimated in Florianópolis, the present study provides an unprecedented set of data

METHODS

In this work, the Delfino Conti road (Figure 1), in Florianópolis/SC - Brazil was used as study case for estimating soil resuspension from vehicle traffic. This road is one of the main accesses to the Federal University of Santa Catarina (UFSC), is adjacent to local commerce and presents an intense vehicular flow throughout the day.

In order to estimate PM resuspension, a method developed by the Environmental Protection Agency was employed (EPA, 2011). The equation applied can be found in Chapter 13 of AP-42, which defines the Emission Factor (EF) of resuspended PM from paved roads as shown in Equation 1:

$$EF = [k * (sL^{0.91}) * (W^{1.02})] * \left(1 - 1.2 \frac{P}{N}\right) \quad (1)$$

Which can be used to calculate emissions from resuspension as indicated in Equation 2:

$$E = EF * TD \quad (2)$$

Where k is the particle size multiplier for particle size range in vehicle kilometers traveled (VKT); sL is the silt loading in grams per square meters (g/m²); W is the average weight of the vehicles traveling the road in tons (t); P is the number of times it has rained at least 0.254 mm in a period; N is the analyzed period; EF is the emission factor in grams per vehicle kilometers traveled (g/VKT); E is the resuspension emission in grams per hour (g/h); TD is the traveled distance in kilometers (km), obtained by multiplying the number of motor vehicles by the road length.

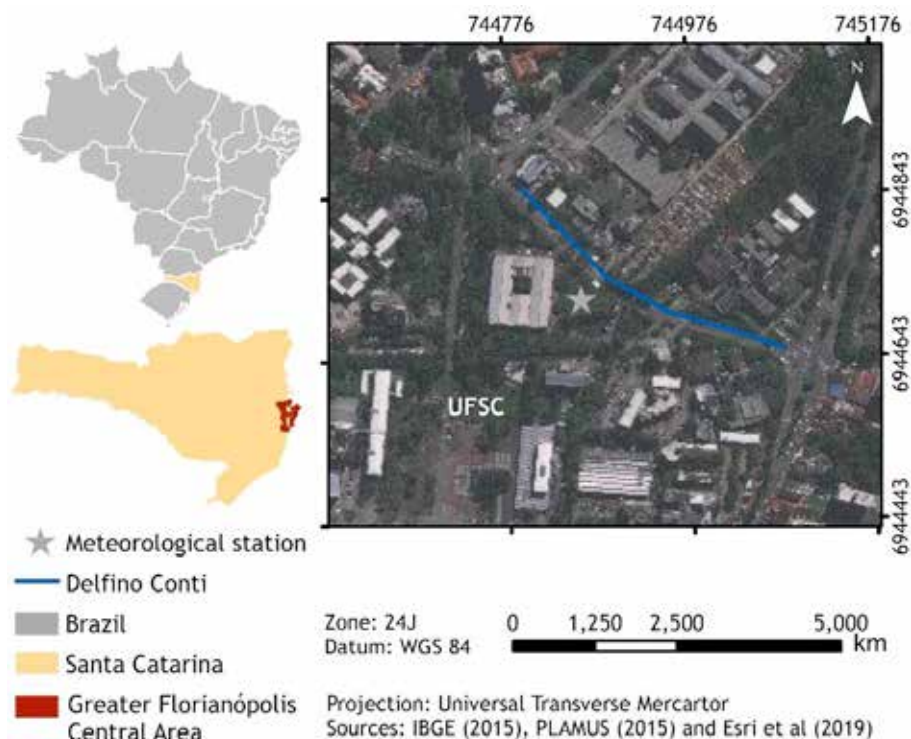


Figure 1. Study area localization

Activity data on light-duty vehicles and trucks during the morning and afternoon peak hours, and the street length, were obtained from the Sustainable Urban Mobility Plan of the Great Florianópolis Area - PLAMUS (2015). The flow of buses during peak hours was obtained through manual counting using the web application Floripanoponto (Consórcio Fênix, 2019). Precipitation data from a six month period, from January to July of 2018, were provided by the meteorological station operated by the Laboratory of Hydrology (LABHIDRO), which is located near the study area, at UFSC. For calculating the average fleet weight, a weighting between light-duty and heavy-duty vehicles (trucks and buses) was calculated. Light-duty vehicles were considered to weight 2.8 tons; and heavy-duty vehicles, 15 tons (MMA, 1995 e MMA, 2013). The silt values varied for each analysis and will be described in the following items. All data manipulation was performed using the software MATLAB.

Temporal disaggregation of emissions according to the hour of the day

From vehicular activity data provided by PLAMUS (2015), the present study conducted a temporal disaggregation of vehicular flow. To distribute vehicular flow throughout the day, a Gaussian adjustment with two terms was fitted to the data (Equation 3). These terms represented the flow in the morning and the afternoon, with peaks

corresponding to the modeled data from PLAMUS (2015).

$$V = a1 * e^{[-(\frac{x-b1}{c1})^2]} + a2 * e^{[-(\frac{x-b2}{c2})^2]} \quad (3)$$

Where V is the vehicle volume curve, $a1$ is the vehicular flow during the morning peak, $b1$ is the morning peak hour, $c1$ is the duration of traffic flow in the morning, $a2$ is the vehicular flow during the afternoon peak, $b2$ is the afternoon peak hour and $c2$ is the duration of traffic flow in the afternoon.

The peak morning and afternoon hours were 8 a.m. and 5 p.m., respectively, as defined by PLAMUS (2015). Both duration of traffic flow were chosen iteratively until the curve presented a realistic shape.

It was possible to estimate the vehicular flow on Delfino Conti road throughout the day, and consequently, estimate hourly emissions. In the same adjustment, the Monte Carlo simulation approach was utilized for a sensitivity analysis, in which random input values were generated for each variable within the Equation 1. Variables values ranged around 10%. For this case, the silt value was fixed as 0.2 g/m², as established by US EPA's AP-42, according to the vehicular activity.

Emissions variability according to the probability of precipitation occurrence

Equation 1 considers that meteorological conditions from the previous hours affects the resuspended material on the subsequent hours. In Equation 1, P/N acts as a correction term according to the precipitation, in which P is the number of rainy events (at least 0.254 mm of precipitation) in a chosen period N . According to the AP-42 method, the probability of rain should be analyzed within intervals from the prior 3 to 12 hours.

Resuspension emissions were analyzed according to the probability of precipitation events on the previous 3, 6 and 12 hours. It aimed to contribute to the averaging time decision on future studies. In that sense, through Monte Carlo simulations, the occurrence of precipitation events for each interval was varied conforming to the meteorological data. The value of silt was also generated randomly, ranging from 0.4 to 1.0 (g/m^2).

FINDINGS AND ARGUMENT

Temporal disaggregation of emissions according to the hour of the day

As expected, the Gaussian distributions in Figure 2 resulted in two emission peaks, respective to the hour of the highest vehicular flow in the morning and afternoon. There is an evident emission intensification before the morning peak and a great reduction following the afternoon peak.

In addition, it is noticeable a great variability of values between peak hours, in other words, between 08 and 17h. Therefore, it is possible to infer that such period presents a higher uncertainty when compared with other hours of the day. The greatest uncertainty interval was found at 1 p.m, where the maximum value found was 174.86 g/h and the minimum, 76.77 g/h .

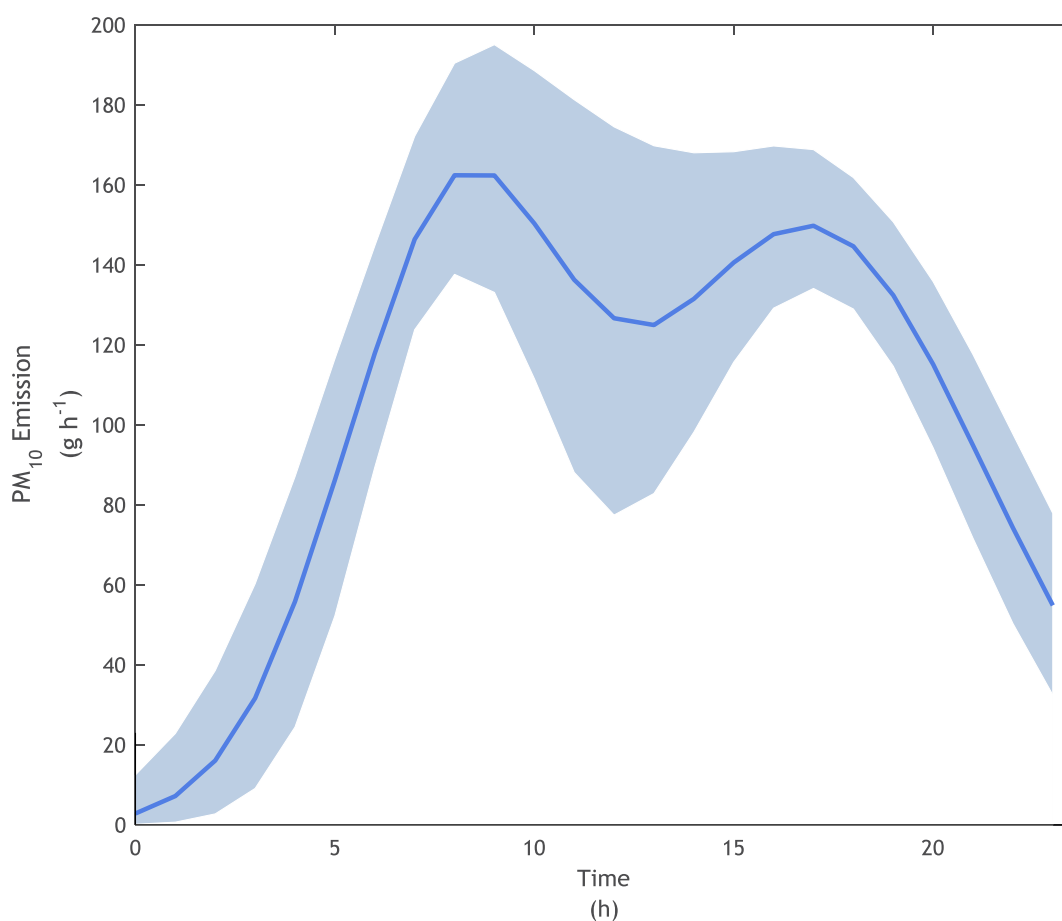


Figure 2. Two term Gaussian adjustment of Particulate Matter resuspension from Delfino Conti road.

Emissions variability according to the probability of precipitation

In general, Figure 3 shows that PM emissions are greater the lower is the probability of raining events on the hours before. The rain has a mitigation effect in respect to emissions rate. Through the results, it was observed lower emissions ratio when the probability of precipitation was higher.

Although the morning vehicular flow in general is higher, in this analyses the emissions did not

presented significant difference comparing the morning and the afternoon hours. The variability of emissions caused by precipitation stands out compared to the variability caused by vehicular flow.

Comparing the three average times utilization, the lower averaging time (3 hours) presented the biggest data variability and median value. Both the averaging times of 3 and 6 hours presented a higher sensitivity to precipitation occurrence than the 12 hours period.

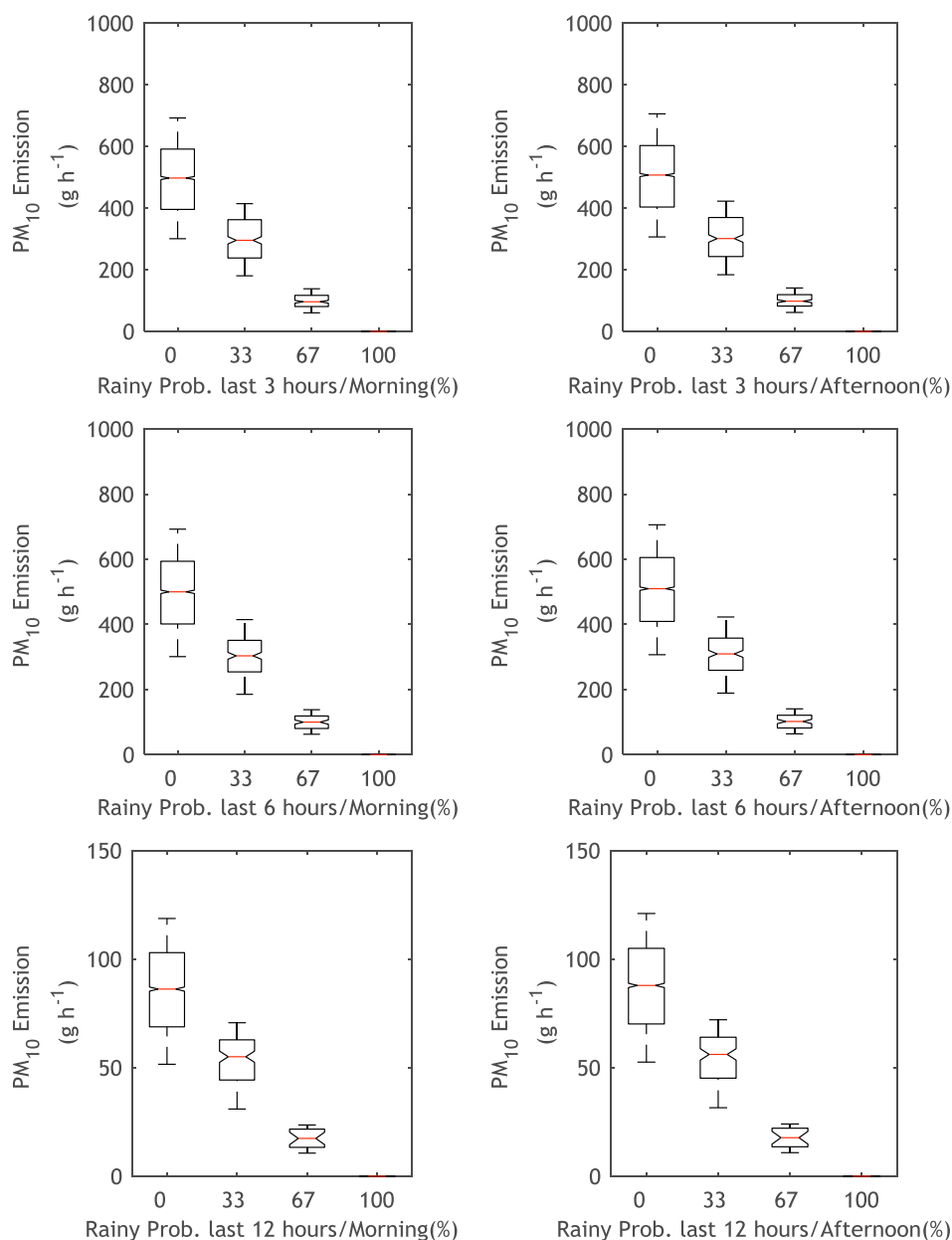


Figure 3. Variability of traffic-related particulate matter emissions from soil resuspension, according to the probability of precipitation events on the prior 3, 6 and 12 hours, during the morning and afternoon peak hours.

CONCLUSIONS

Through the approximation of the daily vehicular flow to a Gaussian curve, it was possible to disaggregate emissions temporarily. The Monte Carlo approach applied to the hourly emissions demonstrated that the biggest uncertainty occurs in between peak hours, from 8 a.m. to 5 p.m. Due to the lack of recent monitored data on vehicular activity, it was not possible to validate results on vehicular flow.

Through Equations 1 and 2 developed by the USEPA AP-42, it was noticeable that the vehicular flow has a direct influence on emissions resuspension. Meanwhile, precipitation events have inverse influence on emissions, reducing them. Through the present study it was possible to evaluate the importance of these parameters.

Until the present time, the Great Florianópolis Region does not rely on a monitoring network to enable validation of emissions estimation. This work reinforces the need of a public air quality monitoring system and development of robust emission inventories. In this case, monitoring results would support the decision on the best averaging time for precipitation events as well as decrease uncertainties on temporal disaggregation.

Understanding air quality and traffic related emissions are hard task in urban centers. This work contributes to the science of emissions inventories and provides valuable information about PM emissions variability and its influencing factors.

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Atmospheric emissions from Pipe Laying Support Vessels in Santos Basin in 2016

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Abstract: Santos basin is the largest offshore sedimentary basin in Brazil and it has potential for large-sized oil discoveries in the pre-salt play, with the possibility to become a major GHG and air pollutant emitter in Brazil. Calculations show that in Santos Basin, in 2016, in cruising regime and using main engines, were emitted 263 tons of NO_x, 20 tons of SO₂, 10 tons of HC and 12,851 tons of CO₂. For maneuvering and port regimes, with main engines, were emitted 2,869 tons of NO_x, 298 tons of SO₂, 406 tons of HC, 243.6 tons of PM and 192,194 tons of CO₂. For auxiliary engines, were emitted 2,145 tons of NO_x, 1,170 tons of SO₂, 62 tons of HC, 46 tons of PM and 106,470 tons of CO₂. As a final result, it was concluded that, in 2016, were emitted to the Santos Basin atmosphere 5,277 tons of NO_x, 487 tons of SO₂, 478 tons of HC, 290 tons of PM and 311,515 tons of CO₂. This research has demonstrated that ship emissions can make a significant contribution to air pollution, being a significant source of CO₂.

Keywords: Offshore supply vessels, greenhouse gases, air pollution, Santos Basin.

INTRODUCTION

Fossil fuels are non-renewable resources that have been used as a source of energy since Industrial Revolution, when there was a need or an intense search for new high performance fuels to assist in large scale production. The main types of fuels are coal, natural gas and oil. For modes of transport oil is the most extensively used fossil fuel.

Brazil has become the 10th largest global oil producer and the largest in Latin America, mainly due to the pre-salt discoveries in 2006, one of the most important made in the world over the last years, as reported by the International Energy Agency (Abelha and Petersohn, 2018). According to the National Agency of Petroleum, Natural Gas and Biofuels (ANP, 2017), pre-salt is a sequence of sedimentary rocks formed more than 100 million years ago from the break-up of the ancient continent Gondwana which formed the current continents of South America and Africa. In deeper regions, after a process which involves high temperatures and pressures, the organic matter accumulated was transformed into oil and gas.

Located between Brazilian states of Santa Catarina and Espírito Santo, pre-salt polygon has an area of approximately 149,000 km² (ANP, 2017). Pre-salt discovery resulted in support vessels significant increase on Brazilian coast. In 2009, pre-salt operation began in Santos Basin (Figure 1), which is the largest offshore sedimentary basin in the country, with more than 350,000 km², that extends from Cabo Frio (state of Rio de Janeiro) to Florianópolis (state of Santa Catarina) (Petrobras, 2019).



Reference: Adapted from Petrobras, 2017

Figure 1. Location Map of Santos Basin

As oil and gas production increased, it was necessary more investments for the renewal of the fleet, with higher demand for offshore supply boats. As reported by the Brazilian Association of Maritime Support (ABEAM, 2017), until 2016, 411 Brazilian shipping companies were authorized by the National Agency for Water Transportation (ANTAQ), with 48 effectively operating in maritime supply.

There are a variety of offshore vessels, and each one serves a specific purpose, as helping in exploration and drilling of oil, providing necessary supplies to the excavation and construction units located at the high seas (ABEAM, 2017). Pipe Laying Support Vessels (PLSV), subject of this study, are complex and highly specialized vessels,

equipped with sophisticated equipment and systems of high value, used for the construction and launch of rigid and flexible lines (ABEAM, 2019).

Undesirable effects may occur as a consequence of increased maritime transport activities, especially with regard to air quality. Marine engines demands density oil consumption for main and auxiliaries engines propulsion and boilers, which result in continuous pollutants emission into the atmosphere, being considered one of the largest global greenhouse gas (GHG) and air pollutant emitters, degrading the environment and affecting human health (Medeiros, 2012). Emissions inventories estimate marine transport as a significant source of air pollution and a contributing factor in global climate change. Ship emissions have local, regional, and global impacts (Corbett e Koehler, 2003). Exhaust emissions from marine diesel engines largely comprise of nitrogen, oxygen, carbon dioxide and water vapour, with smaller quantities of carbon monoxide, sulphur oxides, nitrogen oxides, partially reacted and non-combusted hydrocarbons and particulate matter (Kristensen, 2015).

Thus, the present research aims to estimate the air pollutant emissions in offshore PLSV support vessels in 2016 in Santos Basin.

METHODS

International Panel of Climate Change (IPCC, 2006) and European Commission (EA, 2002) methods were used to estimate the pollutants emitted by the PLSV fleet in Santos Basin.

The applied methodology is based on a bottom-up approach, which considers equipments technical characteristics and working regime, in order to obtain total emitted pollutants, taking into account their emission factors (EF). IPCC Guidelines (2006) have two methodological tiers for estimating emissions, and both assume emission factors to fuel consumption activity data. Tier 1 (IPCC, 2006) was used to estimate pollutants emissions (Equation 1) in this study, considering emission factors obtained by EA (2002).

$$Emission_x = \sum (P_a \times OT_a \times EF_{xabc d}) \quad \text{Eq.1}$$

Where:

P - engine power,
OT - operating time,
EF - emission factor,
x - pollutant,
a - engine type (main or auxiliaries),
b - fuel type,
c - engines speed (low, medium or high speed),
d - ship operating regime (cruise, maneuvers or port).

The engine powers of the PLSVs were obtained from vessel technical manuals available online. All PLSV were considered with three main engines (ME) for propulsion and three auxiliaries engines (AE) (Medeiros, 2012). The auxiliaries engines are used for energy generation (EG), medium speed diesel engine (MSD), and one staying in stand-by (SB) being used only in case of failure of any of the other engines. The fuel consumed by the fleet was marine diesel oil - MDO (Petrobras, 2013).

Information of supply vessels dynamics that attend platforms installation and operation in Santos Basin were acquired by Naval Traffic Monitoring Project (Petrobras, 2017). Vessels are equipped with a tracking system that emits positioning signals which were tracked through Inmarsat C and Inmarsat D+ satellite systems and the AIS (Automatic Identification System) terrestrial system. Monitoring records obtained were processed through a Geographic Information System (GIS). In order to carry out the analysis, vessels with a speed equal to or greater than three knots were considered in cruising, while vessels with a speed below this limit were considered stopped/anchored or stopped/operating. Through vector data obtained by GIS, was possible to determine the distance traveled by each vessel (Petrobras, 2017). Technical manuals also provides vessels full speed, thus with distance and speed is possible to calculate operating time in cruising regime.

Port and maneuver regime operating time was calculated with Equation 2:

$$OT = \sum_1^n \{(DY \times 24) - [CT + TO]\} \quad \text{Eq.2}$$

Where:

OT - operating time,
DY - Days of the year,
CT- Cruising Time (h),
TO - Time Out of BS and no signal (h),
n - number of vessels.

The European Commission (2002) published a report containing emissions estimative for ships based on previous studies. Data from five different engine types and three different fuel types, for all three different activities (cruising, in port and maneuvering), were used in this research. Emission factors, shown on Table 1, were used to estimate air pollutant emissions of nitrogen oxides (NO_x), sulphur dioxide (SO₂), hydrocarbons (HC), particulate matter (PM) and carbon dioxide (CO₂).

Table 1. Emission Factors (g/kW.h)

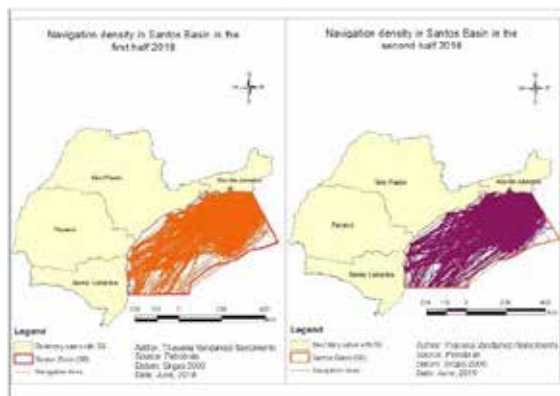
Pollutant	CO ₂	NO _x	SO ₂	HC	PM
Engine/Regime					
ME/cruising	645	13.2	1	0.5	-
ME/maneuvers or port	710	10.6	1.1	1.5	0.9
AE/all regimes	690	13.9	1.1	0.4	0.3

Reference: European Commission, 2002.

FINDINGS AND ARGUMENT

According to Naval Traffic Monitoring Project, Annex II (Petrobras, 2017), four hundred and twenty one supply vessels traveled at Santos Basin in 2016, twenty of these being identified as PLSV. This fleet covered a distance of 130,494.06 km of navigation at an average speed of 23.48 km/h in cruise regime. The total time spent for PLSV in maneuver service and in port was 75,447 hours. The average power of the main engines, used in vessels propulsion, was 3587.9 kW, and of the auxiliary engine, used for the energy generation, 1022.6 kW.

Figure 2 shows the density of navigation of vessels in SB in the first and second semester of 2016.



Adapted from: Petrobras, 2017.

Figure 2. Navigation density map in Santos Basin in 2016

From data collected, it was possible to estimate the amount of pollutant emitted for each operation regime and engine type. Results, in tons, are shown on Table 2. It is noted that CO₂ emitted is higher than the other pollutants, representing 97.95% of total emissions, followed by NO_x with 1.66%, SO₂ with 0.15%, HC with 0.15% and particulate matter with 0.09% of the total. According to the 'Third IMO GHG Study' (IMO, 2014), in 2012, global total shipping emissions were approximately 938 million tons of CO₂, 20.9 million tons of NO_x, 11.3 million tons of SO₂ and

14.4 million tons of PM. Comparing SB results with global ship emissions, CO₂ emitted in the basin corresponds to 0.03% of global emission in 2014, while emissions of NO_x, SO₂ and PM correspond, respectively, to 0.025%, 0.0015% and 0.002%. These are significant proportions considering that study took into account twenty vessels, and data were limited only to Santos Basin.

Table 2. Pollutant emission (ton) in SB in 2016

Pollutant	CO ₂	NO _x	SO ₂	HC	PM
Engine/Regime					
ME/cruising	12,851	263	20	10	-
ME/maneuvers or port	192,195	2,869	298	406	244
AE/all regimes	106,470	2,145	170	62	46
Total emitted in 2016	311,515	5,277	487	478	290

Results also indicate that main engines, in maneuvers or port regime, has higher emission values for all pollutants compared to values emitted by auxiliary engines. This may be due to its high power and operating time, since auxiliaries engines are only used for energy generation.

CONCLUSIONS

According to this study, it was estimated that, in 2016, 311,515 tons of CO₂, 5,777 tons of NO_x, 487 tons of SO₂, 478 tons of HC and 290 tons of PM were emitted in Santos Basin by PLSV vessels. Pollutant emissions show that improvements in efficiency of both engines and marine fuels are important in mitigating emissions growth. More stringent legislation regarding marine fuels could have a significant reduction in the amount of pollutants emitted and GHG.

Thus, further studies are important to develop more efficient engines and cleaner fuels to minimize the pollutants emissions into the atmosphere that cause impacts on the environment and human health.

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Vehicular emission factors in São Paulo evaluated with measurements in traffic tunnels

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ABSTRACT

Nowadays, the air degradation is a common problem in many metropolitan areas. This degradation is noted by effects on human health, including respiratory diseases, with the vehicles being the major source of pollutants emission in São Paulo. Thus, the present work aims to estimate the vehicular emissions factors (EF) of air pollutants and to compare with past studies.

The research was carried out in two tunnels in the metropolitan area of São Paulo (MASP): “Túnel Rodoanel” (TRA), where light-duty vehicles (LDVs) and heavy-duty vehicles (HDVs) were allowed to traffic inside, and “Túnel Jânio Quadros (TJQ), where only LDVs are allowed.

The EF was calculated for CO₂, CO, NO_x, SO₂ and ethanol. HDVs were found as the largest emitters of CO₂, NO_x and SO₂ 1255, 6.9 and 0.05 g/km, respectively. On the other hand, LDVs were found as the largest emitters of CO and ethanol, 4.4 and 0.18 g/km, respectively. Furthermore, in a comparison with past studies performed in São Paulo, in 2011, it was observed a reduction up to 2.4 times on pollutant emissions. This reduction is mainly due to the implementation of public policies which have improved engine technology and the production of cleaner fuels.

Keywords: Emission factors, tunnels, São Paulo, pollutants, fuel

INTRODUCTION

The Metropolitan Area of São Paulo (MASP), one of the largest megacities in the world, has approximately 21 million inhabitants and almost 7 million vehicles. In the MASP, 85% of vehicles are light-duty vehicles (LDVs, running on a mixture 72% gasoline+28% ethanol or ethanol-E100), 3% heavy-duty vehicles (HDVs, running on 92%diesel+8%biodiesel) and 12% motorcycles (CETESB, 2017). These vehicles are responsible for emission of gases, such as CO₂, CO and NO_x.

With the objective of reducing the emission of atmospheric pollutants, the PROCONVE (“Programa de Controle da Poluição do Ar por Veículos Automotores”) was created in Brazil in 1986, implementing more restrictive emission limit at each phase (L1 to L5 to LDV and P1 to P7 to HDV, Andrade et al. 2017). To achieve this goal, new technologies are being used in vehicles, such as catalytic converters, electronic injection, biofuels etc. helping the reduction on air pollutants emissions.

The emission factor (EF), which describes the emitted mass of a compound per distance or per volume of fuel burned, is a good way to estimate the emission of air pollutants. To quantify and verify the reduction on vehicle emissions in the MASP, the EF under real conditions was calculated. For this study, the analyzed gases were CO₂, CO, NO_x, SO₂ and ethanol. Similar measurements were performed in 2004 (Martins et al. 2006) and 2011 (Perez-Martinez et al, 2014).

METHODS

The measurements were carried out in two tunnels in the MASP. The first campaign occurred in “Túnel Rodoanel” (TRA), from October 26 to November 4, 2018. The TRA is located in the northeast of the MASP where LDV and HDV are allowed to traffic inside. The second campaign was carried out in “Túnel Jânio Quadros” (TJQ), during November 3 -13, 2018. The TJQ is located in southwest area and only LDV and motorcycles are allowed. The choice of tunnels to carry out measurements is justified to provide the identification of individual vehicles sources. In both, the pollutants measurements were performed in the midpoint inside the tunnels and the background air concentrations were measured outside the tunnels.

Inside tunnels, CO₂, CO and ethanol were measured with photoacoustic infrared spectroscopy (INNOVA 1412i; LumaSense, Santa Clara, CA), whereas outside tunnels were measured with infrared spectroscopy (Picarro-G1301, Santa Clara, CA). NO_x and CO were measured inside and outside using the same methodologies, 42i analyzer and 48i analyzer (Thermo Fisher Scientific Inc., Franklin, MA). The analyzers were inspected and tested in the laboratory, before and after the field campaigns, in order to provide high-quality measurements.

The EF was calculated by the methodology adopted by Marr et al. 1999:

$$EF = 10^3 \left(\frac{\Delta[P]}{\Delta[CO] + \Delta[CO_2]} \right) \omega_c, \text{ where EF is the emission factor, in g per kg of burned fuel,}$$

ΔP is the concentration of pollutant, in $\mu\text{g}/\text{m}^3$, ΔCO is the concentration of CO, in $\mu\text{g}/\text{m}^3$, ΔCO_2 is the concentration of CO₂, in $\mu\text{g}/\text{m}^3$, ω_c is the weight fractions of fuel carbon, being 0,77 for gasohol and 0,87 for diesel. The EF also can be obtained in g/L and g/km.

RESULTS AND DISCUSSION

The EFs are shown in table 1.

Table 1: CO, CO₂, SO₂, NO_x and ethanol EF estimated for LDVs and HDVs in 2018

	LDVs		HDVs	
	g/kg	g/km	g/kg	g/km
CO	49 ± 13	4.4 ± 1.2	3.8 ± 0.9	1.50 ± 0.4
CO ₂	2753 ± 24	248 ± 2	3184.01 ± 1.50	1255 ± 0.6
SO ₂	0.06 ± 0.03	0.005 ± 0.003	0.13 ± 0.03	0.05 ± 0.01
NO _x	1.7 ± 0.8	0.16 ± 0.07	14.6 ± 4.3	6.9 ± 2.0
Ethanol	2.0 ± 1	0.18 ± 0.09	0.08 ± 0.04	0.03 ± 0.02

The highest values of EF of CO₂ and NO_x were observed for HDVs, while the LDVs EF values were highest for CO and ethanol than HDVs emissions. It is noteworthy that in g/km basis, HDV emit around 10 times more SO₂ than LDV.

Table 2 shows a comparison between studies done in the same tunnels in different periods. In 2011 (Pérez-Martínez, 2014) the EF were higher than the EF estimated for vehicles running in 2018. For instance, the reduction of NO_x by HDVs emissions is approximately 1.7 times, while the reduction in LDVs emissions was 2.4 times, which represent an advance in control of the emission of gases. This improvement is due to the new technologies in vehicles and public policies.

Table 2 - Emission factors comparison expressed in (g/kg)

	LDVs			HDVs		
	CO	CO ₂	NO _x	CO	CO ₂	NO _x
2011	81 ± 41	2964 ± 96	4.2 ± 1.7	7.9 ± 4.1	3177 ± 9	25.8 ± 7.6
2018	49.4 ± 13.4	2753 ± 24	1.75 ± 0.77	3.81 ± 0.96	3184.01 ± 1.50	14.6 ± 4.3

CONCLUSIONS

The present study shows that the vehicular emissions in MASP decrease in the last years. Comparing with past study (2011), it is noted a reduction on EFs, mainly in NO_x and CO EF of both fleets, LDVs and HDVs. It is due to new vehicular technologies, such as catalytic converters, and public policies, such as PROCONVE.

Although the EFs have decreased, the emission of CO₂ still stays elevated, being the major emission in the MASP. Moreover, it is observed the difference between HDVs and LDVs. The first present higher emission values of CO₂ and NO_x than the second, while the LDVs is responsible for highest emission of CO and ethanol.

ACKNOWLEDGMENTS: FAPESP, CAPES, CNPq, CETESB, CET and CCR.

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AIR QUALITY AND POLLUTANT EMISSION OVER LARGE CITIES IN SOUTH AMERICA

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Abstract: Air pollution is the largest and most persistent environmental problem in South America and the world, with exposure to PM_{2.5} considered the highest environmental risk for health. According to the World Health Organization (WHO) estimates, in 2016, 91% of the urban population lived in cities that exceeded the minimum levels established by this Organization. In South America, 3 of the 28 megacities in the world are located: Rio de Janeiro in Brazil (12,830,000), Buenos Aires in Argentina (15,020,000) and São Paulo in Brazil (20,830,000). In the same way, this region has 3 of the 43 major cities in the world: Santiago in Chile, Bogotá in Colombia and Lima in Peru. It is expected that in 2030 these last two cities will become megacities as well. The aim of this work was to present a multicentric review of the long and short-term concentrations of atmospheric pollutants such as: nitrogen dioxide (NO₂), sulphur dioxide SO₂, particulate matter (PM_{2.5} and PM₁₀), carbon monoxide (CO) and ozone (O₃) and. Also, a review of the most recent emissions data available in the South America, was presented. The methodology design involved a compilation, validation and analysis of the hourly pollutants concentrations recorded in the 10 monitoring networks in the period 2010-2017. In the review of atmospheric pollutants emissions, was included a complete analysis of the state of the art of the official emission inventories available. If they are not available, the latest version of the Emissions Database for Global Atmospheric Research (EDGAR) 2012 was used. The most important results show that despite efforts to monitor air quality, in some cities, major lacks were found in the diffusion, consistency and presentation of information provided by environmental authorities. In comparison with the World Health Organization Air Quality Guidelines (WHO-AQG), particulate matter (PM_{2.5} and PM₁₀) always exceeded 10 µg/m³ and 20 µg/m³, respectively. The NO₂ WHO-AQG (40 µg/m³) was exceeded by 4 of the 10 cities that had annual mean information. In the SO₂ case, daily averages concentrations exceeded the WHO-AQG by São Paulo (all years) and Vitória (last two years). Ozone (8 hours averages concentrations) has always been below the WHO-AQG guideline (100 µg/m³). In the inventory emissions review it was found that 6 of the 10 cities considered in this research do not have recent inventories available. The inventories available in South America was updated maximum in 2016, which makes it more difficult for environmental authorities to generate and implemented environmental policies and management efficient air quality.

Keywords: Air quality, pollutant emission, South America, Megacities, Monitoring Networks.

1. INTRODUCTION

Population growth and accelerated urbanization processes in large cities, as well as challenges related to economic development, require growth planning and city governance to ensure proper provision of food, shelter, mobility and other services for the well-being of the population that depend on industrial production, energy generation, and transportation, which are the main activities related to emission of air pollutants that deteriorate air quality (WHO, 2012; Gulia et al., 2015; Boas et al., 2018).

According to the World Health Organization (WHO), in 2016, 91% of the population did not breathe clean air and more than half of the urban population was exposed to pollutant levels that exceeded up to 2.5 times the standards issued by WHO. Also, in 2016, air pollution caused around 4.2 million premature deaths in the world (WHO, 2018).

The number of megacities in the world and the size of their populations increased significantly in the second half of the 20th century (Baklanov et al., 2016). According to UN 2018 Revision of World

Urbanization Prospects (UN, 2018), the urban population has grown rapidly in the last six decades, from 751 million to 4.2 billion in 2018, accounting for 55% of the world's population. Estimates report that, by 2050, this percentage may increase to 68%, in Latin America and the Caribbean, the percentage of urban population is even higher (81%), and it is currently the second most urbanized region in the world, after North America (UN, 2018).

Several studies on climate, pollution and megacities have been conducted in recent years in South America, but there is still little progress in understanding the connection between pollution and climate (considering the impact of half-life pollutants on air quality and climate) and the changes occurring in the processes at the planetary boundary layer (such as heat island effects and thermal stratification in complex terrain) (Andrade-Flores et al., 2016).

Currently, no regional diagnosis of air quality is available in South America, or an evaluation of trends in air pollutant concentrations related to recent years. This study provides current information on the air quality status in South

America and expands the understanding through a multicity review of concentrations of the following air pollutants: nitrogen dioxide (NO_2), sulfur dioxide (SO_2), particulate matter (PM_{10} and $\text{PM}_{2.5}$), carbon monoxide (CO), and ozone (O_3), collected from the monitoring networks of large urban agglomerations in South America in 2017 and the trends since 2010. A state of art review of emissions inventories was carried out.

2. METHODS

The following cities were selected: three megacities or metropolitan regions (MR) with more than 12 million inhabitants (MR of São Paulo, Brazil; MR of Buenos Aires, Argentina; MR of Rio de Janeiro, Brazil), 3 large cities with more than 7 million inhabitants (MR of Lima, Peru; Bogotá, Colombia and MR of Santiago, Chile; and 4 midsize cities with more than 2 million inhabitants (MR of Vale de Aburrá, Medellín, Colombia; Vitória, Brazil; and MR of Quito, Ecuador), located in 6 South American countries.

Hourly air quality data between 2010-2017 were collected in ten metropolitan regions, seven of which are among the most populous in South America. The criteria for city selection were: a) **urban population** (including cities or metropolitan areas with more of 1 million inhabitants), b) **location** (including cities in the study region), and c) **available information** (based on a preliminary search for information in air quality monitoring networks).

For the emissions review, we analyzed the most recent emissions inventory available in the environmental authorities. When it doesn't have availability data, EDGAR Global database for 28 emissions activities in 2012 (EC-JRC,2018) was used.

3. FINDINGS AND ARGUMENTS

3.1 Qualidade do ar

Based on the fact that $\text{PM}_{2.5}$ is considered the fourth risk factor for human health and the highest environmental risks (WHO, 2016b), this work presents the average annual concentrations in 7 cities that have monitoring data (see figure 1).

All cities exceeded the World Health Organization Air Quality Guideline (WHO-AQG), $10 \mu\text{g}/\text{m}^3$. Only Vitória (2014-2016) was below $15 \mu\text{g}/\text{m}^3$, corresponding to WHO Interim Target 3 (IT-3). Interim Target 2 (IT-2) was exceeded in Santiago during the whole period and Medellín exceeded it in the last 6 years; Lima exceeded this value in 3 of total 4 years with records. Interim Target 1 (IT-1) of $35 \mu\text{g}/\text{m}^3$ was exceeded in Medellín in 2013-2017.

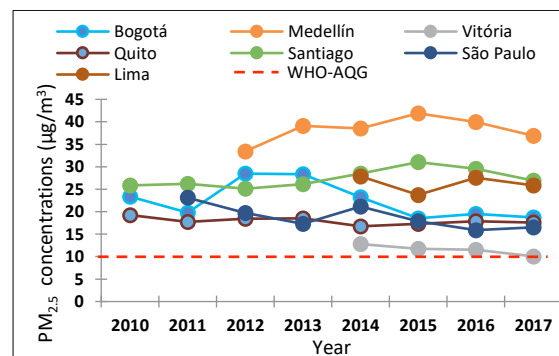


Figure 1. Average annual concentrations of $\text{PM}_{2.5}$ and World Health Organization Air Quality Guideline (WHO-AQG)

A trend analysis (linear adjustment) was performed with data presented in Figure 1; two cities presented reduced annual concentrations of $\text{PM}_{2.5}$ with linear regression slopes of $-0.96 \mu\text{g}/\text{m}^3/\text{year}$ ($R^2 = 0.61$) and $-0.84 \mu\text{g}/\text{m}^3/\text{year}$ ($R^2 = 0.93$) in São Paulo and Vitória, respectively. In Bogotá, although it has no clear behavior that allows a linear adjustment, the concentrations reduced in 2010-2011 and 2012-2015. In Medellín, concentrations presented an increasing trend from 2012 to 2015, reaching the highest value ($41.9 \mu\text{g}/\text{m}^3 \pm 16.6 \mu\text{g}/\text{m}^3$) recorded until today, and then a gradual decrease. Quito and Santiago presented almost constant concentrations in time. In Lima, the annual concentrations do not present a clear linear trend, with values ranging from $23.8 \mu\text{g}/\text{m}^3 \pm 6.5 \mu\text{g}/\text{m}^3$ e $27.9 \mu\text{g}/\text{m}^3 \pm 8.2 \mu\text{g}/\text{m}^3$.

All cities analyzed in this study exceeded the PM_{10} WHO-AQG of $20 \mu\text{g}/\text{m}^3$. For NO_2 , the WHO-AQG was exceeded in all years of the study period in at least one city in the region, except in 2014, when the highest annual concentration was $37.0 \mu\text{g}/\text{m}^3 \pm 8.8 \mu\text{g}/\text{m}^3$ (Santiago). In the SO_2 case, all air quality standards and local and national targets were fulfilled.

Figure 2 shows the current scenario (base year: 2017) of average annual concentrations for $\text{PM}_{2.5}$, PM_{10} , NO_2 and SO_2 in large cities in South America, and their comparisons to World Health Organization Air Quality Guideline (WHO-AQG) (except for SO_2). In 2017, $\text{PM}_{2.5}$ exceeded the limit of $10 \mu\text{g}/\text{m}^3$ in all cities. PM_{10} exceeded WHO-AQG of $20 \mu\text{g}/\text{m}^3$ in all cities as well. NO_2 concentration in Santiago was the highest in the region ($45.09 \mu\text{g}/\text{m}^3$) and the only one that exceeded WHO-AQG value. Vitória had the lowest average annual concentrations of all pollutants, except for SO_2 , and the lowest value of SO_2 was reported in São Paulo. On the other hand, Medellín had the highest average concentrations of $\text{PM}_{2.5}$ and NO_2 , SO_2 and CO .

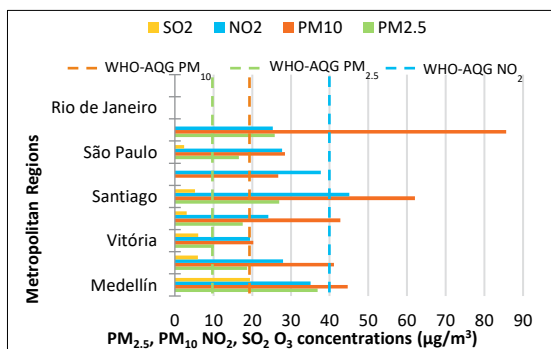


Figure 2. Average annual concentrations in 2017 and World Health Organization Air Quality Guideline (WHO-AQG (Average annual from Buenos Aires are invalids)

3.1 Pollutants emissions

The emissions review showed that the half of the cities evaluated did not have an inventory of emissions and some of the ones that did have corresponded to the maximum base update years of 2016. Vitória has the highest transport emissions of $PM_{2.5}$ and PM_{10} . Santiago is the second largest emitter of $PM_{2.5}$ and PM_{10} . Bogotá has the highest emissions of CO, SO_x, COV and NO_x (See figure 3).

Figure 4 shows that in the 6 cities evaluated with EDGAR database, the highest emissions were CO and NMVOC, in the case of São Paulo these were much higher than those of the other cities, followed by Rio de Janeiro and Buenos Aires. The lowest emissions of all pollutants were found in Lima and Salvador.

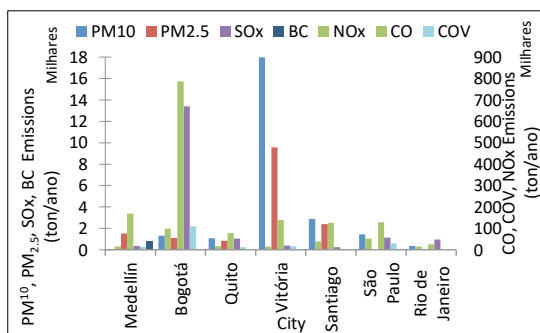


Figure 3. Transport emissions according to the latest official inventories

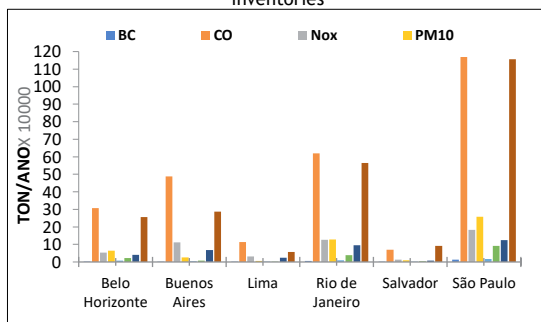


Figura 4. Emissões totais por cada poluente, segundo a base de dados global EDGAR, 2012.

4. CONCLUSIONS

Despite the large number of studies conducted worldwide and dissemination of information by WHO explaining the impacts of $PM_{2.5}$ on exposed populations, and although some cities in South America have reduced since 2010 the annual concentrations of $PM_{2.5}$, such as São Paulo, Vitória and Bogotá, in general, the region does not report a trend in the same direction, as today, the values recommended by WHO and national or local standards (except for Bogotá which in 2017 was below the Colombian standard: $25 \mu g/m^3$) have been continuously exceeded. Cities such as Medellín and Santiago, although in the last 3 years reported a reduction of 11.94% and 13.21%, respectively, in the time series, they always exceeded the national standards and WHO-AQG. The concentrations of PM_{10} and NO_2 in the region seem to remain constant over time, without large fluctuations in annual averages during the study period. PM_{10} exceeded WHO-AQG in most cities, while for NO_2 WHO-AQG was fulfilled most of the time. Except for Medellín and Rio de Janeiro, SO_2 had a clear decreasing trend in South American large cities. CO had a decreasing behavior in 4 of all 10 cities with records.

The quality of inventories sees compromised by the fact that they have been developed using emission factors are drawn to other regions that have extremely different characteristics. In general, the inventories found included the main emission sources identifying clearly the areas assessed, but not included on most of them, the totality of activities in each type of source, and some major sources such as residential, are not evaluated.

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EMISSION OF PARTICULATE MATTER IN PROCESS OF DISCHARGE OF COAL IN A PORT

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Abstract: The present study aims to estimate and analyse the emission of particulate matter (PM_{10} and $PM_{2.5}$) during the storage, transport on a conveyor belt and discharge phases of coal at a port in the municipality of Imbituba, Santa Catarina (SC-Brazil). For what regards the estimation of the emissions during the storage and the transport with the conveyor belt phases, the "Emissions Inventory Guidance Mineral Handling and Processing Industries" with the calculation method for "Wind erosion From Stockpiles" has been employed. Furthermore, the AP 42 methodology of the US EPA (U.S. Environmental Protection Agency) specific for the emission by discharge of coal in port has been used in the discharge step. The simulation of dispersion of the pollutants in the atmosphere has been performed through the AERMOD computational model and the plume generation has been obtained through the QGIS software. The simulation has been performed with mean times of 1, 8 and 24 hours of data and with a simulation period of 1 day and 1 year. The plumes have been computed for both the first and the second highest concentration values resulting from modelling. The results show that the dispersion plume of particulate material is larger the longer the period of simulation, since the pollutants reach greater distances within 1 year of simulation time. Moreover, the lower the mean range of results, the greater the dispersion of the plume because, for an average time of 1 hour, the concentrations are significantly higher than for 8 and 24 hours. Finally, the emission of PM_{10} is more significant than the one of $PM_{2.5}$ for what concerns the discharge of coal in port.

Keywords: Unloading coal, port, particulate matter, dispersion of pollutants.

INTRODUCTION

Air pollution can be defined, according to the Brazilian Ministry of the Environment, as "any form of matter or energy with intensity, concentration, time or characteristics that may make air inappropriate, harmful or offensive to health, inconvenient to public welfare, harmful to materials, fauna and flora or prejudice to safety, use and enjoyment of the property and the quality of life of the community" (MMA, 2019).

Air quality involves the interaction between emissions of air pollutants, topographic characteristics and weather conditions.

In order to guarantee air quality, studies are needed to analyze concentrations of atmospheric pollutants so that the best action plan can be determined with actions of protection, mitigation and reduction of the emissions and of the high concentrations of different substances.

The objective of this work is to evaluate the concentrations of pollutants in the atmosphere from a port, considering the processes of discharging coal, transporting it through a conveyor belt and storing it. For this type of source, the main pollutants emitted are particulate matter with diameters lower than 10

micrometers (PM_{10}) and lower than 2,5 micrometers ($PM_{2.5}$).

The port is located in the municipality of Imbituba, Santa Catarina (SC) and the discharging of coal source is a point source, while the sources of storage of coal and of the conveyor belt are areal sources.

Location of the port and of each stage of the coal discharging process is reported in Figure 1.



Figure 1. Location of the port and of each stage of the coal discharging process.

The results are used to evaluate the pollutant concentrations in the atmosphere, comparing them with the air quality standards of the Brazilian legislation CONAMA No. 491 of 2018. According to the legislation for inhalable particles, such as PM_{10} , the concentration limit as average in 24 hours is 120 micrograms per cubic meter of air and for $PM_{2.5}$, the concentration limit as average in 24 hours is 60 micrograms per cubic meter of air.

METHODS

The first step necessary to carry out the simulation of the dispersion of atmospheric pollutants is the estimation of the emission of each part of the process for each pollutant.

The parts of the process considered in this study are: coal storage, conveyor belt to move the coal and coal discharging.

The "Emissions Inventory Guidance Mineral Handling and Processing Industries" (2000), with the calculation method for "Wind Erosion From Stockpiles", is used for both coal storage and coal conveyor belt to obtain the emission estimation equation. The equation is given below and the resulting unit measure is ton per year.

$$E = E_f \times A$$

Where: E = Particulate matter emissions rate in tons per year; E_f = Emission factor in units of tons of particulate per surface acre; A = Exposed surface area of stockpile in acres.

According to the same file, the emission factor for PM_{10} is 4.05 tons/acre and $PM_{2.5}$ is 1.62 tons/acre.

For the coal discharge process, the equation is obtained from the chapter 13.2.4 of AP-42 of U.S. EPA (2006) and is indicated below:

$$E = k (0,0016 \times \left(\frac{U^{1,3}}{\frac{2,2}{M^{1,4}}} \right) \left(\frac{kg}{Mg} \right))$$

Where: E = emission factor; k = particle size multiplier (dimensionless); U = mean wind speed, meters per second (m/s) (miles per hour); M = material moisture content (%).

The resulting unit of measure is kg of pollutant per Mg of discharged mass.

The value of k is obtained using the table (Table 1) available in the same document.

Table 1. Aerodynamic Particle Size Multiplier (k) for equation

< 30 μm	< 10 μm	< 2,5 μm
0,74	0,35	0,053

Reference: U.S. EPA, 2006.

The emission factors and emission rates for coal discharge are calculated for several values of humidity and wind speed and, in this study, the result coming from the worst situation found is considered.

To simulate the dispersion of the pollutants in the atmosphere, the AERMOD simulation model is used, which is a steady state model that incorporates the air dispersion based on the turbulence structure of the planetary boundary layer (USEPA).

AERMET is the AERMOD processor, which uses as inputs surface and survey weather data. The surface data are obtained through INPE's weather forecasting and climatic studies center (CPTEC), at Florianópolis station (code SBFL), while the survey data considered are those obtained by Florianópolis Airport (FLN) at NOAA RAOBS (ESRL Radiosonde Database), code 83899. The data collected correspond to the entire year 2017.

Two files are prepared: one with discrete receptors chosen based on residences near the port; the other with a cartesian grid of receptors with an area of 50 km x 50 km. The spacing between the receptors is 500 meters.

After obtaining the files, the pollutant plumes are built through the QGIS geoprocessing program.

FINDINGS AND ARGUMENT

The results of the calculations for the estimation of the emission of each step are presented below:

Coal storage: Through Google Earth, it is possible to calculate an approximate area for the coal storage of 36,900 m², that is, 9.12 acres. According to the emission inventory, the effective constants for PM_{10} and $PM_{2.5}$ are respectively: 4.05 tons/acre and 1.62 tons/acre.

Conveyor Belt for Coal: Through Google Earth, a conveyor belt area of approximately 4,600 m², or 1.14 acres, is obtained. The emission factors considered are identical to those considered for the storage stage.

Coal discharging: As mentioned, for the coal discharging part, the AP-42 equation is used and the emission factors and emission rates for coal discharge are calculated for various values of

humidity and wind speed. Finally, the worse case scenario is considered for this study, which is the one with a wind speed of 6.7 m/s and an humidity of 0.25%.

Thus, the final emission rates of each step are presented below (Table 2):

Table 2. Emission rate in g / s

Stage of the process	PM_{10}	$PM_{2,5}$
Coal discharging	1,22	0,18
Conveyor Belt for Coal	0,15	0,059
Coal storage	1,17	0,47

With the results for each source, it can be observed that for PM_{10} , the discharge of coal is the stage that presents the highest rate, followed by the storage stage and, finally, by the conveyor belt. The highest emission rate of the discharging stage may be related to the fact that it is a point source and to the lower rate of the conveyor belt with respect to storage, due to its smaller emission area.

However, for $PM_{2,5}$, the storage is the stage that presents the highest emission rate between the three sources, while the belt continues to be the one with the lowest rate.

In this case, the difference in the rates of storage and transport has a justification similar to the previous one, while the fact that the discharge has no longer the highest rate can be justified by the fact that the unloading process has an emission ratio between PM_{10} and $PM_{2,5}$ higher than the storage.

The plumes generated with the results of the simulation for a mean of 1 hour during all the year 2017 are shown below (Figure 2 and Figure 3).

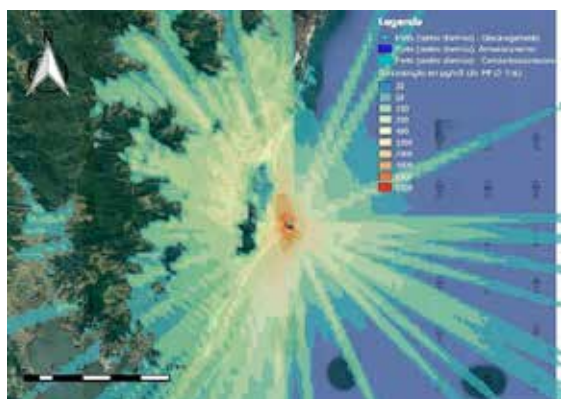


Figure 2. PM_{10} dispersion plume for the first highest value for a mean of 1h

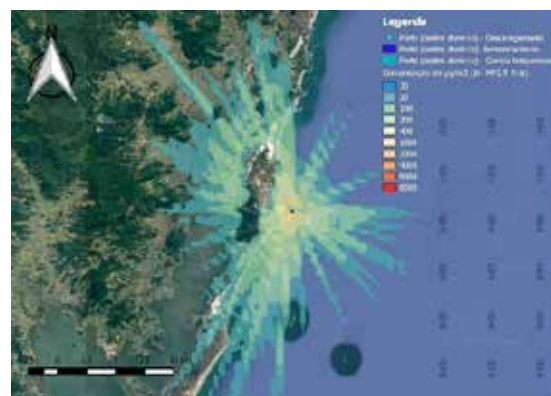


Figure 3. $PM_{2,5}$ dispersion plume for the first highest value for a mean of 1h

The plumes generated with the results of the simulation for a mean of 24 hours mean during the year 2017 are presented below (Figure 4 and Figure 5).

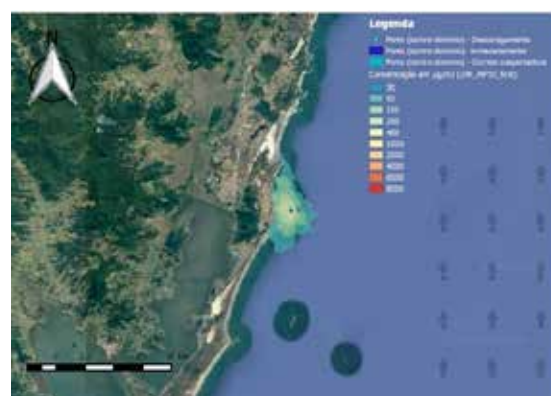


Figure 4. PM_{10} dispersion plume for the first highest value for a mean 24h

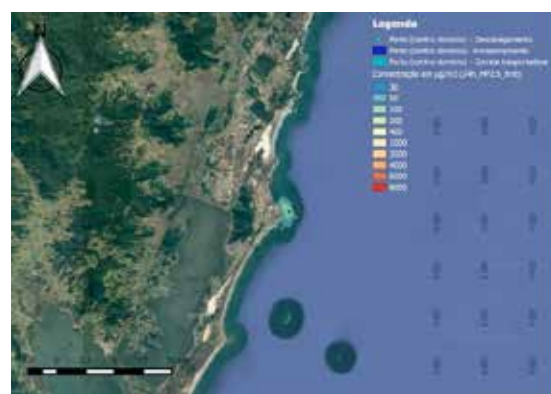


Figure 5. $PM_{2,5}$ dispersion plume for the first highest value for a mean of 24h

Due to the lower emission rate of $PM_{2,5}$ compared to PM_{10} , their concentrations in the atmosphere are also lower.

It can also be observed that the concentrations found in the atmosphere are higher when the results of the mean of 1h are employed, with respect to the results of the mean of 24h. This is due to the fact that the plumes are constructed using the method of calculation of average, which causes the high punctual concentrations to impact more the results the smaller the considered interval for the calculation of average.

With regard to the comparison with Brazilian legislation, there is no standard established for an average of 1 hour in order to consider cases that may be isolated throughout the year. However, there is a standard for the mean in intervals of 24 hours, where the maximum allowed concentration for PM_{10} is $120 \mu g/m^3$, while for $PM_{2.5}$ is $60 \mu g/m^3$.

In this study, the highest concentrations found for PM_{10} reaches values close to 4000 and for $PM_{2.5}$ close to 2000, resulting in concentrations well above that established by CONAMA n° 491/2018.

In this way, emission control measures are necessary in all the steps considered in the port, following the order of priority of the influence on the emission rate. One of the control measures that can be initiated is the sprinkling of water on the coal material.

CONCLUSIONS

In conclusion, according to the dispersion simulation of the pollutants, the emission of particulate material (PM_{10} and $PM_{2.5}$) is quite high in the discharge, transport and storage processes in the coal port, and, for this reason, such activity must be carried out with measures to control the emission of such contaminants.

The values found are well above the limit established by current Brazilian legislation (CONAMA n° 491 / 2018).

Therefore, it is recommended that new dispersion studies should be carried out considering the emission treatment methods, in order to evaluate the best method to be used in these activities.

Also, it is observed that the results of concentration in the dispersion plumes are larger the lower the interval considered for the calculation of the means of the results found, which increases the influence of single and occasional cases occurred throughout the year.

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ESTIMATION AND ANALYSIS OF AIR POLLUTANTS EMITTED FROM GRAY IRON FOUNDRIES

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Abstract: The aim of this paper is to estimate the emission of air pollutants, such as MP_{10} , $MP_{2.5}$, SO_2 , CO, and Pb, during the iron cast process used to manufacture siderurgical products, and also to compare the estimated results with the emission's limits established by the Brazilian legislation. In order to estimate the emissions values, it was applied the specific United States Environmental Protection Agency (USEPA), AP-42, methodology for Iron foundries, while to simulate the dispersion of the pollutants, the AERSCREEN model for dispersion, recommended by the USEPA for preliminary studies, was adopted. For the analysis, it was considered an annual manufacturing capacity of 445.000,00 tons of cast iron products in an industry that operates with cupola furnaces. The dispersion model was simulated for each pollutant, in function of the distance from its source and varying the stack height into 20, 40, 80, and 100 meters. The results have shown that the concentrations of MP_{10} , $MP_{2.5}$, SO_2 and Pb, following the dispersion simulations, exceeded the limits established by the Brazilian legislation, even for the stack height of 100 meters. For the CO, the stack height of 40 meters has shown to be sufficient to drop the pollutant concentration to acceptable levels.

Keywords: Gray Iron Foundries, emission inventory, air pollutants, dispersion of pollutants.

INTRODUCTION

Iron is part of our daily life in such a way, that its production has become an indicator of a country's economic development level (Instituto Aço Brasil, 2019).

The process of iron casting may cause tremendous prejudice due to its emission of air pollutants, thus, impacting directly and indirectly the environment, and the human health.

Emissions released from the iron cast process includes pollutants such as particulate matter (PM), carbon monoxide (CO), sulfur dioxide (SO_2), and lead (Pb), organic compounds, nitrogen oxides, as small quantities of chloride and fluoride compounds. The PM, CO, SO_2 , and Pb are described in the following (US EPA, 2003).

Particulate matter (PM): generated by the incomplete combustion of carbon additives, from the addition of flux, and also due to the dirt and iron oxides (rust) present in iron scraps. It's a complex mixture of solids with reduced diameter,

and of different chemical and physical composition. This pollutant is classified according to the diameter of the particles, due to the relationship between the diameter and the penetration of the particles in the respiratory system (MMA, 2018).

Carbon monoxide (CO): emitted during the process of iron casting, the CO is mostly released due to the incomplete combustion of the coke. The organic material in the iron scraps and the temperature of the furnace, are factors that directly affects the concentration of CO generated (US EPA, 2003).

Sulfur dioxide (SO_2): its emission is primarily due to the sulfur present in the coke (US EPA, 2003). SO_2 is used as the indicator for the group of gaseous sulfur oxides (SO_x), because it is the component of greatest concern (US EPA, 2018).

Lead (Pb): a heavy metal is mostly emitted by mining, metal processing, and by the combustion of aviation fuels. It is commonly found nearby siderurgical manufactures (US EPA, 2018).

Therefore, the aim of this study is to simulate the dispersion of the air pollutants that are emitted during the process of iron casting in siderurgical manufactures.

The analyses of the dispersion will take into consideration the variation in the height of the stack that will be of 20, 40, 80 and 100 m, thus, allowing the correlation between the height of the stack with the influence of the emission in the air quality.

The Brazilian legislation, Resolução CONAMA nº 491/2018, establishes the standards for the air quality trough the country, standards these that will be the base for the analysis of the results from the simulations.

METHODS

In order to estimate the emissions of the air pollutants (PM_{10} , $PM_{2,5}$, SO_2 , CO and Pb), it was applied the AP-42 USEPA (United States Environmental Protection Agency) methodology, chapter 12, section 12.1, from where were obtained the emission factor for each pollutant evaluated in this study (Table 1).

Table 1. Emission factor

Pollutant	Description	Emission Factor (kg/Mg)
PM_{10}	NC	6.2
$PM_{2,5}$	NC	5,8
SO_2	NC	0,65*
CO	NC	73
Pb	NC	0,05-0,6

ND = no data.

S = % sulfur in coke.

Reference: Section 12.10 da AP-42 (U.S. EPA).

According to the technical standard nº 1007 from the CPRH (Companhia Pernambucana de Controle da Poluição Ambiental e de Administração de Recursos Hídricos), a typical composition of the green coke from petroleum presents a sulfur percentage around 0,5% and 7,5%. Also, as stated in the technical guideline of Petrobras (published in 2015), the coke with higher percentage of sulfur, is used more often than the coke with lower percentage of sulfur. Thus, for this study, it was considerate a sulfur concentration of 7%, since it was the worst case scenario to be consider for the release of SO. Therefore, it was possible to determine the emission factor of 4,2 for SO_2 .

To simulate the dispersion of the pollutants from its source of emission, the AERSCREEN model for

dispersion, recommended by the USEPA for preliminary studies, was adopted.

As intended to estimate the emissions from the siderurgical manufactures, it was considered an annual manufacturing capacity of 445.000,00 tons of cast iron products (50,799 tons/h) in an industry that operates with cupola furnaces. For the others pollutants were adopted emission factors considering no control.

The emission rates were calculated according to the following equation:

$$E = A \times EF$$

Where: E = emissions; A = activity rate; and EF = emission factor.

The dispersion model AERSCREEN, was simulated varying the stack height into 20, 40, 80, and 100 meters, thus, were taken into consideration the following parameters:

- Temperature: 1000 K
- Emission velocity: 8 m/s
- Stack diameter: 1 meter
- Local population: 16000 habitants
- Rugosity: 1
- Albedo: 0,16
- Bowen's ratio: 1,7.

FINDINGS AND ARGUMENT

The results from estimated emissions rates for the manufacturing process of iron foundries are shown in Table 2.

Table 2. Estimated results.

Pollutant	Emission factor (kg/ton)	Emission rate (kg/h)	Emission rate (g/s)
PM_{10}	6,2	314,95	87,49
$PM_{2,5}$	5,8	294,63	81,84
SO_2	4,2	213,36	59,27
CO	73	3.708,33	1.030,17
Pb	0,05-0,6	30,50	8,47

Reference: Elaborated by the authors.

Following the dispersion simulations with the AERSCREEN model, it was possible to establish the resulting concentration for each of the pollutants

regarding the distances that varies from 1 to 5 thousand meters, between the receptors and the emission source.

For the PM_{10} , the Federal Legislation CONAMA 491/2018, establish as a limit, a concentration up to $120 \mu g/m^3$, for an average of 24 hours. The higher concentration found during the simulations was for the 20 m stack, with a concentration value of $665,43 \mu g/m^3$, and for a distance of 175 meters from the source. The best case scenario was for the 100 m stack; however, it still exceeded the air quality standards till a distance of 4,6 km from the source of emission. The results for the PM_{10} are shown in Figure 1.

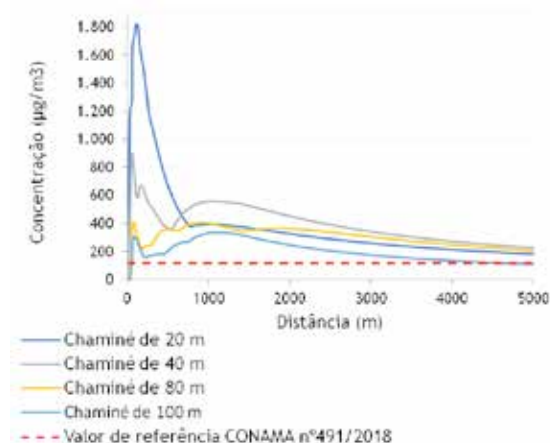


Figure 1. Resultados de dispersão do PM_{10}

As to the $PM_{2,5}$, the CONAMA 491/2018 establish as a limit, a concentration up to $60 \mu g/m^3$, for an average of 24 hours. The Figure 2, shows that this pollutant presented high concentrations for all the scenarios been evaluated, thus, indicating the necessity to consider the use of an emission control.

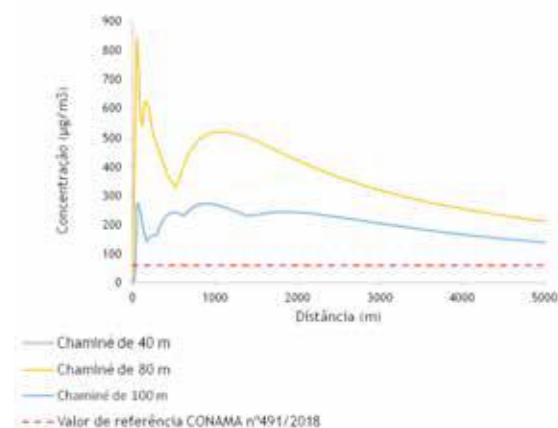


Figure 2. Results for the dispersion of $PM_{2,5}$

For the Pb, the CONAMA 491/2018, establish as a limit, a concentration up to $0,5 \mu g/m^3$, for an annual average. For all the scenarios evaluated, the concentrations obtained exceeded the standard value established by the legislation, even when doing the simulation for a 100 m stack. For the 100 m stack, the concentration obtained was of about $30 \mu g/m^3$ for an approximate distance of 120 meters from its emission source. The results for the Pb are shown in Figure 3.

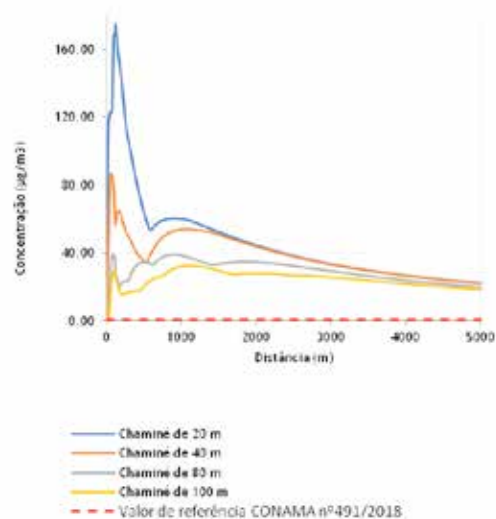


Figure 3. Results for the dispersion of Pb

For the SO_2 , the CONAMA 491/2018 establishes a limit concentration of up to $125 \mu g/m^3$, for an average of 24 hours. For this pollutant, the highest concentration was of $1232,7 \mu g/m^3$ for a distance of 100 m from its emission source. In the same manner as to the other pollutants, the best scenario for the dispersion of the SO_2 was for the 100 m stack. The results for the SO_2 are shown in Figure 4.

For the CO, the CONAMA n° 491/2018 establishes as a limit a concentration up to 9 ppm, for an average of 8 hours. Due to the high limit concentration of CO stated by the legislation, all, but the scenario evaluated for the 20 m stack, remained below the established limit for a distance of 500 m from its source of emission. For the 40 m stack, the concentration of CO exceeded the limit when evaluated for the distances of 50 to 100 meters from its source of emission. The results for the CO are shown in Figure 5.

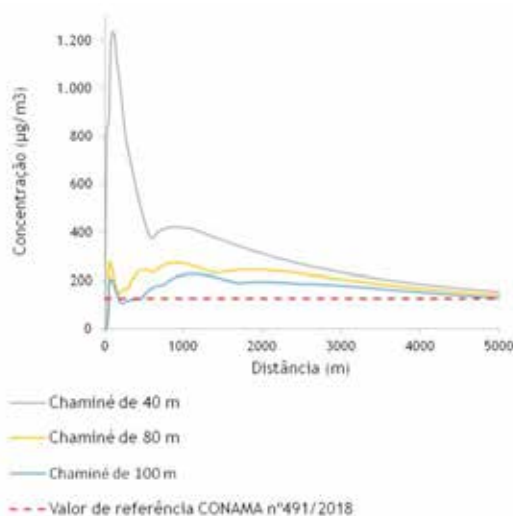


Figure 4. Results for the dispersion of SO₂

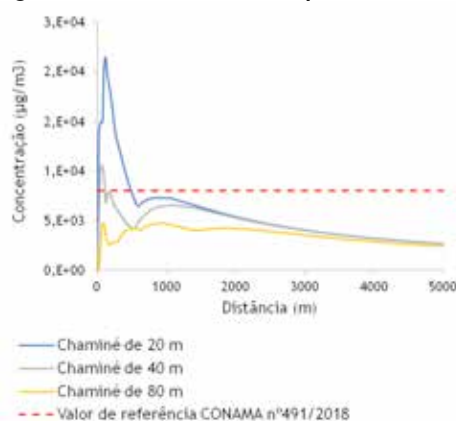


Figure 5. Results for the dispersion of CO

Based on the estimated results, one might conclude that the manufacturing of iron foundries deliver high concentrations of air pollutants, also, it was possible to observe that as higher the stack height, more dispersed were pollutants in the atmosphere.

Among the stack height simulated, the 100 m stack was the one that has shown the best results. However, even for this height, the emissions resulted in concentrations higher than the limit established by the Brazilian Legislation. The maximum stack height evaluated was of 100 m, because for higher heights the stack becomes economically unviable.

Therefore, is reinforced the necessity to adopt control measures regarding the emissions from iron foundry industries. The main pollutants to be taken into consideration for determining the best treatment system are the particulate matter (both MP₁₀ and MP_{2,5}), lead, and sulfur dioxide, due to its

high concentrations in the atmosphere after its emission and dispersion.

Example of possible treatments for the particles are the baghouses and the scrubbers, equipment's that might be used to treat particles such as the PM and Pb. As for sulfur dioxide, a gas, a scrubber is recommended.

One can notice, after running the modeling, that higher concentrations were found for shorter distances, near the source of emission in conditions of atmospheric instability (12 hours); and more distant from the source of emission in conditions of atmospheric stability (1 hour). This is explained by the fact that the solar radiation is most intense during noon, what promotes the heating of the atmosphere, elevating the turbulence and as a consequence, dissipating the plume during conditions of instability, thus, resulting in higher concentrations for the receptors near the source.

CONCLUSIONS

Furthermore, based in the dispersion of the pollutants, we can conclude, that higher the stack height, better the dispersion of the pollutants in the atmosphere, thus, resulting in lower concentrations near the surface from its source of emission.

In view of the violation of the maximum concentrations established by the Brazilian Legislation, is possible to state that the treatment of the gases emitted by the manufacturing of iron cast is required. Thus, for each of the scenarios evaluated in this study, become necessary a new evaluation in order to evaluate the efficiency of the control system to be adopted to treat the pollutants of interest.

Finally, based in this study, it was possible to demonstrate the influence of the atmospheric stability in the dispersion of pollutants, as in moments of instability the pollutant's concentration tends to be higher in receptors near the source, and in moments of stability more distant from the receptors.

In addition, is recommended that for further studies, is taken into consideration, the use of an more advanced dispersion model, that evaluates the particular variables intrinsically to the region where the industry is located. Also, is recommended to consider meteorological variables and use and occupation of the soil, factors this that directly influence in the dispersion of the pollutants in the atmosphere.

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ESTIMATION OF PARTICULATE MATTER EMISSIONS BY TYRE AND BRAKE WEAR AND ROAD ABRASION PROCESSES FROM THE MINAS GERAIS ON-ROAD VEHICLE FLEET

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Abstract: The aim of this study was to estimate the atmospheric emissions of PM (TSP, PM₁₀ and PM_{2.5}) by tyre and brake wear and road abrasion processes in the state of Minas Gerais (Brazil), based on the composition of vehicular fleet for the year 2015. The emission estimation was done following the guidelines of the Brazilian reference methodology, proposed by the Ministry of the Environment, also based on what is proposed in the chapter "Road transport: automobile tyre and brake wear and road abrasion" in the European Union's atmospheric emission inventory. It was observed a TSP emission of 2,928 tons for tyre and brake wear and 2,635 tons for road abrasion processes for the studied year. Regarding the fleet composition, PM was most emitted by heavy vehicles in this analyzed process. In terms of fractions, PM₁₀ accounted for 75.9% of the total emissions for tyre and brake wear processes, and 50.0% for road abrasion. From the total mass of PM₁₀ emitted, 53.6% was related to PM_{2.5}, in the case of tyre and brake wear, and 54.1% in case of road abrasion. These results showed that even with exhaust emissions being zero, vehicular traffic will continue to be a source of particles to the atmosphere via emissions from physical wear of materials. Thus, there is a need of legislation and strategies development for control of non-exhaustive sources. Moreover, methodologies used and results obtained in this study can be used as a emission inventory base to other areas of Latin America and worldwide where there is a lack in studies and data base for these evaluations.

Keywords: particulate matter, tyre and brake wear, road abrasion, emission.

INTRODUCTION

Particles emitted to the troposphere are a direct risk to the environment and human health. Recent studies have shown that in the year 2015, fine particulate matter (PM_{2.5}) ranked fifth among the mortality risk factors worldwide, with 4.2 million deaths associated with exposure to this pollutant (COHEN et.al, 2017).

In the context of urban areas, among the emission sources of particulate matter (PM), vehicles have been considered as one of the main contributors, with emissions occurring due to both exhaustion processes and physical wear of materials (BORGE et al., 2014; HETEM; ANDRADE, 2016).

Despite the emphasis given to exhaust PM emissions, several studies have shown the importance of tyre and brake wear and road abrasion processes in the emission of particles into

the atmosphere. This scenario becomes more relevant when it is considered that the main policy actions in the last decades related to vehicle air pollution control focused mainly on exhaust emissions, requiring a more critical attention at non-exhaustive emission processes (PANT; HARRISON, 2013).

In this context, the aim of this study was to estimate the atmospheric emissions of PM (total, PM₁₀ and PM_{2.5}) by tyre and brake wear and road abrasion processes in the state of Minas Gerais (Brazil), based on the composition of vehicular fleet for the year 2015.

METHODS

Following the methodology proposed by Brazilian Ministry of the Environment (MMA, 2014), particulate matter emissions due to tyre and brake wear and road abrasion were estimated based on

what is proposed in the chapter "Road transport: automobile tyre and brake wear and road abrasion" in the European Union's atmospheric emission inventory (NTZIACHRISTOS; BOULTER, 2016). Based on this methodology, estimates were done according to Equation 1 for each vehicle category.

$$TE = \sum_j N_j \times M_j \times EF_{i,j} \quad (1)$$

Where:

TE = total emissions of TSP, PM₁₀ or PM_{2.5} for the defined time period and spatial boundary [g],

N_j = number of vehicles in category j within the defined spatial boundary,

M_j = average mileage driven per vehicle in category j during the defined time period [km],

EF_{i,j} = mass emission factor for pollutant i and vehicle category j [g/km].

The indices are:

i = TSP, PM₁₀, PM_{2.5}

j = vehicle category (motorcycles, passenger cars, light commercial vehicles, trucks and buses)

For Minas Gerais State, specific parameters for the year 2015, such as N_j and M_j, can be observed in more details in Santos (2018). EF_{i,j} data is shown in Table 1 and 2.

Table 1. EF_{i,j} for tyre and brake wear

Vehicle category	Tyre and brake wear (g.km ⁻¹)		
	TSP	PM ₁₀	PM _{2.5}
Motorcycles	0.0083	0.0064	0.0034
Passenger cars	0.0182	0.0138	0.0074
Light commercial	0.0182	0.0138	0.0074
Semi light trucks	0.0286	0.0216	0.0117
Light trucks	0.0286	0.0216	0.0117
Medium trucks	0.0777	0.059	0.0316
Semi heavy trucks	0.0777	0.059	0.0316
Heavy trucks	0.0777	0.059	0.0316
Buses	0.0777	0.059	0.0316

Table 2. EF_{i,j} for road abrasion

Vehicle category	Road abrasion (g.km ⁻¹)		
	TSP	PM ₁₀	PM _{2.5}
Motorcycles	0.006	0.003	0.0016
Passenger cars	0.015	0.0075	0.0041
Light commercial	0.015	0.0075	0.0041
Semi light trucks	0.015	0.0075	0.0041
Light trucks	0.015	0.0075	0.0041
Medium trucks	0.076	0.038	0.0205
Semi heavy trucks	0.076	0.038	0.0205
Heavy trucks	0.076	0.038	0.0205
Buses	0.076	0.038	0.0205

FINDINGS AND ARGUMENT

Emission estimates for Minas Gerais State vehicle fleet in the year 2015 by tyre and brake wear and road abrasion process can be observed in Tables 2 and 3, respectively.

It was observed a TSP emission of 2,928 tons for tyre and brake wear and 2,635 tons for road abrasion processes in the studied year. Regarding the fleet composition, PM was most emitted by heavy vehicles in this analyzed process.

In terms of fractions, PM₁₀ accounted for 75.9% of the total emissions for tyre and brake wear processes, and 50.0% for road abrasion.

From the total mass of PM₁₀ emitted, 53.6% was related to PM_{2.5}, in the case of tyre and brake wear, and 54.1% in case of road abrasion.

Table 3. PM emission for tyre and brake wear

Vehicle category	Tyre and brake wear (ton.year ⁻¹)		
	TSP	PM ₁₀	PM _{2.5}
Motorcycles	112	86	46
Cars	985	747	402
Light commercial	171	130	69
Semi light trucks	7	6	3
Light trucks	25	19	10
Medium trucks	144	109	59
Semi heavy trucks	564	429	230
Heavy trucks	593	450	241
Bus	327	247	132
Total in 2015	2928	2223	1192

Table 4. PM emission for road abrasion

Vehicle category	Road abrasion (ton.year ⁻¹)		
	TSP	PM ₁₀	PM _{2.5}
Motorcycles	82	40	22
Cars	813	407	223
Light commercial	141	70	37
Semi light trucks	4	2	1
Light trucks	13	7	4
Medium trucks	141	71	38
Semi heavy trucks	552	276	149
Heavy trucks	580	290	156
Bus	319	159	85
Total in 2015	2645	1322	715

Comparing the results presented in this study with PM emissions by vehicle exhausts in Minas Gerais State vehicular fleet also in 2015 (SANTOS, 2018), it is possible to observed in Figure 1 that tyre and brake wear and road abrasion processes, together, accounted for 70.5% of TSP emissions and 51.2% of PM₁₀ emissions. On the other hand, the emission of PM_{2.5} had as its main agent the vehicle exhaust, whose contributions were 63.9% (Figure 1).

These results are in agreement with those observed by Ketzel et al. (2007), who in their studies aiming at the estimation and validation of PM_{2.5}/PM₁₀ emission factors for exhaustive and non-exhaustive emissions, verified that all the models achieved indicated, consistently, that from 50 to 85% of PM₁₀ total emissions were originated from non-exhaustive emissions.

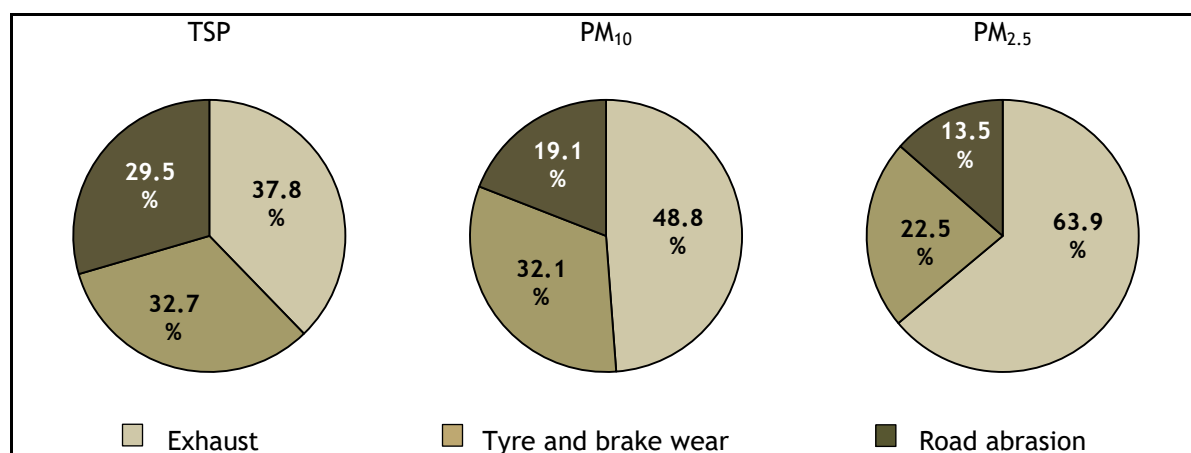


Figure 1. PM emission for tyre and brake wear

CONCLUSIONS

Results obtained in this study showed that even with exhaust emissions being zero, vehicular traffic will continue to be a source of particles to the atmosphere via emissions from physical wear of materials. Thus, there is a need of legislation and strategies development for control of non-exhaustive sources. Moreover, methodologies applied and results obtained in this study can be used as an emission inventory base to other areas of Latin America and worldwide where there is a lack in studies and data base for these evaluations.

ACKNOWLEDGMENT

The authors acknowledge the National Council of Technological and Scientific Development (CNPq), the Research Support Foundation of the State of Minas Gerais (FAPEMIG) and the Coordination for the Improvement of Higher Education Personnel (CAPES) for the financial support.

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SO₂ VEHICULAR EMISSIONS IN MINAS GERAIS STATE (BRAZIL) IN THE YEAR 2015

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Abstract: The aim of this study was to estimate the atmospheric emissions of SO₂ by vehicular fleet in the state of Minas Gerais (Brazil) in 2015, as well as compare these results with the realities of other localities in Brazil and worldwide. The emissions of SO₂ from the combustion of gasoline and diesel in vehicles' engines were estimated according to the chapter "EEA Guidebook for Emissions from Road Transport" present in the inventory of atmospheric emissions of the European Union. This methodology considers that all sulphur present in the fuel is completely converted to SO₂ during the burning process. It was verified that in relation to the type of fuels, diesel was the one that most emitted SO₂, representing 93.2% of the total emissions of this pollutant by Minas Gerais vehicular fleet. Once trucks and buses are only supplied by diesel, the contribution of this type of fleet represented 87.8% of SO₂ emissions by vehicles in Minas Gerais during 2015. Compared to other world realities, the observed per capita emission results for Minas Gerais (0.23 kg.inhab.year⁻¹), were very close to other realities in Brazil, such as São Paulo State and Metropolitan Area of Rio de Janeiro, whose values were 0.11 and 0.18 kg.inhab.year⁻¹, respectively. However, when compared to the international scenario, these values were much higher than those observed in the European Union, in the United States and in Canada, whose values were 0.01, 0.07 and 0.04 kg.inhab.year⁻¹, respectively. These differences can be related to the more restrictive legislation regarding to the presence of sulphur in fuels in these evaluated countries. The obtained results indicate the necessity of policies implementation in Brazil regarding the control of vehicular emissions, aiming air pollution minimization.

Keywords: SO₂, vehicle, diesel, gasoline, emission, Minas Gerais.

INTRODUCTION

Sulphur dioxide (SO₂) is an air pollutant of significant environmental impact, associated with acid rain, industrial smog and as a precursor to the formation of secondary particulate matter in the atmosphere (MARTINS; ANDRADE, 2002; WHO, 2006). Among the effects of SO₂ on health, worsening of asthma symptoms and an increase in hospital admissions due to respiratory problems are constantly reported (WHO, 2006).

Burning of fossil fuels containing sulphur is the main source of this pollutant. Fossil fuels, mainly coal and oil, contain amounts of sulphur that vary according to their source, typically between 1% and 5% (WHO, 2006). Thus, during the burning of these fuels by industries, thermoelectric power plants, industrial boilers, oil refining, and for the vehicular fleet in urban areas, sulphur is converted to SO₂.

In many countries, the removal of a significant portion of the sulphur present in fuels has occurred

during its refining process, in order to prevent the subsequent emission of its gases formed during combustion processes (CARVALHO et al., 2015). In Brazil, for example, some recent efforts have been made in this direction, with the publication of resolutions n°. 40/2013 and n°. 30/2015 of Agência Nacional do Petróleo (National Petroleum Agency).

One way to assess the effectiveness of these policies and to diagnose the scenario of atmospheric emissions of SO₂ in urban areas is through emissions estimation. In view of this context, the aim of this study was to estimate the atmospheric emissions of SO₂ by vehicular fleet in the state of Minas Gerais (Brazil) in 2015, as well as compare these results with the realities of other localities in Brazil and worldwide.

METHODS

The emissions of SO₂ from the combustion of gasoline and diesel in vehicles' engines from the Minas Gerais vehicle fleet in the year 2015 were estimated according to the chapter "EEA

Guidebook for Emissions from Road Transport” (NTZIACHRISTOS; SAMARAS, 2016) present in the inventory of atmospheric emissions of the European Union. Thus, exhaust emissions by type of fuel were estimated according to Equation 1. This methodology considers that all sulphur present in the fuel is completely converted to SO₂ during the burning process.

$$E_{SO_2,m} = 2 \times k_{S,m} \times FC_m \quad (1)$$

where:

$E_{SO_2,m}$ = emissions of SO₂ per fuel m [g],

$k_{S,m}$ = weight related sulphur content in fuel of type m [g/g fuel],

FC_m = consumption of fuel m [g].

Regarding the input parameters for the calculation of SO₂ emissions, it is important to note that for automotive gasoline in Brazil, the sulphur content considered was 50 mg.kg⁻¹, which is the maximum allowed value regulated by resolutions n°. 40/2013 and n°. 30/2015 from the National Petroleum Agency (ANP, 2013a; 2015). In the case of diesel, this inventory considered that one for road use (ANP, 2017a). In accordance with the provisions of resolution n°. 50/2013 (ANP, 2013b), since 2014 in Brazil, two types of diesel are marketed for road applications, according to the maximum permitted sulphur content: S-500 diesel, up to 500 mg. kg⁻¹ and S-10 diesel, with up to 10 mg.kg⁻¹.

Data on actual consumption of gasoline and diesel S-10 and S-500 were obtained from the database of the National Petroleum Agency (ANP, 2017b) and they can be observed in Table 1.

Table 1. Minas Gerais fuel consumption in the year 2015

Months	Gasoline (m ³)	Diesel (m ³)	
		S-10	S-500
January	433,680	131,650	432,402
February	348,164	113,046	375,747
March	370,247	134,750	440,833
April	365,154	134,167	435,981
May	339,249	136,406	432,199
June	344,771	142,567	444,774
July	355,110	152,714	468,514
August	322,727	147,039	455,392
September	322,028	150,228	455,712
October	343,622	156,692	478,153
November	331,251	139,433	419,843
December	420,428	142,820	408,006
Total	4,296,429	1,681,512	5,247,557

For an evaluation of the SO₂ emission for each vehicle category of the Minas Gerais vehicular

fleet, total fuel consumption data were associated to the specific consumption by each vehicle category, according to the size of its fleet, specific consumption per kilometre and average annual mileage. Better details regarding these procedures can be observed in Santos (2018).

In order to compare SO₂ vehicular emission in Minas Gerais to the realities of other regions of the country and the world, the per capita emission rates were calculated. For this, the total SO₂ emission in each evaluated area (São Paulo State, Rio de Janeiro Metropolitan Area, European Union, United States of America and Canada), published in their respective inventories, was related to the populations of each area in the given base year of the inventory.

FINDINGS AND ARGUMENT

From the results, for the year 2015, it was observed an emission of 4,760 tons of SO₂ by Minas Gerais vehicular fleet (Table 2). Regarding the fleet composition, the highest values were observed for semi heavy and heavy trucks, which were, 1,334 and 1,398 ton.year⁻¹, respectively.

Table 2. SO₂ emission in Minas Gerais vehicular fleet in 2015

Vehicle category	Fuel	SO ₂ emission (ton.year ⁻¹)
Motorcycles	Gasoline	18
	Flex-Gasoline	6
	Flex-Ethanol	0
Cars	Gasoline	79
	Ethanol	0
	Flex-Gasoline	186
	Flex-Ethanol	0
Light commercial	Gasoline	8
	Ethanol	0
	Flex-Gasoline	27
	Flex-Ethanol	0
	Diesel	259
Semi light trucks	Diesel	18
Light trucks	Diesel	100
Medium trucks	Diesel	274
Semi heavy trucks	Diesel	1,334
Heavy trucks	Diesel	1,398
Urban bus	Diesel	647
Micro bus	Diesel	96
Highway bus	Diesel	309
Total		4,760

It was verified that in relation to the type of fuels, diesel was the one that most emitted SO₂, representing 93.2% of the total emissions of this

pollutant by Minas Gerais vehicular fleet (Figure 1). Once trucks and buses are only supplied by diesel, the contribution of this type of fleet represented 87.8% of SO₂ emissions by vehicles in Minas Gerais during 2015 (Table 2).

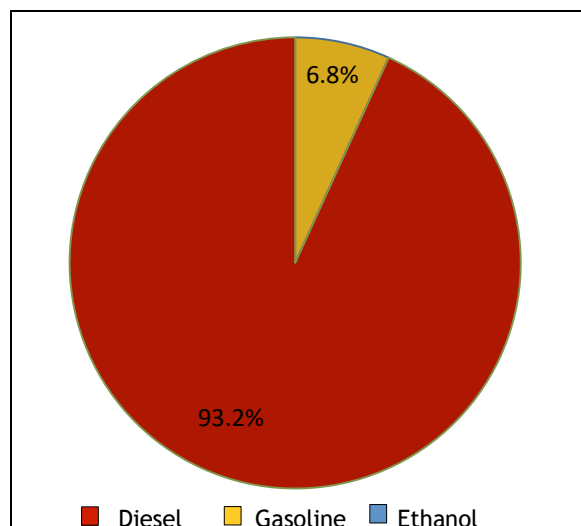


Figure 1. Percentages of vehicle SO₂ emission per type of fuel in Minas Gerais in 2015

Compared to other world realities, the observed per capita emission results for Minas Gerais (0.23 kg.inhab.year⁻¹), were very close to other realities in Brazil, such as São Paulo State (CETESB, 2016) and Metropolitan Area of Rio de Janeiro (VENTURA; PINTO, 2016), whose values were 0.11 and 0.18 kg.inhab.year⁻¹, respectively. However, when compared to the international scenario, these values were much higher than those observed in the European Union (EEA, 2018), in the United States (US EPA, 2018) and in Canada (GOVERNMENT OF CANADA, 2018), whose values were 0.01, 0.07 and 0.04 kg.inhab.year⁻¹, respectively.

These differences can be related to the more restrictive legislation regarding to the presence of sulphur in fuels in these evaluated countries. For example, In Brazil, as previously reported, gasoline is marketed with a sulphur content of up to 50 ppm (50 mg.kg⁻¹), while diesel may contain 500 ppm (S-500) or 10 ppm (S-10). On the other hand, for the world scenario, several policies are focused on the limitation of sulphur levels in diesel and gasoline. In the European Union, considering road vehicles, diesel and gasoline were limited to 10 ppm of sulphur, according to Directive 2003/17/EC of the European Parliament and of the Council of the European Union. Canada, whose standards are developed by the Canadian General Standards Board (CGSB) and implemented by "Environment Canada" has at its current standards the definition of 15 ppm of sulphur in diesel and 10 ppm in gasoline. In the case of the USA, the use of diesel

with a maximum sulphur content of 15 ppm for road vehicles was standardized in 2006. In the case of gasoline, also since 2006, the emission control program for light vehicles has required the average standard of 30 ppm of sulphur. All these factors may have contributed to the lower indicators of vehicle SO₂ emission per capita in these countries and regions of the world, compared to Brazil.

CONCLUSIONS

The emissions of SO₂ by Minas Gerais vehicular fleet have the greatest contributions of heavy vehicles (especially trucks) supplied with diesel. The observed values for Minas Gerais State in 2015 and other regions of Brazil were higher than those verified in countries of North America and European Union. These differences in emissions may be related to the higher or lower allowable sulphur limits in the fuels according to the policies of each of these sites evaluated. The obtained results indicate the necessity of policies implementation in Brazil regarding the control of vehicular emissions, aiming air pollution minimization.

ACKNOWLEDGMENT

The authors acknowledge the National Council of Technological and Scientific Development (CNPq), the Research Support Foundation of the State of Minas Gerais (FAPEMIG) and the Coordination for the Improvement of Higher Education Personnel (CAPES) for the financial support.

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ASSESSMENT OF INDIVIDUAL DRY BULK TERMINALS FUGITIVE PARTICULATE EMISSIONS' INFLUENCE ON LOCAL AIR QUALITY

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Abstract:

Dry bulk exports, mostly from vegetal origin, have great economic importance for Latin America; and this activity's nature makes it a potential source of fugitive emissions. Historically, development of residential areas close to seaports has occurred, and this fact increases the relevance of air quality assessment in these areas, specially concerning particulate matter. Therefore, this research's objective is to conduct the assessment of particulate emissions in a Latin-American port, besides indicating possible control measures that can contribute to local air quality improvement. The selected study area included eight dry bulk terminals within the port. The sources and emissions inventory was developed from the Bottom-Up perspective, using the emission factors from AP-42- Compilation of Air Pollutant Emission Factors (US EPA, 2003) for the target parameters TSP, PM₁₀, and PM_{2.5}. The technological differences among terminals were taken into account through the analysis of presence of emission control systems in each source or activity. Therefore, specific emission control efficiency percentages were adopted. The emissions were calculated on the annual scale for each terminal, and finally it was possible to compare the contributions of each terminal on the resulting total emissions. Based on the inventory data, one of the terminals was selected and the diagnosis and prognosis were performed through atmospheric dispersion modeling, which was conducted using the AERMOD regulatory model. The prognostic scenario considered the technical improvements to be made at the terminal in order to improve local air quality.

Keywords: Port emission inventories; dry bulk terminal emissions, port air quality management, emission control measures.

INTRODUCTION

Atmospheric emissions, especially fugitive emissions of particulate matter, are very common and relevant in port areas, as is the case of the port considered in this study. In the region there are several terminals that carry bulk cargo handling, with potential to generate atmospheric emissions and whose control is complex. There are also the contributions of mobile sources such as motor vehicles, ships and other vessels, and even natural sources (eg, marine spray). In this scenario, there is a possibility that concentrations of pollutants in ambient air become high, especially with respect to particulate pollutants. This concern with the air quality in the environment was the motivating factor of the present study, in which one tries to know and estimate, in a quantitative way, the influence of the activities of the terminals on the levels of air pollution in the environment.

METHODS

The sources of atmospheric emission to be evaluated in the study were initially defined, in order to later verify their possible impacts on the local air quality. To achieve this goal, it was necessary to define the area to be covered by the inventory and the modeling; that is, to delimit the scope. To do this, the following steps were followed: identification of the terminals in operation in the port; definition of the types of

cargo to be studied; spatial delimitation of the study area. In this way, the scope of this study was delimited to a group of eight terminals in a port in Latin America, destined to the export of vegetal bulk cargo.

The substances evaluated in this study were defined according to the characteristics of the atmospheric emissions expected for the various sources present in the enterprises, focusing on the loading and unloading of grain at the terminals. The pollutants evaluated were the Total Particulate Material (PM), linked to the air quality parameter TSP (Total Suspended Particles), as well as its fractions: PM₁₀ and PM_{2.5}.

1) Atmospheric Emissions Inventory

The present inventory was developed using the Bottom-Up approach, based on emission factors, where emissions are calculated individually for each source, resulting in a greater level of detail, representativeness and accuracy.

Emission factor is a representative value that relates the amount of pollutant emitted to the atmosphere with an activity associated to the emission of this pollutant. The Compilation of Atmospheric Pollutant Emission Factors, better known as the AP-42 (Compilation of Air Pollutant Emission Factors), is a publication that provides a comprehensive list of emission factors.

The basic equation of the emission estimation algorithm according to EPA (1999; 1997b) for uncontrolled emission factors can be expressed as:

$$E = A \times FE \times (1-ER / 100)$$

Where: E is the emission estimate for the source; A is the activity level; FE is the uncontrolled emission factor (obtained from chapter 9.9.1- Grain Elevators and Processes of the AP-42); and RE is the overall efficiency of emission reduction, expressed as a percentage (%) and equal to the efficiency of the control mechanism.

With regard to emission control systems, the particulate removal efficiency considered for each type of system, as well as the technical justification, is presented in Table 1. These explanations for each index range were based on observations made in the field as well as on references from the specialized literature.

Table 1. Particulate removal efficiency.

Sources	Efficiency considered	Justification
Grain receiving (truck and railcar)	60 - 85%	The efficiency of 99% can be considered for complete systems, including two side walls, doors, roof, underground flaps below the grate and dust aspiration (DUBENETZKY & SINHA, 1998).
Emission sources with fabric filters	95 - 98%	The US EPA (2011) reports that the efficiency of pulsed jet fabric filters ranges from 95,0 to 99,9%.
Storage bin (vent)	90%	According to the EPA, this emission factor appears to be overestimated (US EPA, 2003). Also, taking into account the silo geometry that restricts the size of the vent, a control efficiency of 90% was applied.
Grain shipping (ship)	70 - 85%	Although the ship-loaders do not have fabric filters installed, the terminals have some measures to reduce emissions (e.g., dust suppressor, telescopic tube, sprinkling of vegetable oil).

2) Atmospheric Dispersion Modeling

The atmospheric pollutant dispersion modeling carried out the diagnosis and the prognosis of the possible impacts, by mapping the maximum concentrations expected over the entire study area, considering the influence of topography (SRTM digital topography data from the study domain area, 15 km by 15 km, with horizontal resolution of 90 m) and the variation of meteorological conditions (series of data - five years - measured by surface meteorological station, as well as in radiosondes). The diagnosis used emission rates based on the current terminal situation. In the other hand, the prognosis used emission rates that consider the technological improvements to be made in the terminal. In order

to evaluate the results, these were then compared to the current air quality standards, with their attendance throughout the study area, as well as at discrete receptors representative of locations that are sensitive to possible changes in air quality. The AERMOD model and its components (AERMET and AERMAP) of the United States Environmental Protection Agency (U.S. EPA) were used as a mathematical dispersion modeling tool.

FINDINGS AND DISCUSSION

1) Atmospheric Emissions Inventory

The results of the estimation of the theoretical atmospheric emissions of the eight terminals are presented in Figure 1. The values obtained here allowed to classify the terminals, in ascending order, based on the percentage contribution of each terminal in the total estimated emission. These results also made it possible to analyze which terminals are more and less efficient in terms of atmospheric emissions control.

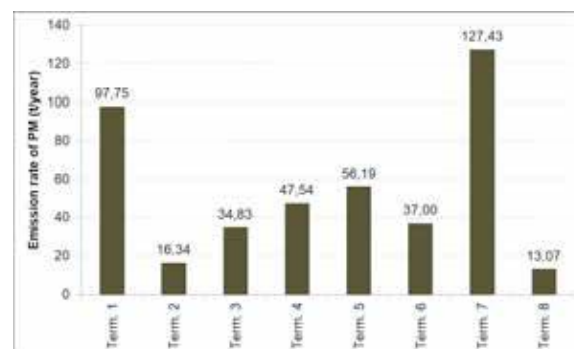


Figure 1. Emission rate of PM (t/year).

Taking into account the use of atmospheric emission control systems, the sum of the total emissions of the 8 terminals is of the order of 430 t/year of PM, being approximately 30% originated in Terminal 7, 23% in Terminal 1, and 13% of Terminal 5. Regarding PM₁₀ and PM_{2,5}, the emission proportions correspond approximately to the percentage of particulate matter, since they are fractions of the total particulate.

Figure 2 compares the percentages of handling and emission of particulate matter at the terminals. As already expected, the terminals with the highest handling are also those that contribute the highest percentage of emission. It is important to note that Terminal 2 and Terminal 8 were the terminals with the lowest emission rate in comparison to their handling. This is due, in addition to the adoption of control systems, to the type of product that has lower emission factors.

When analyzing the emission normalized by the handling of each terminal, it was verified that the terminal with the largest mass fraction of PM loss is Terminal 6, where approximately 23,75 g/t of product are lost to the atmosphere in the form of

emissions. This corresponds to approximately 0,0024% of the mass handling. It should be noted that Terminal 3 and Terminal 4 present a 0,0019% PM loss ratio. This result also indicates that there is a similarity between the efficiencies of atmospheric emissions control systems at these terminals.

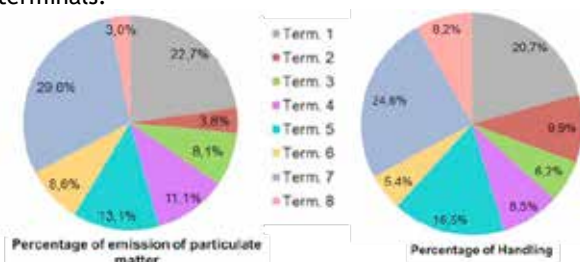


Figure 2. Comparison between handling and emission.

2) Atmospheric Dispersion Modeling

The result of the evaluation of the 8 solid bulk terminals showed that the pollutant levels predicted for the current scenario of operation exceed the short and long term air quality standards for TSP ($240 \mu\text{g}/\text{m}^3$) and PM10 pollutants ($120 \mu\text{g}/\text{m}^3$) (CONAMA, 2018). In the case of PM_{2.5}, standards were met throughout the domain, in the short term and in the long term. Figure 3 shows the result for the TSP emission diagnosis considering the eight terminals. The results of the modeling were shown to be consistent with the monitoring data available for the region.

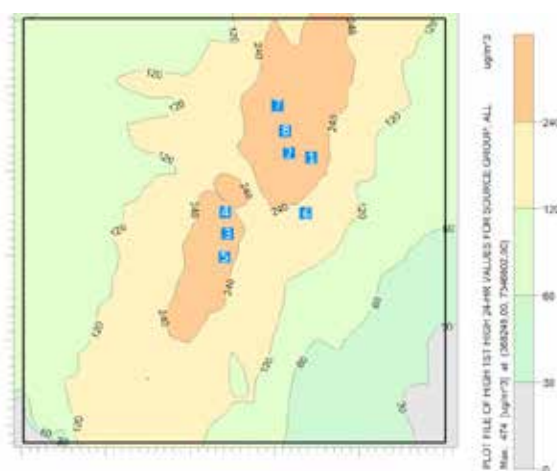


Figure 3. Maximum daily concentration of PM (considering the eight terminals).

Terminal 3 has been selected for a more detailed study of atmospheric dispersion modeling since there are already improvements projects to be carried out in order to reduce emissions of particulate matter to the atmosphere and thus collaborate with local air quality. In the diagnosis (current situation) the terminal presents PM emissions for equal to 1,95 g/s, which

results in maximum hourly concentrations of $192 \mu\text{g}/\text{m}^3$. On the other hand, in the prognosis (situation considering the adoption of technical improvements) the emission of the terminal is about 80% lower than the current one, which results in maximum concentrations of $20 \mu\text{g}/\text{m}^3$. Therefore, it is concluded that the adoption of measures such as fabric filters, point filters, dust suppressors, vegetable oil sprinkler systems, and shiploaders accessories are essential to ensure good air quality in the study region.

CONCLUSIONS

When analyzing the results of the emissions inventory and the atmospheric dispersion modeling, it is observed that the eight terminals have a significant participation in the maintenance of the local air quality. Modelling indicated that the eight terminals together exceed the legally established air quality standards for the PM and PM₁₀ parameters, without considering the contribution of other sources such as other terminals, vehicles and marine spray. Therefore, since air quality must be maintained by the group of sources, it is recommended that the emission prevention and control actions in the terminals under study be maintained and improved. In addition to the implementation of emission control systems, it is essential to pay attention to the operational procedures during the activities, in order to maximize the efficiency and effectiveness of the control systems to be installed. It is important to review and, if necessary, update the maintenance plan of emission control equipment (fabric filters, point filters, dust suppressors, vegetable oil sprinkler systems, and shiploaders' accessories), favouring preventive maintenance instead of corrective maintenance; as it is essential to properly train all operators of these systems to ensure their correct use.

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PARTICULATE COMPOSITION ANALYSIS IN DRY BULK TERMINALS TO INVESTIGATE SOURCES' PARTICIPATION

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Abstract:

In seaport regions with great number of dry bulk export terminals, there are many activities and stages with potential to generate atmospheric emissions. The pollutants which cause the most visible impact are the particulates, and the presence of varied emission sources (anthropogenic and natural, fixed and mobile) make the air quality analysis complex. Therefore, the objective of this study was to analyze the chemical composition of particulate matter to obtain indication of different emission sources' participation on the resulting air quality. The study area included two vegetal dry bulk export terminals and its residential vicinities. TSP and/or PM_{10} sampling was conducted using Hivols in two points located close to fugitive emission sources (with the goal to characterize emission's composition), and three points on receptors around the terminals (with the goal to characterize the imission's composition, on the receptors). Bearing in mind that the product handled in these terminals is of vegetal origin (and thus, organic), the contributions of other external emission sources (such as marine aerosols, unpaved roads and vehicular emissions) were investigated through chemical analyses. The analytical methods employed were termogravimetry (SMWW 2540 E), to analyze inorganic material mass, and Flame Atomic Absorption Spectrometry (FAAS), to determine 23 metal concentration on sampling filters. The results pointed that the proportion of organic material varied from 54 to 90% on the receptor's samples, and was influenced by meteorological conditions. On the fugitive emission samples, the organic percentage was 63%, and 27% inorganic. The predominant metallic elements, both on emission and imission samples, were Na, K, Al, Fe, Ca, and Ba, which can be originated on the handled product itself, as well as on other external sources, such as marine aerosol. In conclusion, even though the emissions from terminals' activities represent the greater participation on the analyzed samples, this activities are not the only sources responsible for the particulate resulting concentration on the atmosphere.

Keywords: Port dry bulk emissions, particulate matter chemical characterization, port air quality management, source apportionment.

INTRODUCTION

In seaport regions with great number of dry bulk export terminals, the pollutants that cause the most visible impact are the particulates - Total Suspended Particles (TSP) and Particulate Matter less than $10\mu m$ (PM_{10}). Yet there are many activities with potential to generate atmospheric emissions. The presence of varied emission sources (anthropogenic sources, such as cargo handling; natural sources such as marine aerosol; fixed sources like terminal structures; and mobile sources such as light and heavy vehicles, ships and other marine vessels) makes the air quality analysis and management very complex.

Therefore, the objective of this study was to analyse the chemical composition of particulate matter collected in the surrounding of two vegetal dry bulk terminals to obtain indication of different emission sources' participation on the resulting air quality.

METHODS

The study area included two vegetal dry bulk export terminals and its residential vicinities. The study was carried out during a few weeks in the winter of 2018, corresponding to the maximum activity rates at the terminals. During the

monitoring campaign, the cargo handled was soybean grain and soybean meal (Terminal 01) and corn grain (Terminal 02).

1) Sampling method and points

TSP and/or PM_{10} sampling was conducted using Hivols in two points (FUG-01 and FUG-02) located close to fugitive emission sources (with the goal to characterize emission's composition), and two points (AQ-01 and AQ-02) on receptors around the terminals (with the goal to characterize the imission's composition, the air quality on the receptors). Collection lasted for 24h+-1h and was done on glass fiber filters (GF/A 8X10in WHATMAN). The wind direction and speed was measured locally in each sampling point in order to aid in interpretation of results.

2) Chemical analyses: inorganic content

Bearing in mind that the product handled in these terminals is of vegetal origin (and thus, mostly organic), the contributions of other external emission sources (such as marine aerosols, unpaved roads particles and vehicular emissions) were investigated through chemical analyses. The first analytical method employed was termogravimetry (SMWW 2540 E), to analyze inorganic material mass, and allow the calculation

of organic mass by subtraction of the total mass (SMEWW, 2017).

3) Chemical analyses: metals

Besides, some samples were subject to Flame Atomic Absorption Spectrometry (FAAS), in order to determine 23 different metal concentrations on sampled Hivol filters: Al, As, Ba, B, Cd, Ca, Pb, Co, Cu, Cr, Sn, Fe, Li, Mg, Mn, Mo, Ni, K, Ag, Se, Na, V and Zn.

FINDINGS AND DISCUSSION

1) Points close to fugitive sources (emission composition)

Table 1 shows the results for inorganic and organic fractions of PM₁₀ in the two points close to fugitive emission sources. The results showed that on point FUG-02 (located close to shiploader of Terminal 2) the proportion of organic material was higher than inorganic, and varied from 54 to 90%. This percentage was maximized when the meteorological condition transported emissions from the shiploader to the sampling point FUG-02.

Table 1. PM₁₀ Inorganic and Organic fractions (%) on points close to fugitive emission sources.

Terminal	Terminal 1	Terminal 2	
Point	FUG-01	FUG-02	
Location	Close to receiving area	Close to shiploader	
Day	Jul. 28th	Jul. 28th	Jul. 29th
PM ₁₀ Inorganic %	27	46	<10
PM ₁₀ Organic %	63	54	>90

On the FUG-01 point, located close to the receiving area, the organic percentage was 63%, and 27% inorganic. This inorganic material may be generated from the terminal activity (soil particles that come together with grain received by truck or rail; or even metal particles caused by abrasion of grain on structures); or from external sources.

Concerning the concentration of metals, no heavy metals were identified in these samples. The predominant metallic elements were Na, K, Al, Fe, Ca and Ba, which can be originated on the grain itself (COELHO & FRANÇA, 1995; BRAMUGY & CHIBALE, 2013), or on external sources (mostly marine aerosols).

2) Points close to community (emission composition)

Figure 1 shows the resulting TSP and PM₁₀ fractions on AQ-01 point, located in the influence area of Terminal 1. The results show that the particulate composition (organic/inorganic fractions) varies considerably between different granulometries (TSP and PM₁₀), and also between samples taken on

different days, also displaying the influence of meteorological conditions.

In this point, the organic fraction was around 81% for PM₁₀. For TSP, the organic fraction was in average 48%, yet ranged from 23% to 73%. This wide range indicates that there is relevant influence from many different external sources, natural or anthropogenic, and that the air quality concentration levels are not caused exclusively by vegetal dry bulk cargo handling (which is expected to generate a higher organic fraction, because of material's organic origin).

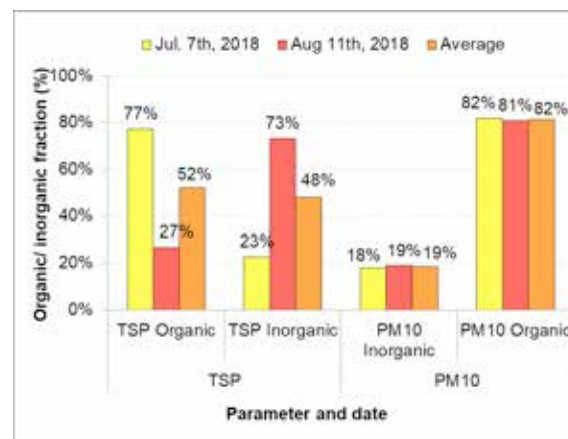


Figure 1. TSP and PM₁₀ Inorganic and Organic fractions (%) on point AQ-01 (community around Terminal 1).

About metallic concentrations, the results were similar to the fugitive emission points: practically there were no heavy metals, and the predominant metallic elements were Na, K, Fe, Ca and Ba.

Figure 2 shows the resulting TSP and PM₁₀ fractions on AQ-02 point, located in the influence area of Terminal 2.

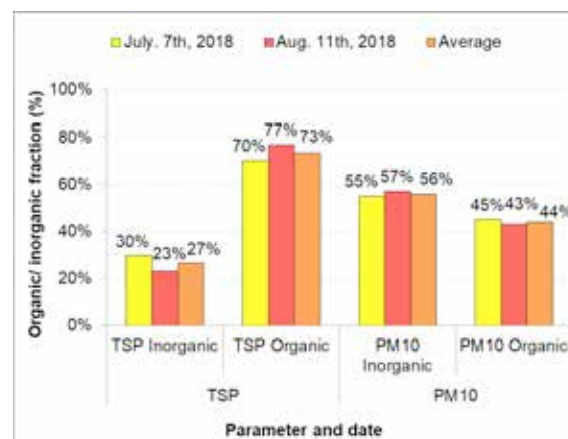


Figure 2. TSP and PM₁₀ Inorganic and Organic fractions (%) on point AQ-02 (community).

Compared to Figure 1, Figure 2 showed less variability in organic/inorganic composition. In the larger particles (TSP), the organic fraction prevailed with an average of 73%, against 27% inorganic. In the other hand, for PM₁₀, the inorganic fraction was slightly higher (56%) than the organic (44%).

This result may be related to the fact that vehicular emissions, whose composition is inorganic, lay mostly in the fine particulate (below 10µm) (GEIGER & COOPER, 2010). Therefore, considering the fine particles, the participation of sources external to the terminal is more relevant than in the TSP.

Concerning the metals' concentrations, just as in the other samples mentioned, the predominant metallic elements were Na, K, Al, Fe, Ca and Ba. Nonetheless, in point AQ-02 some other elements were detected: B, Zn, and Cu.

Table 2 displays examples of key elements that may indicate particulate emission sources. the elements that were found in the analyzed samples are marked in bold.

Table 2. Examples of key elements in particulate that can be indicators of emission sources.

Emission source	Related elements
Geologic (soil and rosck of earth crust)	Na, Mg, Al, Si, K, Ca, Sc, Ti, Mn, Fe, Ga, Rb, Sr, Zr
Diesel combustion	Fine particulate: V, Ni, Mo
Vehicular emissions	Fine particulate: Br e Pb
Smelting (Cu, Ni, Pb)	Cu, As, Cd, Pb, In, Sn, Sb
Marine aerossol	Na, Cl
Biomass combustion	Organic carbon, elementary carbon, K, Cl, Zn
Iron and steel industry	Fine particulate: Fe, Co, Cr, Ni, Mg

Reference: Adapted from GEIGER, COOPER (2010).

In the study area, the following emission sources mentioned in Table 2 are present, with its related elements: geologic sources (soil), indicated by the presence of Mg, Al, K, Ca, Fe, elements that are present in the earth crust; and marine aerossols given the close proximity with the sea and coast, which is confirmed by the high levels of Na.

Even though diesel combustion and vehicular emissions are present sources in the study area, as indicated by the relevant inorganic fraction of PM₁₀ (see Table 1 and Figure 2), these elements were not found in the samples analysed through FAAS, probably due to the fact that concentrations of these indicator elements (V, Ni, Mo, Br and Pb) were below the detection threshold of the analytical method.

CONCLUSIONS

The analysis of results in the points located close to fugitive emission sources (FUG-01 and FUG-02) displayed that there is a parcel of inorganic material even in locations where the contribution of organic sources was expected to be higher. The inorganic participation ranged from 27 to 46% considering the samples taken in 2 different days. On the other hand, the percentage of organic contribution clearly increased in meteorological conditions that carried the emissions from the shiploader to the sampling point FUG-02.

The results in air quality in the surrounding of terminals (imission: points AQ-01 and AQ-02) showed that, even though the emissions from terminals' activities (organic fraction) represent the greater participation on most samples, these fractions may vary widely (27 to 73%, for TSP in AQ-01). This shows that these activities are not the only sources responsible for the resulting concentration of TSP and PM₁₀ in the atmosphere. The influence of terminals' activities seems to be more relevant in the coarse (TSP) than in the finer fraction (PM₁₀); the inorganic fraction of PM₁₀ was higher than organic in point AQ-02. This may be explained by a higher influence of vehicular emissions, considering the fine particles.

The metallic concentration in all samples pointed to the relevant participation of geological sources (indicated by the presence of Na, Mg, Al, K, Ca, Fe) and marine aerossols (Na). No heavy metals were detected, nor elements indicators of vehicular emissions or diesel combustion, even though these sources are present in the study area. Finally, due to the variability of composition influenced by meteorological variables and sampling locations, it is recommended to analyse a higher number of samples in order to be able to draw more consistent conclusions about source apportionment in this region.

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AN EVALUATION OF ATMOSPHERIC EMISSIONS DUE TO BIOMASS BURNING IN BRAZILIAN STATES

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Abstract:

The biomasses burning are seen as important factors of ecological disturbance, causing health, social and economical impacts. On the environment, biomass burning can lead to vegetation degradation, erosion, changes in the hydrological cycle, soil impoverishment, serious human health problems and influences on climate changes. There are many studies about wild fires/biomass burning in Amazon region. However, none of them quantify the total amount of pollutants emitted by each jurisdiction or state in Brazil. It is essential to know where the critical areas are and the major controlling factors of biomass burning in Brazil. This is valuable information for environmental managers towards impact control. The objective of this work is to evaluate the emission of carbon monoxide from biomass burning in the Brazilian states in 2016. In the present work the FINN (Fire INventory from NCAR) model will be used to estimate biomass burning emissions in Brazil. This model was developed by the National Center for Atmospheric Research of the United State. FINN is based on the detection of hotspots and burned area around the world captured by the MODIS system (Moderate Resolution Imaging Spectroradiometer). GEOS-chem emission factor and speciation was employed in this work. Daily basis data of fire event between January 1 and December 31, 2016 was considered. The north of the country are the states that emit the most carbon monoxide by burning biomass, Pará in absolute number of hot spots in the region with 59013 detections. In relation to the emission by territorial area appear Acre, Rondonia and Roraima with 16.11Mton/km².year, 13.29Mton/km².year and 9.59Mton/km².year, respectively as the largest emitters. In the Amazon, fire is widely used for the initial conversion of extensive areas of natural vegetation into agricultural fields and pasture areas, and for the subsequent maintenance of deforested areas.

Keywords: Atmospheric pollution, emission estimate, biomass burning, FINN.

INTRODUCTION

The biomass burning have posed a significant challenge to air quality and resource management worldwide due to the uncertain nature of their occurrence, intensity and duration, and the complex relationships among the ecological, hydrological and atmospheric factors that drive them. Reliable estimates of how the areas of forest fires will be burned and the factors that imply the occurrence of the events help to guide sound policies on the management of air quality and natural resources, which is still very precarious in Brazil (RUSSO, 2013).

Information on the location and extent of the areas affected by fire is necessary to assess the effects of biomass burning on atmospheric chemistry, ecosystem functioning, and human health. (SHIMABUKURO et al., 2015).

Brazil is currently among the ten most polluting countries in the atmosphere (KANSKI, 2015). Unlike the other countries, where the main source of emissions is the burning of fossil fuels, the emissions

of greenhouse gases in Brazil come mainly from the fire originated in the tropical forests, representing about 75% of the total volume of CO₂ released in the country. In the Amazon, more than 10 million people are exposed to high levels of pollution due to anthropogenic causes (MMA,2004; LELIEVELD et al., 2015; PEREIRA et al., 2016; ALVES et al., 2017).

Among the main substances studied in air quality assessments, biomass burning is responsible for considerable emissions of particulate matter (PM), sulphur dioxide (SO₂), nitrogen dioxide (NO₂), volatile organic compounds (VOCs) and carbon monoxide (CO) (BOND et al., 2005; WIEDINMYER et al., 2011).

Many studies present the spatial and temporal distribution of biomass burning using different types of data processing and remote sensing. However, no papers have quantified the total emission of pollutants emitted by each jurisdiction or state in Brazil. It is essential to know where the critical areas and the main control factors of the biomass burning in Brazil are. This is valuable information

for environmental managers in relation to impact control.

The objective of this work is to evaluate the atmospheric emissions from biomass burning in the Brazilian states in 2016, based on the FINN (Fire Inventory from NCAR) model.

METHODS

In the present work, the atmospheric pollutant emission estimates of the FINN (Fire Inventory from NCAR), developed by the National Center for Atmospheric Research of the United States, were used. The model estimates the emissions originated by the biomass burning by means of global detections of heat sources captured by MODIS (Moderate Resolution Imaging Spectroradiometer), with spatial resolution of 1km². The trace gases and particles from the burnings can be estimated by means of equation 1:

$$E_i = A_{(x,t)} \times B_{(x)} \times FB \times ef_i \quad (1)$$

Where, E_i represents a emission estimate for the pollutant i , $A_{(x,t)}$ is an area burned at time t and at location x , $B_{(x)}$ is a biomass charge available to burn in the local x , FB is a fraction of biomass burned at x , ef is the emission factor of pollutant i .

To estimate emissions, FINN can work with three emission factor and speciation databases, MOZART-4, SAPRC99, and GEOS-chem. For the present study, the 2016 data were used based on GEOS-chem.

FINDINGS AND ARGUMENT

Figure 1 shows a high concentrated concentration of fires spots mainly in northern (Amazon Rainforest) Brazil, where a large number of biomass burning events were recorded mainly in the states of Pará (PA) with 59.013 and Tocantins (TO), with 33.381 fire spots .

According Morton (2008), more than 40% of all high-confidence MODIS fire detections within Amazonia were associated with deforestation.

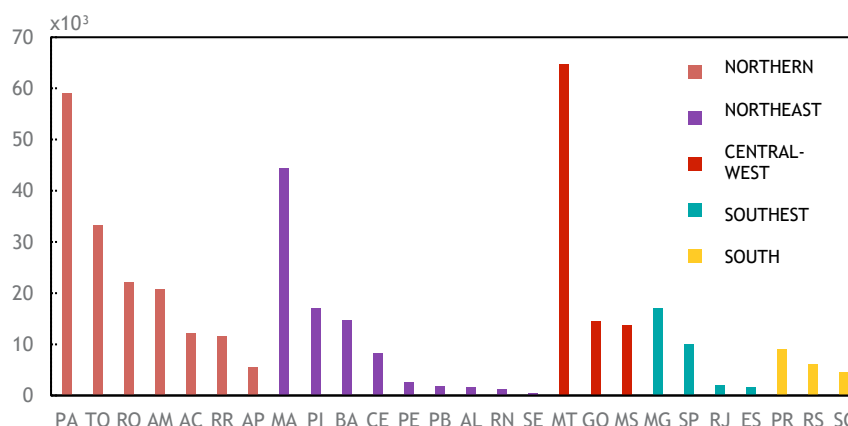


Figure 1. Number of fire spots by Brazilian state for the year 2016. Northern: Pará (PA), Tocantins (TO), Rondônia (RO), Amazonas (AM), Acre (AC), Roraima (RR) and Amapá (AP). Northeast: Maranhão (MA), Piauí (PI), Bahia (BA), Ceará (CE), Pernambuco (PE), Paraíba (PB), Alagoas (AL), Rio Grande do Norte (RN) and Sergipe (SE). Central-West: Mato Grosso (MT), Goiás (GO) and Mato Grosso do Sul (MS). Southeast: Minas Gerais (MG), São Paulo (SP), Rio de Janeiro (RJ) and Espírito Santo (ES). South: Paraná (PR), Rio Grande do Sul (RS) and Santa Catarina (SC).

The state of Mato Grosso located in the central-west region is among the highest concentration of detections in Brazil, with 64.783 fire spots in 2016. Concentrated fire activity in the state is consistent due to the peak of deforestation of agricultural land, promoted by the high prices of soybean exports (Morton et al., 2006).

In the Amazon, fire is widely used for the initial conversion of extensive areas of natural vegetation into agricultural fields and pasture areas, and for the subsequent maintenance of deforested areas (COCHRANE et al., 1999; GIGLIO et al., 2006). In contrast, the Cerrado biome is an ecosystem that

has plant species adapted to fire (PIVELLO, 2011). However, occurrences of natural fires are extremely rare, with the great majority of the events of fires resulting from the use of anthropogenic fire, that is, deliberate (COCHRANE et al., 1999).

Based on these heat sources and on data obtained from the FINN emission estimation model, Figure 2 below shows the emission rates of the atmospheric pollutant carbon monoxide, one of the nine atmospheric pollutants present in the current resolution (CONAMA n°. 491 of 2018) that provides on air quality standards in Brazil.



Figure 2. Emissions estimated by FINN in all Brazilian states in the year 2016 for the polluting carbon monoxide.

The behavior of emissions follows a pattern similar to other pollutants, that is, the state that emits more carbon monoxide tends to emit a larger amount for the other pollutants.

Despite the large amount of detection of burning spots in some states of the Amazon Forest, other states stood out for the amount of emission of carbon monoxide. Following the premise that the estimation of emission of a shipper is dependent on the combustible material, the occurrence of fire in areas of dense forests will lead to higher emissions.

In this way, we present in Figure 3 the relation between the emission of carbon monoxide by the territorial area of each state.

In this scenario, Acre with 16.11Mt/km².year, Rondônia, 13.29Mton / km².year and Roraima with 9.59Mton / km².year, occupy respectively, first, second and third position among the states with the highest amounts of carbon monoxide emitted by territorial area. Santa Catarina emerges in the southern region as the largest emitter of carbon monoxide by territorial area, with 5.32Mton/km².year.



Figure 3. Estimation of FINN model performance for the CO pollutant by territorial area for each unit of the federation in 2016.

Other atmospheric pollutants are listed in Table 1. Carbon dioxide (CO₂) , nitrogen dioxide (NO₂), sulphur dioxide (SO₂) , methane (CH₄) and particulate matter (PM_{2,5}) are listed.

Table 1. CO₂, NO₂, SO₂, CH₄ AND PM_{2,5} EMISSIONS ESTIMATION FOR EACH BRAZILIAN STATE IN 2016.

	UF	CO ₂ (Mton/ year)	NO ₂ (Mton/ year)	SO ₂ (Mton/ year)	CH ₄ (Mton/ year)	PM _{2,5} (Mton/ year)
Northern	PA	159.66	0.35	0.04	0.48	8.67
	AM	101.54	0.22	0.02	0.31	5.60
	RO	58.04	0.13	0.01	0.17	3.15
	AC	53.64	0.12	0.01	0.16	2.95
	RR	45.54	0.10	0.01	0.14	2.49
	TO	15.84	0.03	0.00	0.02	0.59
	AP	8.79	0.02	0.00	0.03	0.47
Norwest	MA	23.76	0.05	0.01	0.05	1.05
	BA	8.35	0.02	0.00	0.01	0.35
	PI	7.04	0.01	0.00	0.01	0.24
	CE	2.91	0.01	0.00	0.00	0.09
	PE	0.93	0.00	0.00	0.00	0.03
	AL	0.68	0.00	0.00	0.00	0.02
	PB	0.63	0.00	0.00	0.00	0.02
	RN	0.44	0.00	0.00	0.00	0.01
	SE	0.16	0.00	0.00	0.00	0.00
Central-west	MT	83.53	0.18	0.02	0.23	4.24
	MS	6.26	0.01	0.00	0.01	0.27
	GO	5.97	0.01	0.00	0.01	0.21
Southwest	SP	6.91	0.01	0.00	0.02	0.30
	MG	7.38	0.01	0.00	0.01	0.29
	ES	1.16	0.00	0.00	0.00	0.05
	RJ	0.97	0.00	0.00	0.00	0.04
South	PR	14.54	0.03	0.00	0.04	0.75
	SC	9.61	0.02	0.00	0.03	0.52
	RS	8.71	0.02	0.00	0.02	0.45
Total (Brazil)		632.99	1.35	0.12	1.75	32.94

The most recent national inventory of atmospheric emissions by road vehicles published in Brazil in 2013 shows that the emission of carbon monoxide amounts to approximately 1.5 Mton/year, compared to the biomass burning at 34 Mton/year. As for the emission of CO₂, 632.99 Mton/year are from the fires, and the vehicle emits about 210 Mton/year.

Regarding the NO_x , about 1 Mton/year are issued by the automotive, near the estimated of the fires with 1.35 Mton/year of NO_2 . On the other hand, the emission of CH_4 emissions was higher when compared to fires, with 40 Mton/year versus 1.75 Mton/year. All the particulate matters inventoried in the combustion of automotive vehicles in the Brazilian study represent similar values with the emissions of the fires presented in this study, 36 Mton/year of the vehicles and approximately 33 Mton/year of the heat sources.

CONCLUSIONS

This article provides an overview of the emission of carbon monoxide along the Brazilian territory. The spatial records of the emission of carbon dioxide and monoxide, methane, particulate matter, nitrogen dioxide and sulphur dioxide in the states of the Amazon region are clearly characterized in large potential areas for the emission of other compounds harmful to human health and the environment.

As the fire activity in deforestation is still an expansive practice in the northern region of the country besides burnings in areas of arable and pastureland management, these emissions can continue for several years.

Other states like Mato Grosso and Santa Catarina present great potential in the propagation of atmospheric pollutants mainly because they are units that have in agriculture their main source of economy. The intra-annual variation of the fire distribution (SHIMABUKURO et al., 2015), corroborates the hypothesis that the practice of burning in the preparation of the soil is responsible for the emissions of greenhouse gases.

Overall, the results of our study demonstrate that the results of our study demonstrate that biomass burning remains an important contributor to the emission of air pollutants in Brazil. There is the occurrence throughout the territory, however the Amazon region is where the largest records coincide. When compared to pollutants emitted by motor vehicles and burned, in general the pollutants from combustion are in larger quantities. Continued research over a historical series of data is needed to obtain more consistent information.

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EXHAUST VEHICULAR EMISSIONS IN SANTA CATARINA - BRAZIL: IDENTIFICATION OF CRITICAL SITES

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Abstract: An inventory of vehicular emissions was elaborated for the state of Santa Catarina (SC) - Brazil. Carbon Monoxide (CO), Hydrocarbons (HC), Nitrogen Oxides (NO_x), Particulate Matter (PM) and Nitrous Oxide (N₂O) emissions were estimated using a probabilistic Top-Down approach for the year of 2016. The method employed considered the fleet size and age, fuel consumption and the emission factor of each city in SC. In Santa Catarina the vehicles are responsible for the emission of 133,334.37 ton.year⁻¹ of CO, 17,844.03 ton.year⁻¹ of HC, 92,830.42 ton.year⁻¹ of NO_x, 4,044.37 ton.year⁻¹ of PM and 802.38 ton.year⁻¹ of N₂O. The present study identified that light vehicles are the main responsible for the emission of CO (61%) and HC (45%). Heavy vehicles, which correspond to 5% of the states's fleet, emit most part of PM (98%) and NO_x (92%). N₂O is emitted in similar proportion by light and heavy vehicles. The variability of emissions among SC's cities is explained by the degree of urbanization, industrialization, size of the fleet, economic factors and regional characteristics. Among the mesoregions, the Itajaí Valley is the largest contributor of CO from vehicle exhaustion (25%), HC (24%), N₂O (24%). The western part of the state emits most of the NO_x (24%) and PM (25%), since it has an important industrial activity and large heavy-duty fleet. Considering the emissions among municipalities, Joinville, Blumenau, Itajaí, Florianópolis, Chapecó, Jaraguá do Sul, Guaramirim, São José, Balneário Camboriú, Navegantes, Itapema, Criciúma and Maracajá are the most important emitters. These cities are the major target for vehicular emissions control in Santa Catarina.

Keywords: Emission Inventory, Vehicular Emissions, Top-Down, Santa Catarina.

INTRODUCTION

Air Pollution is recognized as the greatest environmental risk to health, especially in low-income areas. Currently, 4.2 million premature deaths worldwide annually are linked to atmospheric pollution (WHO, 2014). In addition, the deterioration of air quality contributes to climate change and disruption of the ecological balance.

Among the sources of air pollution, traffic-related emissions (exhaustion and resuspension) account for a significant proportion of the pollutants found in the local atmosphere in urban areas. In developing countries, traffic emissions are becoming a big problem, given the increasing number of vehicles and fuel consumption.

Santa Catarina is one of the 27 federative units of Brazil, and is located in the South Region of the country. The state has 295 municipalities distributed in an area of 95,737.954 km². The estimated population for the year 2017 is 7,001,161 inhabitants, resulting in the 9th highest population density in the national ranking, with 65.27 inhabitants per km². The state of SC has a fleet of 4,772,160 vehicles, the 6th largest national fleet, with a predominance of a light vehicles (IBGE, 2017).

In Santa Catarina, automotive vehicles are the main mode of transport, either for private, commercial and industrial use.

The establishment of regulations to reduce vehicular emissions is essential for improving environmental health. Regulations and control strategies should be based on an air quality

management system, which the development of emission inventories is the first step.

The inventories are used to guide the air quality intervention strategies, quantify the main emitted substances, identify the best available control technologies and provide future perspectives.

The objective of this work is to elaborate an exhaust vehicular emission inventory from Santa Catarina - Brazil, focusing on the identification of critical sites.

METHODS

The licensed vehicle fleet in Santa Catarina is segregated in 4 categories (light, light commercial, motorcycle and heavy) and 3 different types of fuel (Gasoline C, Ethanol and Flex-Fuel). We used data from the National Department Traffic Statistical- DENATRAN for the year of 2016. These data were employed to categorize the fleet of the respective year (DENATRAN, 2016). A top-down probabilistic approach was used to estimate emissions. The Emission Factors of CO, HC, NO_x, PM and N₂O were provided by the Environmental Company of the State of São Paulo - CETESB (CETESB, 2016). Fuel consumption was provided by the National Agency of Petroleum, Natural Gas and Biofuels - ANP (ANP, 2016). MATLAB was employed for data manipulation and analysis. A general formulation of probabilistic Top-Down approach used in this work is presented in Equation 1.

$$Ex_k = \sum_{j=1}^{j=x} \sum_{i=1}^{i=y} P_{(j,i)} \times FEx_{j,i} \times A_{j,i} \times Cm_k \times S_{\%}$$

Being $E_{x,k}$ is a emission of pollutant x to city k in g/year; $P_{(j,i)}$ a conditional probability of the vehicle

using fuel j , and be of year i ; $FE_{x,j,i}$ the pollutant emission factor x for each vehicle using fuel j and is of year i in g/year; $A_{j,i}$ the autonomy of the vehicle using fuel j and is of year i in km/L. Cm_k the amount of fuel m in liters consumed in city k (in fuel units); $S\%$ the percentage of fuel consumption m per type of vehicle.

FINDINGS AND ARGUMENT

The present study identified that light vehicles are the major contributors of CO (61%) and HC (45%) exhaust vehicle emissions. Heavy vehicles, which correspond to 5% of the state's fleet, emit most part of PM (98%) and NO_x (92%). N₂O is emitted in similar proportion by light and heavy. Motorcycles have the second largest fleet in SC (. Its emission factor and its autonomy are the smallest among the all categories. However, due to the high vehicle-use intensity, the motorcycles have high fuel consumption. Therefore, the emissions of this category are significant for CO (18%) and HC (21%), as shown in Figure 1.

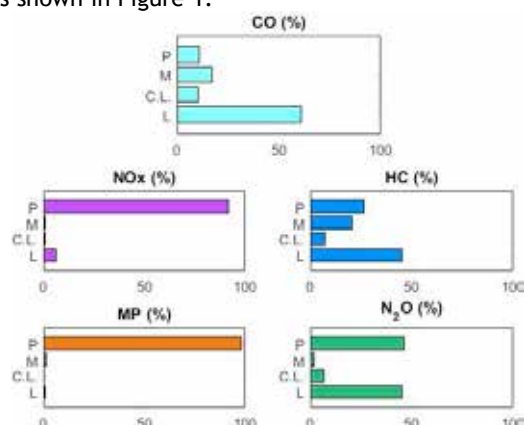


Figure 1. Percentage contribution of emission of pollutants in each category

The variability of emissions between the cities of Santa Catarina is high. It is explained by the degree of urbanization, industrialization, size of the fleet, economic factors and regional characteristics. Urbanized cities with large fleets have emission profiles with higher emissions of Carbon Monoxide and Hydrocarbons, while more industrialized cities emit mostly Nitrogen Oxides and Particulate Matter.

Table 1 shows the total emissions by year, fleet size and territorial area of each region in SC. It is verified that Greater Florianópolis presented the lowest emission per vehicle between the regions. This could be explained by the latest fleet and pollution control technology implemented in Greater Florianópolis, when compared to other regions. The Serrana region fleet has the greatest emission potential. However, this region represents the lowest consumption, fleet and the largest territorial area. The emissions found for each region is probably related to economical factors, Human Development Index (HDI) and other regional characteristics.

Among the mesoregions, the Itajaí Valley is the largest contributor of CO emitting (25%), HC (24%) and N₂O (24%) in SC. The western part of the state emits most of the NO_x (24%) and PM (25%), since it has an important industrial activity. The north of the state is the second largest emitter of all pollutants, due to intense urbanization and industrialization. Figure 2 presents the percentage of emission in Ton/Year from each mesoregion of the state of Santa Catarina.

Table 1. Emission of pollutants in mesoregions of Santa Catarina

EMISSION UNIT	POLLUTANT	ITAJAI VALLEY	WEST	NORTH	SOUTH	GREATER FPOIS	SERRANA
Ton.ano ⁻¹	CO	27.413	20.786	20.882	16.869	14.885	9.158
	HC	3.341	2.856	2.830	2.252	1.684	1.162
	NO _x	18.358	22.287	21.239	16.244	6.487	7.397
	PM	766	998	928	702	246	351
	N ₂ O	195	160	170	133	111	49
kg.veic ⁻¹ .year ⁻¹	CO	22.85	24.12	24.82	23.49	19.85	36.95
	HC	2.78	3.31	3.36	3.14	2.25	4.69
	NO _x	15.3	25.86	25.24	22.62	8.65	29.84
	PM	0.64	1.16	1.10	0.98	0.33	1.42
	N ₂ O	0.16	0.19	0.20	0.19	0.15	0.20
Ton.km ⁻¹ .year ⁻¹	CO	2.093	0.761	1.311	1.735	2.022	0.410
	HC	0.255	0.105	0.178	0.232	0.229	0.052
	NO _x	1.401	0.816	1.333	1.671	0.881	0.331
	PM	0.058	0.037	0.058	0.072	0.033	0.016
	N ₂ O	0.015	0.006	0.011	0.014	0.015	0.002

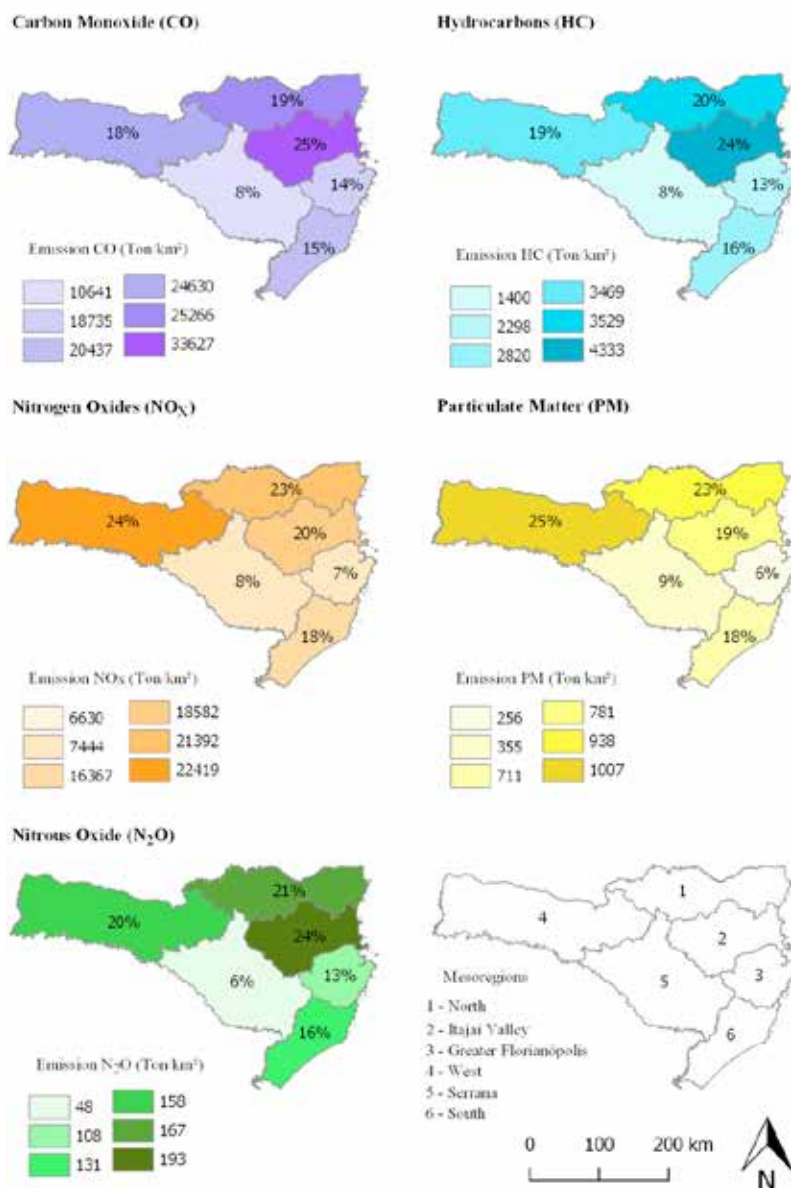


Figure 2. Percentage contribution of emission of pollutants in each mesoregion

When considering total emissions per unit of area and number of vehicle, the Itajaí Valley is the major emitter of CO, HC and N₂O among the Santa Catarina mesoregions. The South region is the most important emitter of NO_x and PM pollutants. It is known that the southern part of the state has strong industrial and urban activities. The regions of Greater Florianópolis and North are one of the major emitters by unit of area.

When segregating by cities, Joinville, Blumenau, Itajaí, Florianópolis, Chapecó, Jaraguá do Sul, Guaramirim, São José, Balneário Camboriú, Navegantes, Itapema, Criciúma and Maracajá are the critical sites for vehicular emissions controlling in SC, as shown in Figure 3.

It can be observed that the cities with the highest pollutants emission are located in the northern region of the state (Joinville, Guaramirim and Jaraguá do Sul). The city of Joinville, the largest city in the state, is the highest emitter of CO, HC and N₂O. In the mesoregion of the Itajaí Valley, the municipalities of Itajaí and Blumenau are the major contributors of vehicle emissions. In the Greater Florianópolis, the state capital (Florianópolis) emits the highest proportion of exhaust-vehicular pollutants. In the western part of the state, the city of Chapecó emits the most part of NO_x and PM.

Carbon Monoxide (CO)



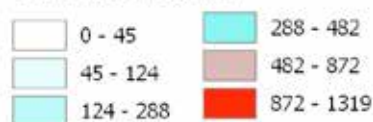
Emission CO (Ton/Ano)



Hydrocarbons (HC)



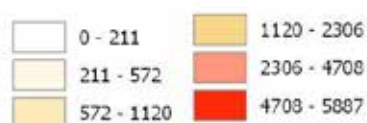
Emission HC (Ton/Ano)



Nitrogen Oxides (NO_x)



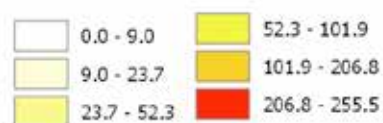
Emission NO_x (Ton/Ano)



Particulate Matter (PM)



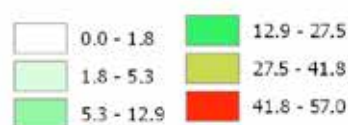
Emission PM (Ton/Ano)



Nitrous Oxide (N₂O)



Emission N₂O (Ton/Ano)



0 100 200 km



Figure 3. Estimation of pollutant emissions in the municipalities of Santa Catarina.

CONCLUSIONS

This study shows that the light vehicle emits the most part of CO and HC in SC, while the NO_x and PM predominantly emitted by heavy vehicles. N₂O is emitted with similar proportions between light and heavy-duty.

The Itajaí Valley is the most important contributor of air pollutants from exhaust-vehicular emissions in SC. This mesoregion also represents the higher rates per unit of area. The Greater Florianópolis region, South and North are also important emitters. The West region of Santa Catarina is among the three major emitters (ton/year). However, this region accounts for the largest area in SC, explaining this relatively high emissions obtained. The city of Chapecó concentrates the most part of pollutants emitted in West/SC.

The evaluation of emission per unit area is especially interesting, as it demonstrates the emissions accumulation in a given territory.

Among the cities of Santa Catarina, those with the highest urbanization and industrialization are the largest emitters. This work showed that the municipalities of Joinville, Blumenau, Jaraguá do Sul, Guaramirim, Florianópolis, São José, Criciúma, Lages and Chapecó are the critical sites for controlling vehicular emissions in SC.

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Session 03

Model Development

HOURLY OZONE CONCENTRATION FORECASTING USING DEEP LEARNING

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Abstract: The goal of this work is to build and evaluate a deep learning-based model to forecast tropospheric ozone levels hourly, up to twenty-four hours ahead, using data from the automatic air quality monitoring system in the metropolitan region of Vitória city, Espírito Santo, Brazil. To train, validate and test the model, observational data of air pollutant concentrations and meteorological parameters were used as the input variables of the model, once they represent the state of the atmospheric fluid in terms of its properties and chemical composition throughout the time. Several architectures of neural networks were tried and evaluated, using 60% of data for training and validating the models and the remaining 40% for testing. Using statistics of the predictions over the test data to evaluate the model performance, the forecasts for the next hour returned a Pearson correlation coefficient (r) of 0.848, a Regression coefficient (R^2) of 0.719 and a Factor of two (Fac2) of 0.918. For forecasts of 24 hours ahead, the model obtained a r coefficient of 0.645, R^2 of 0.415 and Fac2 of 0.807. Considering the model as a whole, taking into account all the forecasts from 1 to 24 hours ahead, the results presented r coefficient of 0.659, R^2 of 0.435 and Fac2 of 0.820, indicating a reasonable performance for the forecasting model.

Keywords: deep learning, artificial neural networks, forecast, air quality, ozone

INTRODUCTION

Ozone (O_3), which is a secondary pollutant in the troposphere, is one of the photochemical oxidants causing air quality problems. It is formed from chemical reactions between gases emitted by natural and anthropogenic sources, such as nitrogen oxides and volatile organic compounds in the presence of solar radiation. O_3 can cause harmful impacts on human health and on the environment. It could irritate the respiratory system, reduce lung capacity, and aggravate asthma problems and chronic lung diseases (Filippidou and Koukoulia, 2011). Moreover, it could damage plants causing several types of symptoms including chlorosis and necrosis, affecting its growth and agricultural production (Emberson *et al.*, 2018).

At the end of 2018 the Brazilian National Council for the Environment (Conselho Nacional do Meio Ambiente - CONAMA) has introduced a new resolution establishing updated air quality standards and, more specifically, ozone concentration thresholds for attention, alert and emergency levels (Brazil, 2018). Therefore, it is important to develop a powerful forecasting model that could help authorities and the population to take preventive measures and avoid imminent health risks, even before the attention limits are reached. With that in mind, this work aims to build and evaluate a deep learning-based model to forecast tropospheric ozone levels hourly, up to twenty-four hours ahead, using data from the automatic air quality monitoring

system in the metropolitan region of Vitória city, Espírito Santo (ES), Brazil. Figure 1 illustrates the region where the monitoring station used in this study is installed, with the red target indicating its location.



Figure 1. Location of the monitoring station in Cariacica, metropolitan region of Vitória, Espírito Santo, Brazil. Source: Google Maps

In the machine learning field, there are currently many different artificial neural network architectures available for implementation, being essential to examine which one best fits the problem that needs to be solved. Previous works used recurrent neural networks (RNN) to predict daily maximum concentrations of tropospheric ozone in the city of Palermo, Italy (Brunelli *et al.*, 2007), and in the Mexicali (Mexico)-Calxico (USA)

border area (Salazar-Ruiz *et al.*, 2008). In Biancofiore *et al.* (2015), RNN models were applied to predict O_3 concentration at time $t+\Delta t$, where Δt can be 1, 3, 6, 12, 24 and 48 h. A convolutional neural network (CNN) was employed in Eslami *et al.* (2019) to predict the hourly ozone concentration on each day using parameters from the previous day. Eight separated multilayer perceptron (MLP) networks were used in Agirre *et al.* (2007) to forecast the values of the variables $O_3(t+k)$, being $k = 1, 2, \dots, 8h$, at two rural stations located in the Autonomous Community of the Basque Country (North Central Spain). A MLP predictor was built in Tamas *et al.* (2014) using one single output to forecast O_3 concentration 24 hours ahead in Corsica, France, in order to be able to anticipate pollution peaks formation. In Coman *et al.* (2008) two MLP models were evaluated. The “dynamic” model used a cascade of 24 multilayer perceptrons arranged so that each MLP feeds the next one, and the “static” model was a classical single MLP with 24 outputs. For both configurations, the outputs were ozone concentrations for a 24h horizon.

The present research focus on multilayer perceptron neural network models, due to its simplicity and large application for short-term forecasts. Prior studies that used this type of network to forecast hourly concentrations of ozone aim attention on MLPs with one single hidden layer, which can lead to models with limited representational power. Moreover, few of them uses a single model to forecast hourly ozone concentrations for all time steps ahead in a 24h horizon. The proposed model employ this approach, since it can take advantage of a shared internal representation for all the forecasts and obtain a better generalization of the problem. Additionally, in the performed simulations the best results were achieved with deeper network topologies.

METHODS

The data used in the experiments is publicly available and was gathered from the Automatic Air Quality Monitoring Network (Rede Automática de Monitoramento da Qualidade do Ar - RAMQAr) owned by the State Institute of Environment and Water Resources of Espírito Santo (Instituto Estadual de Meio Ambiente e Recursos Hídricos do Espírito Santo - IEMA-ES). The monitoring station chosen for this study is located in Cariacica, a city in the metropolitan region of Vitória, ES, Brazil. This station measures hourly averages of the twelve atmospheric pollutant concentrations and meteorological parameters displayed on Table 1.

Data from year 2002 were collected and treated to eliminate records with invalid or missing measurements in one or more sensors. Furthermore, only valid data and hourly sequences with at least twenty-four consecutive samples were kept in order

to make possible the generation of ozone concentration ground truth targets, required on supervised machine learning algorithms for the model fitting. These steps discarded most part of the data and resulted in a data set with 1,036 samples and their corresponding targets divided into three continuous periods referring to the months of February, March, October and November of 2002.

Table 1. Parameters measured in Cariacica's air quality monitoring station.

Parameter	Unit
Particulate matter below $10\mu m$ (PM_{10})	($\mu g/m^3$)
Total suspended particulate matter	($\mu g/m^3$)
Sulphur dioxide (SO_2)	($\mu g/m^3$)
Nitrogen monoxide (NO)	($\mu g/m^3$)
Nitrogen dioxide (NO_2)	($\mu g/m^3$)
Nitrogen oxides (NO_x)	($\mu g/m^3$)
Carbon monoxide (CO)	($\mu g/m^3$)
Ozone (O_3)	($\mu g/m^3$)
Temperature	($^{\circ}C$)
Humidity	(%)
Scalar wind direction	($^{\circ}$)
Scalar wind speed	(m/s)

In the machine learning domain, one of the main objectives is to create computational models with the ability to generalize well the extracted attributes to new data. Poor generalization is often characterized by overfitting, and a common method to avoid that is to evaluate a model by splitting a data set into two. The first one is the training set, on which the model is built and optimized. The second is the test set, on which the finished model is evaluated with unseen data (Reitermanová, 2010). For this research, 621 data points were separated for the training and validation set, and the remaining 415 data points were used as test data. This division was done in such a way that the two batches of data have samples of the three continuous periods of the full data set.

Multilayer perceptron networks have a flexible topology and among their main parameters are the number of layers and the number of neurons in each layer. At least three layers are required: an input layer, a hidden layer, and an output layer. The definition of the number of layers and neurons is variable, and the best composition is problem-specific (Russel and Norvig, 2010). Since the model objective is to predict tropospheric ozone levels hourly, up to twenty-four hours ahead, the output layer of the proposed model is composed by twenty-four neurons, one for each hour in advance. Several network designs were tested varying the number of hidden layers and nodes in each hidden layer. Besides, different nonlinear activation functions were experimented on nodes in the hidden layers, keeping the output neurons with linear activation function. In order to choose a good set of

parameters for the training procedure, some optimization algorithms and values of learning rate and batch size were tried.

The models' performances were measured based on statistics such as the mean absolute error (MAE), mean squared error (MSE), Pearson's correlation coefficient (r), regression coefficient (R^2) and factor of two (Fac2). These metrics are described in the following equations:

$$MAE = \frac{1}{n} \sum_{i=1}^n |O_i - F_i| \quad (1)$$

$$MSE = \frac{1}{n} \sum_{i=1}^n (O_i - F_i)^2 \quad (2)$$

$$r = \frac{\sum_{i=1}^n (O_i - \bar{O})(F_i - \bar{F})}{\sqrt{\sum_{i=1}^n (O_i - \bar{O})^2} \sqrt{\sum_{i=1}^n (F_i - \bar{F})^2}} \quad (3)$$

$$R^2 = \frac{(\sum_{i=1}^n (O_i - \bar{O})(F_i - \bar{F}))^2}{\sum_{i=1}^n (O_i - \bar{O})^2 \sum_{i=1}^n (F_i - \bar{F})^2} \quad (4)$$

$$Fac2: 0.5 \leq \frac{F_i}{O_i} \leq 2 \quad (5)$$

where O_i is the observed value, $\bar{O}$ is the mean of all observed values, F_i is the forecasted value, $\bar{F}$ is the mean of all forecasted values and n is the number of samples. The factor of two returns the percentage of predictions in which the ratio $\frac{F_i}{O_i}$ are in the range [0.5, 2].

The best obtained model has seventeen inputs composed by five temporal variables, namely the year, month, day, hour and minute of the samples, and by the twelve parameters measured in the air quality station. The wind representation was converted from scalar values of direction and speed to vector components U and V , using equations (6) and (7). This transformation was made because the scalar representation could mislead the model, since direction values close to 0 degrees or to 360 degrees indicate that the wind is blowing in the same direction, although these values are numerically distant.

$$U = speed * \sin((270 - direction)(\frac{\pi}{180})). \quad (6)$$

$$V = speed * \cos((270 - direction)(\frac{\pi}{180})). \quad (7)$$

Before model fitting, all inputs and their ground truth targets were normalized between -1 and 1. This procedure changes the data to a common scale, avoiding that one input have excessive importance in consequence of its value range (Tamas *et al.*, 2014). Once the output of the model is obtained, the variables are de-normalized.

To measure the efficiency of the proposed neural network the Persistence model was used as a reference, since it is commonly used as a baseline to evaluate the performance of a forecasting model. In this predictor, the forecasts for all time steps ahead are set as the current value, which can be expressed mathematically as $y(t+\Delta t) = y(t)$, where y is the forecast target and t is time (Zucatelli *et al.*, 2019).

All computational procedures were implemented using the *Python* language and some data science libraries like *pandas*, *matplotlib* and *scikit-learn*. Experiments with artificial neural networks were performed using the *TensorFlow* platform through its *Keras* high-level API (Application Programming Interface).

FINDINGS AND ARGUMENT

Table 2 summarizes the topology and characteristics of the MLP neural network that achieved the best results in the metrics evaluated. The training of this network used the Feedforward Backpropagation algorithm with Adadelta optimizer, learning rate of 0.394 and mean squared error as the loss function.

Table 2. Multilayer perceptron neural network topology.

Layers	Nodes	Function	Params.
Input layer	17	N/A	0
1 st Hidden layer	17	ReLU	306
2 nd Hidden layer	81	ReLU	1,458
3 rd Hidden layer	81	ReLU	6,642
4 th Hidden layer	81	ReLU	6,642
5 th Hidden layer	81	ReLU	6,642
6 th Hidden layer	81	ReLU	6,642
7 th Hidden layer	81	ReLU	6,642
8 th Hidden layer	81	ReLU	6,642
Output layer	24	Linear	1,968

A comparison between the metrics of the evaluated ozone forecasting models, using the test data set, is shown in Table 3. Values close to 0.0 are best for the MAE and MSE and values close to 1.0 are adequate for the r , R^2 and Fac2. A Pearson's correlation coefficient of -1.0 implies a negative linear correlation between the forecasted and the ground truth values, and a value of 0.0 implies that there is no linear correlation between these variables (Zucatelli *et al.*, 2019).

Table 3. Comparison table between ozone forecasting models using performance metrics over the test data set.

Model	MSE	MAE	r	R^2	Fac2
Persist.	299.6	13.1	0.171	0.029	0.623
MLP	104.7	7.6	0.659	0.435	0.820

The values of the metrics introduced on Table 3 refers to the models as a whole, considering all the

24 predictions at the same time. Thus, the proposed multilayer perceptron is an effective model, surpassing the Persistence model in all considered metrics as expected due to its simplicity. Table 4 and Table 5 presents the statistics for some forecasting horizons of the MLP model and of the Persistence model, respectively.

Table 4. MLP model metrics over the test data set for some forecasting horizons.

Step	MSE	MAE	r	R ²	Fac2
T+1	54.2	5.54	0.848	0.719	0.918
T+2	84.8	6.99	0.752	0.565	0.848
T+3	93.6	7.35	0.717	0.514	0.846
T+6	111.8	8.01	0.639	0.409	0.824
T+9	104.9	7.42	0.647	0.418	0.814
T+12	104.0	7.40	0.650	0.423	0.822
T+15	104.6	7.54	0.654	0.428	0.812
T+18	107.5	7.70	0.680	0.463	0.822
T+21	110.6	7.91	0.682	0.466	0.795
T+24	111.3	7.88	0.645	0.415	0.807

Table 5. Persistence model metrics over the test data set for some forecasting horizons.

Step	MSE	MAE	r	R ²	Fac2
T+1	32.8	4.2	0.909	0.827	0.949
T+2	88.6	7.0	0.755	0.571	0.860
T+3	152.3	9.3	0.581	0.337	0.769
T+6	314.9	13.4	0.135	0.018	0.663
T+9	372.8	14.8	-0.038	0.001	0.578
T+12	376.1	15.1	-0.046	0.002	0.537
T+15	397.3	15.9	-0.099	0.010	0.528
T+18	377.5	15.3	-0.044	0.002	0.516
T+21	273.6	12.7	0.242	0.058	0.612
T+24	190.9	10.0	0.474	0.224	0.723

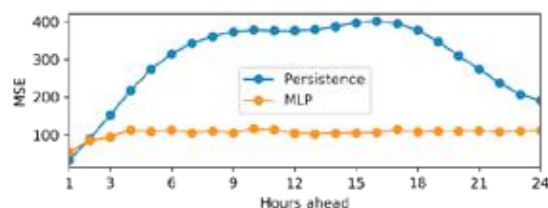


Figure 2. Comparison between MLP and Persistence models using mean squared error.

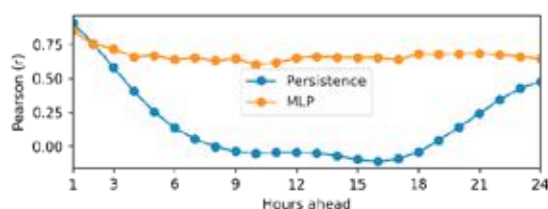


Figure 3. Comparison between MLP and Persistence models using Pearson's correlation coefficient.

With exception of the predictions for the first two hours ahead, in which the models have similar

results, the neural network outperforms the Persistence model in all other time horizons. This is shown on Figure 2 and Figure 3, where the mean squared error and the Pearson's correlation coefficient are used as metrics, respectively. Besides, the prediction errors of the MLP model have a more stable behaviour along the forecasted time steps. The MLP model accuracy is graphically shown in Figure 4, Figure 5 and Figure 6, where ozone concentration forecasts are displayed for 1 hour ahead, 12 hours ahead and 24 hours ahead in a period of approximately 6 days of measurements. The blue lines represent the actual ozone concentrations and the orange lines represent predictions of ozone concentrations.

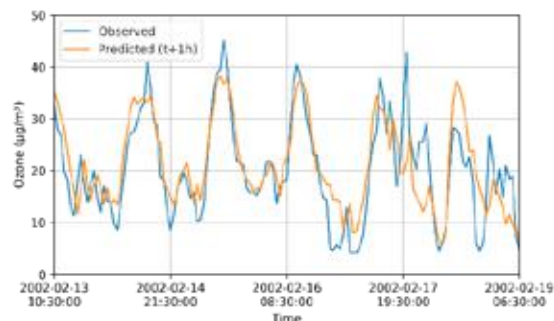


Figure 4. MLP predictions 1 hour ahead for a six-day period in February 2002.

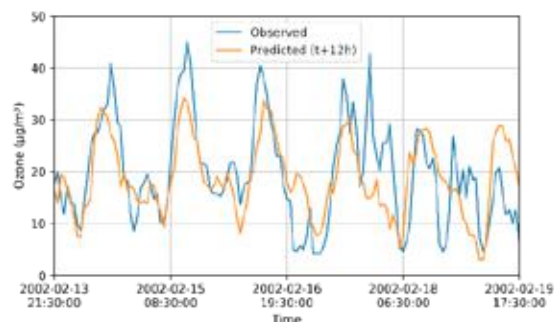


Figure 5. MLP predictions 12 hours ahead for a six-day period in February 2002.

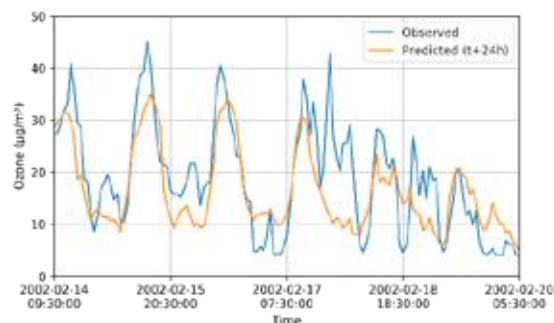


Figure 6. MLP predictions 24 hours ahead for a six-day period in February 2002.

CONCLUSIONS

The amount of data used in this study was relatively small compared to the scale generally used in the deep learning field, where thousands and even millions of samples are often applied in model training. Furthermore, only data from a few months of a single year were used, indicating that greater generalization and better performance can be achieved with a larger number of samples that better represent the behavior of tropospheric ozone over time.

However, the results indicated a reasonable performance for the proposed forecasting model, which can be used by authorities and citizens to take preventive measures that avoid imminent health risks due to O₃ exposure. Moreover, it has been shown that deep learning techniques can be successfully applied to hourly forecasting of ozone concentrations in urban areas. Once such models are trained and fit to the data, the inference process, i.e. the forecasting procedure, has a very low computational cost, meaning that it can be used as an alternative approach in comparison with numerical modelling systems, which require much more computational power.

ACKNOWLEDGEMENTS

This work was partially supported by the Bahia State Research Support Foundation (Fundação de Amparo à Pesquisa do Estado da Bahia - FAPESB), in the form of a Development of Technological Innovation grant for L. Alves in the project "Implantation of Infrastructure Research in Simulation and Computational Modelling in the State of Bahia using High Performance Processing", developed at Senai CIMATEC Supercomputing Center for Industrial Innovation.

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DEVELOPMENT OF A LOW-COST COLLABORATIVE PLATFORM FOR MONITORING AIR POLLUTION IN HIGH RESOLUTION

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Abstract: Air pollution poses a tremendous threat to human health and the environment, and urgent actions need to be taken to mitigate its effects. In order to implement effective measures and policies for that matter, trustful data must be available. One way of collecting data is by on-site measuring of air pollutants. Currently, this is achieved with very expensive and complex monitoring stations, which poses great difficulty for a more spread use of this instruments and for increasing spatial resolution air quality monitoring. The objective of this work is to develop a low cost collaborative IoT platform for monitoring air quality in high resolution. This platform aims the creation of a framework to promote air pollution monitoring at lower costs and complexity. A web system was developed to provide access to the data collected by low cost monitoring system which represents a node of a monitoring network. Data can be accessed from any mobile device or desktop computer in real time. Likewise, a low cost air quality monitoring node was developed for measuring NO₂, O₃, SO₂ and CO and sending this information to the web platform for visualization and processing. This work shows a first step towards on improving an air quality monitoring network in Brazil, thanks to its low cost and simplicity of implementation.

Keywords: Air pollution, air quality monitoring, internet of things, low cost sensors, ubiquitous sensing.

INTRODUCTION

Air pollution is the world's worst environmental health risk, according to the United Nations Environment Programme (UNEP, 2014). Its direct relation with different types of cancer as well as respiratory, cardiovascular and neurological diseases has already been shown by the World Health Organization (World Health Organization, 2005). In Brazil, several studies confirm the increase of the number of death caused by respiratory and cardiovascular diseases related to air pollution in vulnerable groups like elders and children (Toledo and Nardocci, 2011). Within these groups, those with lower socioeconomic conditions showed the highest rates of mortality.

However, despite of this scenario, air quality monitoring along Brazilian territory is still very limited. According to Oyama and Zamboni (Oyama and Zamboni, 2017) only 10 of the 26 Brazilian states actually perform air quality monitoring. There are a few governmental and independent initiatives to make air quality data more easily available (CETESB, 2019; INSTITUTO DE ENERGIA E MEIO AMBIENTE, 2019; INSTITUTO ESTADUAL DE MEIO AMBIENTE E RECURSOS HÍDRICOS, 2019). The air quality monitoring networks that have been implemented cover just some points of few Brazilian cities, and their performance over time is very often compromised due to lack of

maintenance and qualified staff. All this may result in deficient estimations of air pollution and poorly effective air quality management policies.

All the factors stated above, make the finding of alternative solutions for air quality monitoring crucial issue.

In that sense, the rise of lean and reliable low-cost sensors, and embedded platforms during the last decades, along with the establishment of the Internet of Things (IoT), has lead to a paradigm shift on the way of monitoring air pollution (Snyder *et al.*, 2013; Kumar *et al.*, 2015). Basically, the shift consists on combining these technologies, in order to making air quality monitoring simpler and cheaper, minimizing the impacts of their use on accuracy and reliability.

New methodologies, based on that paradigm, have arisen (Castell *et al.*, 2017; Liu *et al.*, 2019), but current state of the art makes them incapable of substituting reference monitoring stations which have traditionally been used for these purposes.

However, promising results have been shown on alternative applications, e.g.: supplementing existing reference monitoring data; source identification and characterization; and community education, awareness and engagement

in air quality issues (Williams *et al.*, 2014). In addition, low cost technologies have fostered the popularity of ubiquitous sensing, which has allowed the implementation of gas sensor networks with higher spatial resolution than traditional reference stations (Kumar *et al.*, 2015).

The objective of this work is to develop a low cost collaborative IoT platform for monitoring air quality in high resolution, at lower costs and lower complexity.

METHODS

A web platform was developed for providing access to real time data collected by low cost air quality monitoring systems (nodes). This platform can be accessed from mobile devices or desktop computers. The communication model is represented in the diagram on Figure 1.

Within the server, a Back-end application links the monitoring nodes to a Database, and the Database to a Front-end application. The Back-end application is also responsible for data processing, filtering and selection. It also puts the information into the Database for storage, and gets it from there for visualization through the Front-end application. Front and Back-end interaction is achieved via HTTP protocol.

The Front-end application provides an interface for final users visualization of the data collected by the monitoring nodes. Data may be visualized on maps or as time series (reports).

As a first step towards the implementation of a low cost air quality monitoring network, a low cost air quality monitoring node was developed, which measures ozone (O_3), carbon monoxide (CO), nitrogen dioxide (NO_2) and sulfur dioxide (SO_2).

The node is composed by four SPEC digital gas sensors for IoT: the DGS-03 968-042, the DGS CO 968-034, the DGS NO_2 968-043, and the DGS SO_2 968-038. Each sensor also provides readings of temperature and relative humidity.

Figure 2 illustrates the structure of the monitoring node. A NodeMCU 1.0 (ESP-12E module) board manages all the control, data acquisition and communication tasks. This board is based on the Espressif ESP8266 microcontroller, which is a highly integrated Wi-Fi System-on-Chip (SoC) integrating WiFi functionalities to a 32-bits RISC processor. The NodeMCU communicates with sensors over a RS485 serial bus, and collects the readings of gas concentration, temperature and humidity of each one of them. The information collected is then sent to the web platform, using the Rest convention over HTTP protocol, for online visualization and processing.

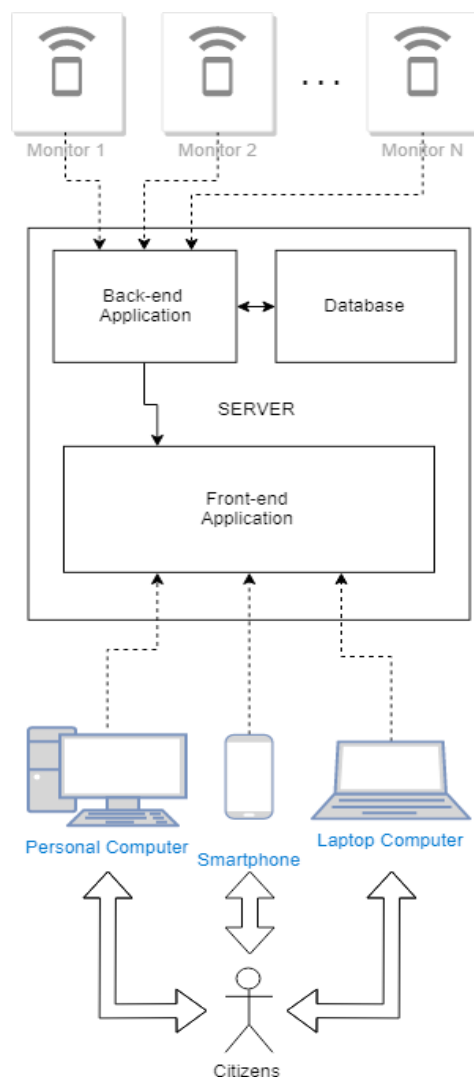


Figure 1. Communication model

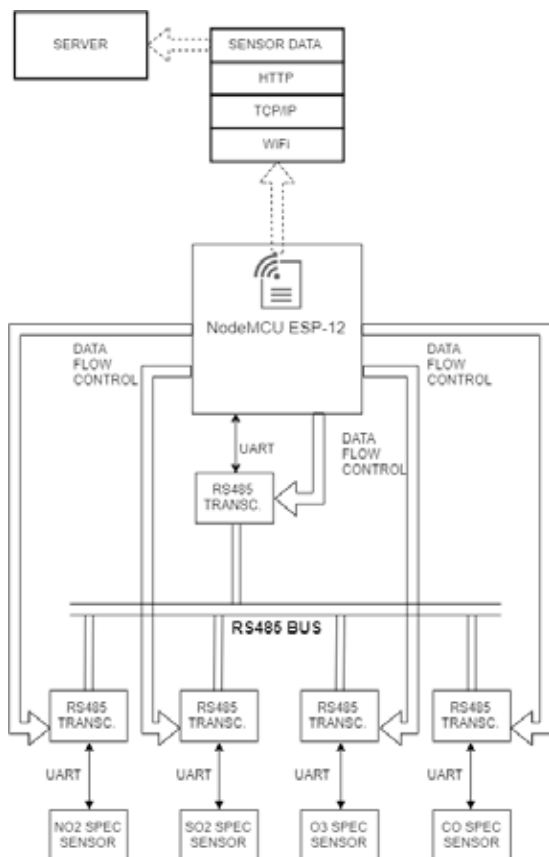


Figure 2. Monitoring node control and communication structure

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A collaborative IoT platform for air quality monitoring in high resolution was developed. A low cost air quality measurement node was also developed and installed at Federal University of Santa Catarina (UFSC). The web interface is user friendly; it presents interactive graphics of air quality monitoring stations over time, notifications, reports and other functionalities. It is expected that new sensors may be incorporated to the IoT platform, by several agents, as long as they satisfy pre-defined measuring requirements.

The collaborative platform, as the low cost monitoring network continues to expand. It would allow collecting air quality information in high spatial and temporal resolution with great potential of application along Brazilian cities. The data obtained may complement readings from reference stations, or bring preliminary air quality information where reference stations may be unfeasible. It may also contribute to involve citizens in environmental problems, like air pollution, and the searching for solutions to them.

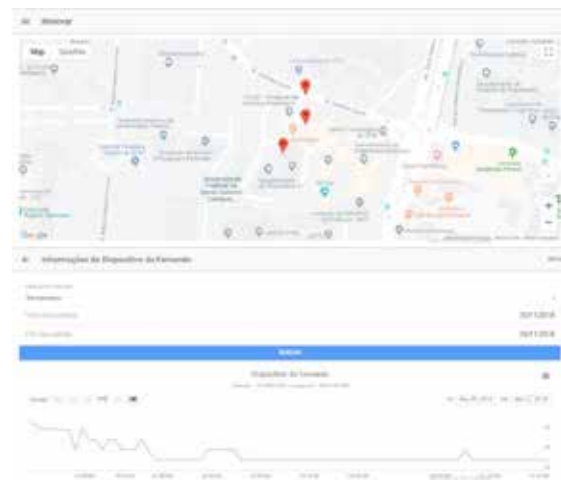


Figure 3. Web platform for real-time monitoring



Figure 4. Air quality monitoring node

CONCLUSIONS

The development of a low cost collaborative IoT platform for high resolution air quality monitoring was presented. The platform aims for the implementation of a framework for promoting air pollution monitoring at lower costs and complexity. All hardware and software is open and publicly available in order to encourage communities, schools and universities to engage in spreading a low cost air quality monitoring network. It is expected that air pollution data, with acceptable levels of accuracy and spatial resolution, will be available in an intuitive way.

Future works include the installation of 10 replicates of this node on different locations in the city of Florianópolis, SC. Likewise, the reliability of the readings from these sensors must be evaluated in terms of precision, repeatability, and robustness to real world conditions.

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ESTIMATING TOTAL SUSPENDED PARTICLES AND SETTLEABLE PARTICULATE MATTER USING CMAQ AEROSOL MODULES

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Abstract: In its original version CMAQ includes dynamics and transport of particulate matter (PM) up to 10 μm . This condition is intrinsically associated with issues of interest to developers and practitioners around world. Major concerns are directed to PM smaller than 10 μm , which are known to be of greatest concern to environmental and health conditions. However, specifically in the Grande Vitória (GV), in addition to the PM smaller than 10 μm , for reasons, such as discomfort of the population and dirtiness caused by dust deposition, there is also a concern with PM larger than 10 μm (super-coarse PM, SCPM), because total suspended particles (TSP) concentrations and settleable PM (SPM) deposition. Therefore, to suit GV's population expectations and needs, we have developed a complement to the CMAQ's original source code to enable the assimilation of SCPM emissions and their integration into transport, dispersion and deposition processes. This innovation enabled the CMAQ to calculate TSP concentrations and calculate SPM deposition including SCPM. The hypothesis assumed for the treatment of SCPM considers these particles are mostly (almost entirely) generated by mechanical processes and do not come from gaseous transformations (nucleation, condensation). Therefore, by origin and definition, they are included as coarse mode particles. Changes made in the source code are the inclusion of a new PM species to input super-coarse PM in emission file, called PMSC, and a new PM species for the transport calculations through the routines of the CMAQ, called APMSC. These changes did not alter the way that CMAQ compute the other species included in previous source code, all original algorithm was preserved and we focused only in the changes implemented in terms of SCPM. Obviously, whatever the physical process to be represented there are certainly exceptions, arising from an intrinsic condition of any atmospheric computational model: the attempt to represent the complex reality of atmospheric phenomena is supported by simplifications. That is, this case is not the only one and isolated, several parts of the CMAQ model are based on simplifying assumptions. Considering the assumptions and complements, we have obtained positive results based on the comparisons between TSP and SPM data modeled vs. measured by GV air quality network, that showed good agreement. We understand that the innovations made to include the computation of TSP concentrations and SPM deposition flow reached the adequate objective for the study of the GV air quality and analysis of the impacts arising from PM emission sources, especially considering the expectations of the population in terms of SPM.

Keywords: dust, deposition, improvement, model, particles, super-coarse.

INTRODUCTION

The Grande Vitória (GV) region located in the state of Espírito Santo, southeast of Brazil, has several issues regarding settleable particulate matter (SPM). Many people complain about settleable particles annoyance (Melo et al. 2015) what they call "black dust", in an association with particles emitted by mining and steel making factories. Due this issue, the environmental agency of Espírito Santo (IEMA) has a manual network measurement of SPM deposition flux based on ASTM D1739 - 98(2017) Standard Test Method for Collection and Measurement of Dustfall (Settleable Particulate Matter) in 10 sites over the GV region.

In this context, we believe CMAQ could be useful as a tool to assist in knowledge where are the areas most impacted and how is the deposition flux relation with industrial emission, adapting CMAQ to be able reading super coarse PM emissions (particulate matter larger than 10 μm , PMSC) and calculate advective transport (vertical and horizontal). In this paper, we present a study case of CMAQ modeling considering PMSC in GV region.

Add PMSC is the key for a representative SPM model since a mass of one super coarse particle is equivalent up to thousand small particles. CMAQ treats aerosol physics as a three-modal lognormal distribution to represent the Aitken, accumulation

and coarse mode (Binkowski and Roselle 2003). Each mode represents distinct populations of particles, distinguished by size or chemical composition (Whitby and McMurry 1997). CMAQ uses moment dynamic equation (MDE) approach to process affecting aerosols, internal and external process.

METHODS

A new aerosol specie was added in CMAQ aerosol module code to represent PMSC. Few changes also were made on the module that treats aerosol emissions. CMAQ uses lognormal parameters chosen by Binkowski and Roselle (2003) (D_g and σ_g) as (0.03 and 1.7) for Aitken mode, (0.3 and 2.0) for accumulation mode and (6.0 and 2.2) for coarse mode. We added an option size distribution as (20 and 2.2) for coarse mode to be used for particles emitted by fugitive sources like wind erosion and paved road sources.

GV emission inventory used in this study was adapted from emission inventory provided by IEMA (2011). PM emissions from vehicles both exhaust and paved roads and industrial are the major sources at region (Table 1). The study area (34 x 42 km, LL = 335588, 7726368; UR = 391299, 7800766, 23K, WGS84) was characterized as a computational domain subdivided in cells of 400 m. Figure 1 shows the delimitation of the study area for the CMAQ

modeling (Byun and Ching 1999) and the computational domains used for the WRF (Skamarock et al. 2008).

Table 1. PM emission rates (kg/h) of GV sources in 2010

Source	PM	PM ₁₀
Vehicles (exhaust and paved roads emissions)	2,904.78	1,389.81
Industrial	909.47	587.51
Logistics (ports and airports)	60.39	58.96
Others	27.73	13.24
Total	3,898.37	2,049.52

Adapted from IEMA (2011).

The WRF simulations were driven by GFS data with 0.5° spatial resolution and 6 h temporal resolution to generate the required initial and boundary conditions. The WRF output files were processed with the Meteorology-Chemistry Interface Processor (MCIP) which creates the required meteorological input data to run CMAQ. The Carbon Bond Five mechanism (CB05) was used as chemical mechanism for CMAQ, simulation and average concentrations obtained in GV were used for initial conditions (ICONS) and boundary conditions (BCONS). However, as PMSC has a short lifetime on atmosphere this specie was not considered as relevant to boundary conditions.

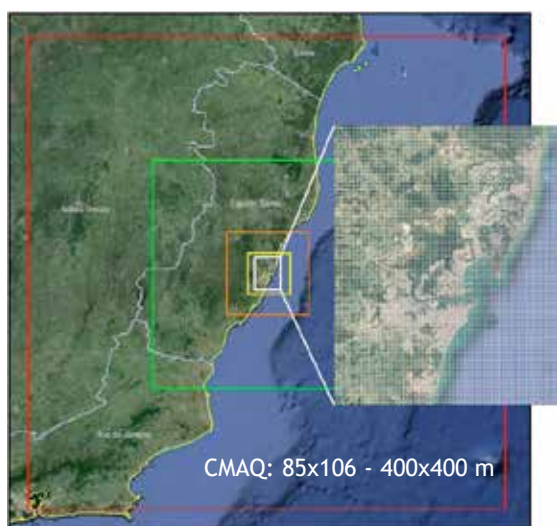


Figure 1. WRF and CMAQ domain study

The simulation considers the entire year of 2011, hourly. Calculated air concentrations were used to evaluate how CMAQ represents deposition flux on GV region.

FINDINGS AND ARGUMENT

Concentrations and deposition flux modeled using CMAQ were compared to air quality network stations over GV region, as shown by Figure 2.



Figure 2. Location of IEMA air quality network stations in GV.

Each location analyzed indicates a peculiar behavior of PM concentration and SPM deposition flux (Table 2). In station 1, CMAQ overestimated PM concentrations in 26% whereas overestimated deposition flux by 5%. In station 4, PM was overestimated by 4% and deposition flux underestimated by 21%. PM₁₀ has the same pattern, in station 1, CMAQ underestimated PM₁₀ in 3% and overestimated PM in 26% whereas station 5 overestimated PM in 2% and underestimated PM₁₀ by 20%.

Table 2. Comparison particle concentrations (µg/m³) and deposition flux (g m⁻²/30-day) between CMAQ results and Air Quality Network - AQN in GV.

Local	PM		PM ₁₀		Deposition flux	
	AQN	CMAQ	AQN	CMAQ	AQN	CMAQ
1	59.3	74.5	35.8	34.9	12.6	13.2
2	26.2	35.8	21.3	21.1	4.1	3.1
3	45.9	45.7	20.7	23.5	7.3	7.1
4	49.5	51.6	30.6	26.2	11.7	9.2
5	51.4	52.5	32.7	26.3	8.9	7.7
6	50.4	59.5	28.1	29.3	9.2	10.5
7	nd	43.3	nd	21.7	6.1	7.5
8	85.2	75.8	45.7	36.3	11.8	13.4
HS	nd	35.7	nd	19.2	7.5	6.8
IB	nd	30.7	nd	17.2	6.3	6.1

nd - no data available, HS: Hotel SENAC, IB: Clube Ítalo Brasileiro. Stations 1 to 8 corresponds to IEMA air quality monitoring network.

According to emission inventory, emissions from vehicles (paved roads and exhaust) and industrial are responsible for more than 96% of dust emission, as expected, these urban areas are most impacted by PM concentrations and deposition flux (Figure 3).

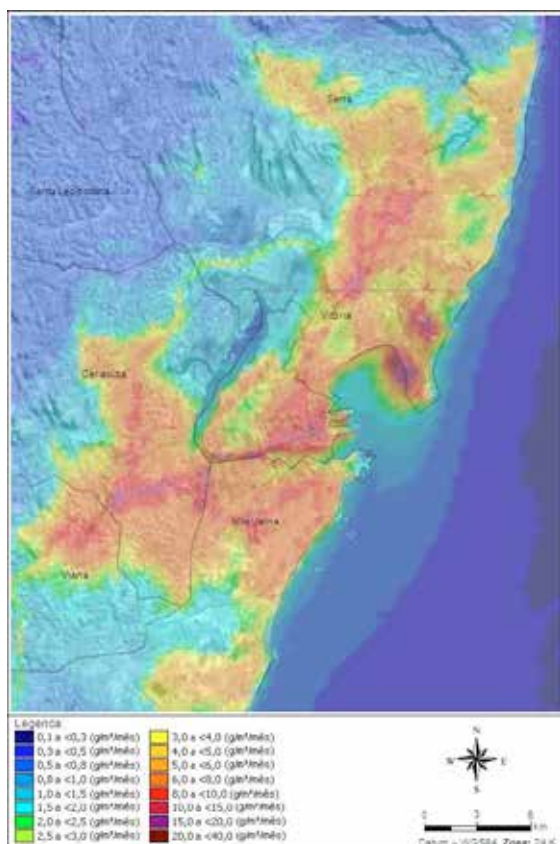


Figure 3. Average SPM deposition flux ($\text{g m}^{-2}/30\text{-day}$) modeled by CMAQ considering PMSC.

CONCLUSIONS

The first try using PMSC species to understand settleable particles dynamic showed CMAQ has potential to be a good tool helping to identify sensitive areas do measure PM concentrations and PM deposition flux.

We need more investigation to define coarse mode parameters, which are used in aerosol emission module, considering GV peculiarities. The values used in this study was a first guess and perhaps one solution could be inserting a size distribution data by each source type to represent emissions moments (M_0 , M_2 and M_3) instead of one fixed to all sources in the mode.

Besides, when modeling microscale resolution to obtain good results it needs a representative emission inventory, considering significative microscale sources. Also, it required WRF model considering high resolution terrain and land use data.

It is recommended more investigate to understand PMSC dynamic in short events, a WRF study to validate microscale resolution and sensitive modeling tests to understand PMSC boundary conditions influence.

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DEVELOPMENT OF A WEB PLATFORM AND KNOWLEDGE DATABASE FOR INDUSTRY EMISSION SELF REGISTER

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Abstract: Atmospheric pollution is one of the main causes of mortality due to respiratory and cardiovascular diseases. Historically, industries have been considered as important emitters. Santa Catarina is one of the Brazilian states without emission inventories, despite having a large industrial activity. Therefore, a development of a web based system for helping in the elaboration of industrial emission inventories may benefit Santa Catarina and many other Brazilian states. The objective of this work is to present the first user-friendly web system for registering the emissions from industries in the state of Santa Catarina, Brazil. The web system would provide a central database containing consolidated information about industry emissions within the state. Moreover, it makes this information more accessible for government and researchers. This system will help in the development of Industrial Emission Inventories. The software application was divided in two parts. One is responsible for user interaction and was build as a plug-in for Wordpress, while the other is a process for managing and storing information. With this architecture it is possible to change the user interface and to make integrations with other systems. Both parts were programmed mainly in PHP language and communication between them is achieved through POST methods. The proposed web based system provides an easy and automatic way to produce up-to-date industrial emissions inventories. Although it is based on state legislation only for industrial activity, it has a potential for expansion along Brazilian territory due to its flexibility and easy usage.

Keywords: Air pollution, emissions inventory, industrial emissions, web system.

INTRODUCTION

Atmospheric pollution is pointed as the main causes of respiratory and cardiovascular diseases. According to OMS, air pollution causes around 3.7 millions of premature death per year on worldwide, with 88% of them occurring in underdeveloped and developing countries (WHO, 2014). Since 2018, according to the resolution CONAMA 491/2018, every Brazilian state is responsible for elaborating its own Air Quality Management System (AQMS). Any AQMS is essential to the identification and quantification of major emitters. All this information is generally found in emission inventories, but only few Brazilian states actually elaborate them. Moreover, improving and periodically updating the emission inventories require an exhaustive work and considerable amount of resources, due to difficulties in collecting data in Brazil.

It is known that information access and its accuracy are essential elements for research and decision making processes. Nowadays, web systems provide great advantages in terms of the usability and easing of data access. In that sense, the development of an automated system for regular registration of emissions from industries is an efficient way for improving the availability and robustness of emission inventories.

This work proposes a new intuitive web system for elaborating and regularly updating industrial emission inventories. This software would keep a temporal record of emissions from all registered industries. This platform could be implemented in any Brazilian state.

METHODS

Programming Languages and Methodologies

The system was programmed mainly in PHP 7 language, which also allows to managing other programming languages. The system was designed in two modules: core and view. For that reason, a “Model View Control” (MVC) methodology was applied. The modules were built to run independently in different servers. The communication between modules is done using HTTP POST method with specific requisition patterns.

Core is constituted by “Model and Control” and follow object oriented programming. It is responsible for receiving, processing, sending, managing and storing data. Also, it contains traces of SQL in order to manage the database.

On the other hand, View is the interface of core and user. It contains JavaScript, HTML and CSS languages. The architecture is shown in Figure 1.

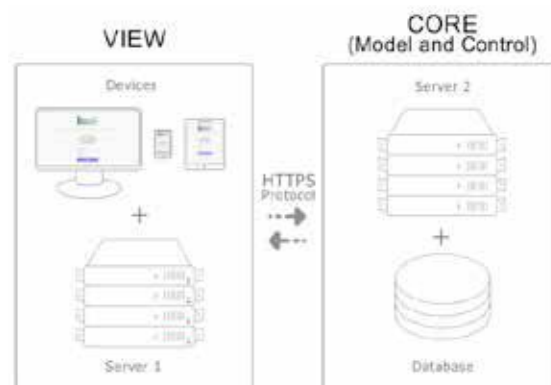


Figure 1. MVC structure and location of servers.

This view was created as a Wordpress plugin and it was improved using web framework Bootstrap v3.0. Another functions like fields completion were implemented using Leaflet JavaScript library and external APIs.

All communication is done using SSL certificates and HTTPS protocol, granting security during data transportation. Other strategies were used to prevent cyber-attacks.

Program Requirements

The program requirements were brought up by researchers of *Instituto de Meio Ambiente de Santa Catarina (IMA)* and *Laboratório de Controle e Qualidade do Ar (LCQAR)*.

Potential emitting activities were listed according to CONSEMA 98/2017 and 123/2018. The list of pollutants was created according to CONAMA 382/2016, CONAMA 436/2011 and SEMA 016/2014. The first version of the system was implemented.

Program structure

Users can create an account, register an Industry, register emission sources (chimneys) into each industry and manage this information (Figure 2). Address, Brazilian registry of legal entity (CNPJ), business name and activity are the main information required for registering new industries. For a new chimney to be registered, the system requires geographical coordinates (latitude and longitude), amount of emitted pollutant, operation time (hours of day, days of week and months of year), height of chimney, diameter of chimney, velocity and temperature of emission. The information of each source is registered in a database, permitting a temporal analysis of air pollutant emissions.

Pre-validation of input data is automatized by specific algorithms, which decreases human validation effort and prevents the database to

receive inconsistent or incorrect data, although, human validation is still necessary at some degree.

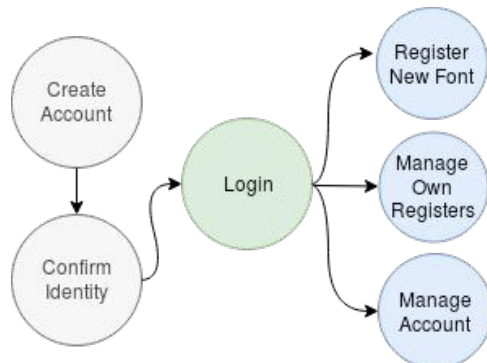


Figure 2. Functionality flow chart.

To secure data transport between modules, an HTTPS protocol is used (Figure 3).

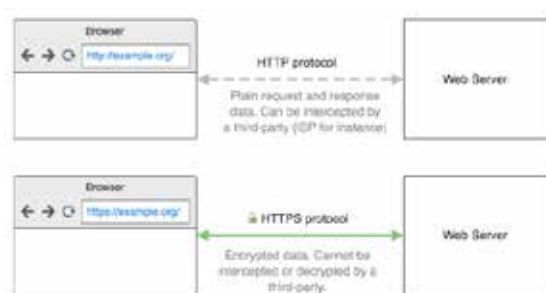


Figure 3. HTTP vs HTTPS.

Reference: AdGuard website, 2009.

Facilitating user access to the system is one of the most important aspects that needs to be checked when implementing self registering system interfaces. Thus, Bootstrap framework, external libraries and APIs were used to improve user interaction on view module. Also, autocomplete fields improve user experience and facilitates data validation.

Historical records of emission levels is an important information that needs to be considered on governmental analysis and air quality management. The system works creating temporal registers for each update of emission sources and industries on database. It allows temporal and geographical analysis of pollutants emitted by sources. Moreover, researchers can use this information to improve their Air Quality Models, and government may improve politics concerning air quality management.

Thanks to its decentralized core, the system, can support different views and serve as API for another web systems (see Figure 4). New versions can make possible the support for another states requirements (by specific laws) or can be generalized to all Brazilian territory.

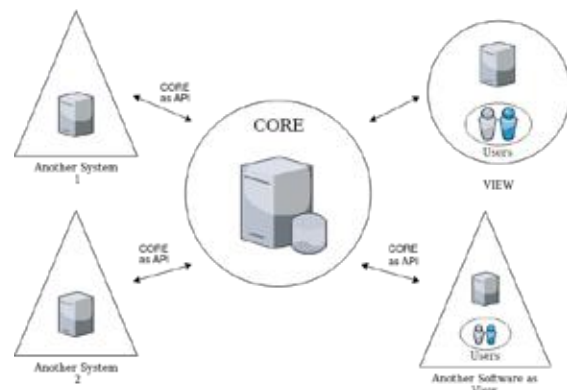
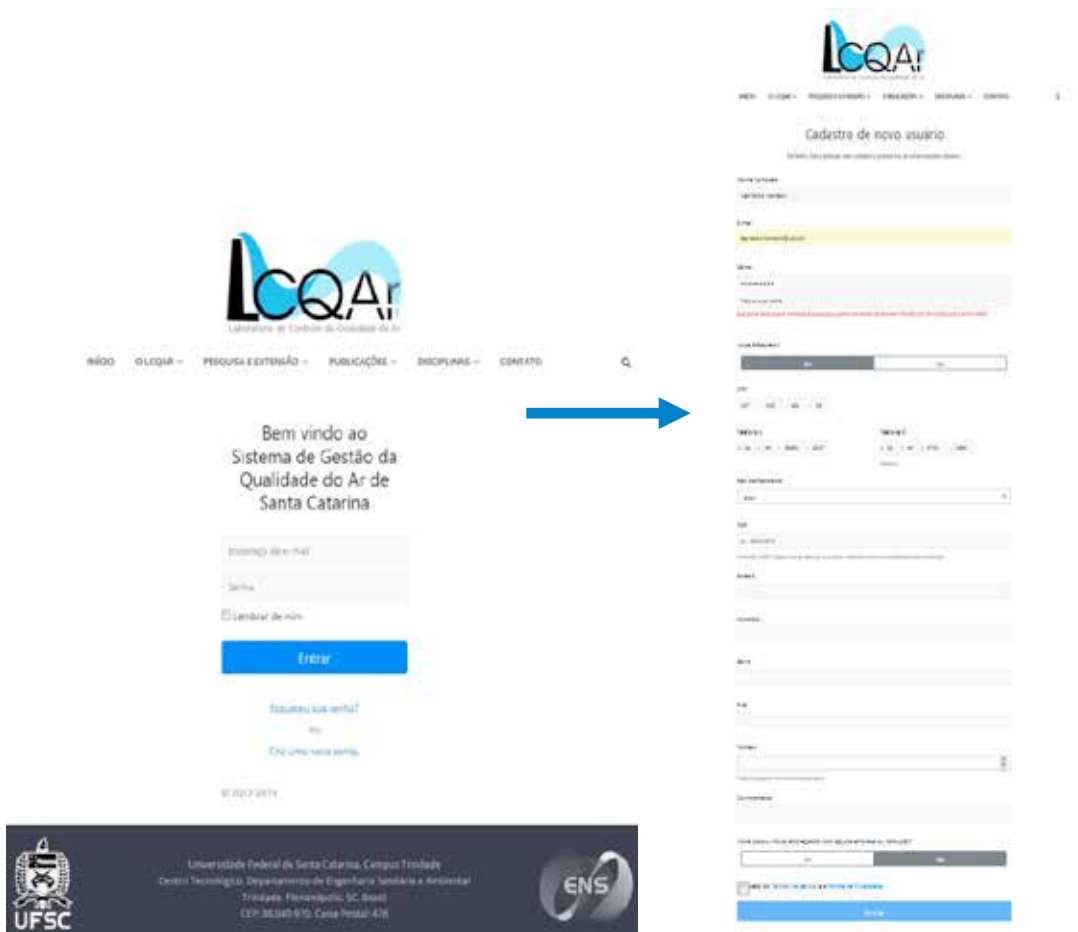


Figure 4. Core communication possibilities.

FINDINGS AND ARGUMENT

As an illustration of system functionality, figures 5 and 6 show the "create account" page of the emission inventories web system, and an example of a new source registration, respectively.



The image shows two screenshots of the LCQA website. The left screenshot is the login page, titled 'Bem vindo ao Sistema de Gestão da Qualidade do Ar de Santa Catarina'. It features a login form with fields for 'Email (e-mail)' and 'Senha', a 'Lembrar de mim' checkbox, and a blue 'Entrar' button. Below the button are links for 'Esqueceu sua senha?' and 'Criar uma nova conta'. The right screenshot is the 'Cadastro de novo usuário' (New User Registration) page. It contains a form with fields for 'Nome completo', 'E-mail', 'Senha', 'CPF', 'Data de nascimento', 'Sexo', 'Endereço', 'Cidade', 'UF', 'CEP', 'Telefone', and 'Complemento'. A blue arrow points from the login page to the registration page.

Figure 5. Creating an account on the web system of emission inventory

The image displays the 'Sistema de Gestão da Qualidade do Ar de Santa Catarina' (Air Quality Management System of Santa Catarina) interface. It is divided into three main sections, connected by blue arrows indicating the workflow.

Top Left: System Home

- Logo: LCQA (Laboratório de Controle da Qualidade do Ar)
- Navigation: HOME, O QUE É?, PROPOSTA DE INSTALAÇÃO, PUBLICAÇÕES, SISTEMAS, CONTATO
- Title: Sistema de Gestão da Qualidade do Ar de Santa Catarina
- Welcome message: Bem-vindo (sempre o que você deseja fazer)
- Buttons:
 - Adicionar fonte
 - Modificar informações
 - Criar dados para modelo
 - Consultar história de dados

Top Right: Data Entry Form

- Form fields:
 - Nome do ponto de emissão
 - Endereço atual e nome da rua (obrigatório)
 - Insira a altura da chaminé
 - Agora o diâmetro da chaminé
 - Insira a velocidade da saída da chaminé
 - Insira a temperatura de saída da chaminé
 - Indique a Latitude e Longitude do seu ponto de procura e clique sobre ele no mapa
 - Latitude
 - Longitude
 - Ver no Mapa
- Map: A map showing the location of the chimney.
- Form fields (continued):
 - Esta chaminé funciona, em média, quantos meses por ano?
 - Jan, Fev, Mar, Abr, Mai, Jun, Jul, Ago, Set, Out, Nov, Dez

Bottom Left: Calendar and Pollutant Selection

- Form fields:
 - Esta chaminé trabalha, em média, quantos meses por ano?
 - Jan, Fev, Mar, Abr, Mai, Jun, Jul, Ago, Set, Out, Nov, Dez
 - Esta chaminé trabalha, em média, quantos dias por semana?
 - Domingo, Segunda-feira, Terça-feira, Quarta-feira, Quinta-feira, Sexta-feira, Sábado
 - Quais as horas que a chaminé inicia e encerra a emissão, normalmente, durante os dias de funcionamento?
 - De [] até []
 - De [] até []
 - De [] até []
- Form fields (continued):
 - Clique nos poluentes que sua chaminé emite e preencha a quantidade
 - Material Particulado
 - NOx (como NO2)
 - SOx (como SO2)
 - Emissão Radiativa Total (como SO2)
 - CO (óxido de Carbono)
 - Pb (Chumbo)
 - Fluoretos Totais
 - SO2 (óxido de Enxofre)
 - Cl2 (cloro)
 - SO3 (óxido sulfúrico)
 - Cl (cloro)

Bottom Right: Pollutant List and Document Upload

- Form fields:
 - HCl (Ácido Clorídrico)
 - Carbono total
 - Substâncias gasosas orgânicas (Classe I)
 - Substâncias gasosas orgânicas (Classe II)
 - Dibenz-p-dioxinas (TEQ)
 - Dibenz-p-furanos (TEQ)
 - H2S (Sulfeto de Hidrogênio)
 - NH3 (Amônia)
 - Hexano
 - THS (como SO2)
- Form fields (continued):
 - Adicione o documento usado como base para preencher os dados acima em formato PDF.
 - Escreva com um arquivo
 - Adicionar
 - ☐ Aceito os Termos de Serviço e a Política de Privacidade.
 - Enviar
 - Sair

Figure 6. Adding a source on the web system of emission inventory

CONCLUSIONS

The need for information to elaborate Industrial Emissions Inventory of Santa Catarina has led the development of a new intuitive web system that permits self-registering of emission sources by users and industries. A first version was completed, which facilitates user access and experience.

All the information that would be generated, will be available for researchers and government. It is expected that the system will contribute to create diagnostics and to manage air quality. Likewise, new versions of the system could be implemented on different states, according to regional laws, or be extended to all Brazilian territory.

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Session 04

Model Evaluation and Analysis

INVESTIGATION OF RUN SEGMENTS IN WRF FOR A DRY MONTH IN MESOSCALE

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Abstract: Many works have been investigating the practice of breaking up the meteorological simulations of different models into several segments (days, weeks and month) in order to better represent the winds, temperature, water mixing ratio, and rainfall, for example, since a long-term continuous simulation may generate systematic error growth in long integrations. This work aims to investigate the influence of three run segments (5.5, 10.5, and 15.5 days) and a non-segmentation run on WRF results, comparing the temperature, specific humidity, wind speed and wind direction against 51 meteorological station in Minas Gerais (Brazil) for August 2015. Two nested computational domains with spatial spacing of 25 km and 5 km were used. Statistic indices and the Kruskal-Wallis test were used to determine if there are significant differences among the cases. The results showed that dividing the simulation into segments did not significantly alter the results for all the four variables investigated. However, as the runs are independent of each other, they can be integrated in parallel, what reduces the total time to complete the modelling. One-month simulation with non-segmentation showed to be adequate to be applied in WRF. Nevertheless, to improve the results it is recommended parametrization tests and evaluate the possibility of using nudging technique.

Keywords: WRF, run segments, mesoscale, Minas Gerais.

INTRODUCTION

One of the main objectives of the study of atmospheric contaminants behavior is to be able to mathematically describe their spatial and temporal distribution after being released into the atmosphere. This is performed through air quality modeling, that rely on meteorological fields as one of its main inputs (Seaman, 2000; Kumar et al., 2017).

Meteorological parameters, such as temperature, wind speed, wind direction and humidity are functions of time and space, that affect transport, diffusion, transformation and removal processes (dry and wet deposition) of chemical species. Meteorological processes, such as horizontal and vertical transport, turbulent mixing, convection, and diffusion, control or influence the behavior of emissions, chemical gas species and aerosols. In addition, the formation of secondary pollutants is directly affected by relative humidity, solar radiation, temperature and cloud presence (Seaman, 2000; Zhang et al., 2015).

For air quality modeling, numerical models that generate the meteorological fields are used, such as the Weather Research and Forecasting (WRF) model (Skamarock et al. 2008). However, long-term continuous simulation (i.e. one year) may generate systematic error growth in long integrations. Therefore, the practice to break up the simulation time into several segments has been investigated (Pan et al., 1999; Qian et al., 2003; Lo et al., 2008).

In this context, and considering the continuous development of the WRF model over the years, with new parametrizations, better topography data, and

finer gridded operational global analysis and forecast data, this paper aims to evaluate WRF results for August 2015, a dry month, in mesoscale 5-km grid spacing, testing four run segmentation scenarios (5.5-day, 10.5-day, 15.5-day, and non-segmentation). The results may be valuable to define the best approach to adopt in WRF for mesoscale grids, and in consequence, improve air quality model results. Hourly results were statistically compared to 51 surface meteorological monitoring stations.

METHODS

The simulations of the meteorological fields were performed using WRF v. 3.9.1.1. Two nested computational domains (Figure 1) were used covering Minas Gerais state (586,522.1 km²) (Brazil): the larger domain (D01) has a grid spacing of 25 km with 75 × 65 grid cells in the longitudinal and latitudinal extensions, respectively, forming a domain of 1,875 × 1,625 km, centered at 18.389° S; 45.569° W coordinates. The second domain (D02) has a grid spacing of 5 km with 311 × 261 grid cells in the longitudinal and latitudinal extensions, respectively, forming a domain of 1,555 × 1,305 km. The vertical structure was represented by 32 vertical levels, with the nearest layers being more refined.

Topography data provided by the United States Geological Survey (USGS) GMTED2010 and land use from Moderate Resolution Imaging Spectroradiometer (MODIS), both with a resolution of 30 arcsec, were used. The initial and boundary conditions were obtained from the National Center for Environmental Prediction (NCEP) Global

Forecast System (GFS) final (FNL) with a six-hour time resolution, 26 vertical levels, and a horizontal resolution of 0.25×0.25 degrees (ds083.3). Table 1 summarizes the spatial, physical and dynamic parameters used in WRF. The Cumulus parametrization was applied just for the coarse domain. The physical parametrizations were based on previous tests, and the time step used was 150 s.

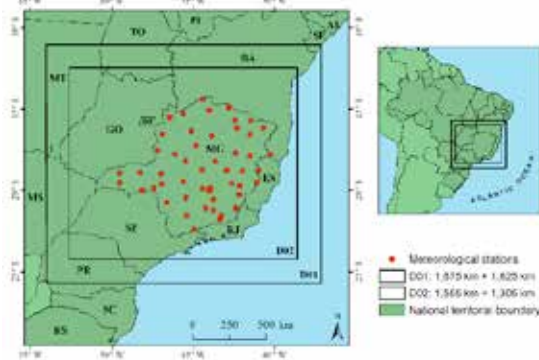


Figure 1 - WRF domains and meteorological monitoring stations.

Table 1: Spatial, physical and dynamic parameters for WRF.

Spatial parameters		
Grid spacing	25 km	5 km
Column numbers	75	311
Row numbers	65	261
Vertical layers	32	
Grid center	18.389° S; 45.569° W	
Physical and dynamic options - WRF v. 3.9.1.1		
Microphysics	WDM5	
Longwave Radiation	CAM scheme	
Shortwave Radiation	CAM scheme	
Surface Layer	Revised MM5 Monin-Obukhov	
Land Surface	Noah-MP Land Surface Model	
Planetary Boundary layer	Shin-Hong	
Cumulus	Grell-Freitas	
Diffusion/dissipation/ advection	3rd order Runge-Kutta	
Turbulence and Mixing	2nd order diffusion term	
Eddy coefficient	1st order Smagorinsky scheme	

It was considered a run with non-segmentation (ID 1), and three overlapping segmentations: 5.5-day (ID 2); 10.5-day (ID 3); and 15.5-day (ID 4). The meteorological modeling validation was performed by comparing hourly modeled results with surface data observed by 51 meteorological stations of the National Institute of Meteorology in Brazil (INMET) over Minas Gerais (Figure 1), using the statistical indices and benchmarks suggested by Emery et al.

(2001): Mean Bias (MB); Mean Error (ME); Root Mean Square Error (RMSE); and Index of Agreement (IOA). In order to compare the study cases, the Kruskal-Wallis non-parametric statistic test (Kruskal and Wallis, 1952) was performed. The significance of the teste considered was 0.05.

FINDINGS AND ARGUMENT

Regarding synoptic events, just one high pressure event occurred in August 2015 (Aug. 05th). The presence of high pressure is expected because it is a climatological positioning in winter. Therefore, the period chosen for this analysis can be considered representative for the dry season.

The benchmarks for specific humidity are presented in Figure 2 (left side), which was well simulated in all cases. Regarding the 51 meteorological stations, for MB two stations presented values outside the benchmark ($\leq \pm 1 \text{ g kg}^{-1}$) for ID 1, one station for IDs 2 and 3, and three stations for IDs 4. For ME, a similar distribution of the index was observed for all IDs, and except for one, all stations attended the benchmark ($\leq 2 \text{ g kg}^{-1}$). From the hypothesis test, there were no significant differences among all cases. The p-value found was 0.4019 for MB, 0.9630 for ME, and 0.3238 for IOA. This means that dividing the simulation into segments did not significantly alter the specific humidity results.

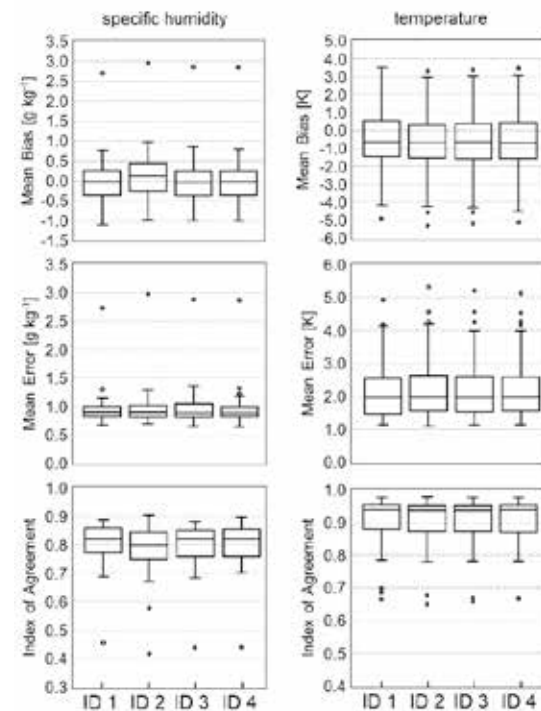


Figure 2 - Benchmarks for specific humidity (left side) and temperature (right side) for non-segmentation (ID 1), 5.5-day (ID 2), 10.5-day (ID 3), and 15.5-day (ID 4) segments.

Figure 2 (right side) shows the benchmarks for temperature. For MB, less than a quarter of the stations reached the benchmark interval ($\leq \pm 0.5$ K). All cases presented the median ME near the benchmark (2.0 K). For IOA, all IDs presented most of the meteorological stations attending the requested value (> 0.8). From Kruskal-Wallis test, it was observed no statistical relevant differences among the IDs for all three benchmarks. The p-value found was 0.9280 for MB, 0.9797 for ME and 0.9712 for IOA.

The results for wind speed are shown in Figure 3 (left side). For MB, just a fifth of meteorological stations reached the benchmark ($\leq \pm 0.5$ m s⁻¹). The median was above 1.2 m s⁻¹, with the mean value around 1.0 m s⁻¹, showing an overestimation of the wind speed. Shimada et al. (2011) found that the annual mean wind speed simulated by the WRF had a “remarkable positive bias” near surface. Moreover, using other PBL schemes did not reduce the positive bias. Avolio et al. (2017) and Albuquerque et al. (2018) also found an overestimation of the wind speed, for all PBL schemes tested in the study of Avolio et al. (2017). Previous parametrization tests carried out in the present work corroborate the results found by Shimada et al. (2011) and Avolio et al. (2017). The PBL schemes tested showed to be insensitive to reduce the wind speed bias. The cases also presented similar results for IOA and RMSE, including the variability of indices. Statistically, there was no difference among all cases studied for MB, IOA and RMSE (p-value of 0.0.9965, 0.9998, and 0.9984 respectively).

The benchmarks for wind direction are presented in Figure 3 (right side). Around 11 of the 51 monitoring stations reached the benchmark for MB ($\leq \pm 10$ degrees). MB results were between -20 and 20 degrees in around 50% of the stations, while median and mean were around -20 degrees. It can be understood that the model tends to move, on average, wind anticlockwise in a wind rose. The ME benchmark (< 30 degrees) was reached for few stations (3 or 4), with mean and median values around 51 degrees. Around 50% of the meteorological stations presented CCC above 0.5, value obtained as median for all cases. From the hypothesis test, there were no significant differences among all cases. The p-value is 0.9989 for MB, 0.9987 for ME, and 0.9998 for CCC.

Jiménez and Dudhia (2013) showed that differences between observed and modeled wind direction depend on wind speed, with higher velocities leading to better representation of the direction. Additionally, simulations in a complex terrain domain present “larger systematic differences between model and observations”. Zhang et al. (2013) and Mughal et al. (2017) also concluded that

complex terrain affects the wind speed and wind direction predictions. Minas Gerais is a plateau where altitude varies from 100 to 2800 m, and flows are relatively weak, despite the model overestimation of wind speed. Hence, a limitation of the model to better represent the wind direction can be inferred. From previous parametrization tests, different PBL schemes showed to be inefficient in improving the wind prediction.

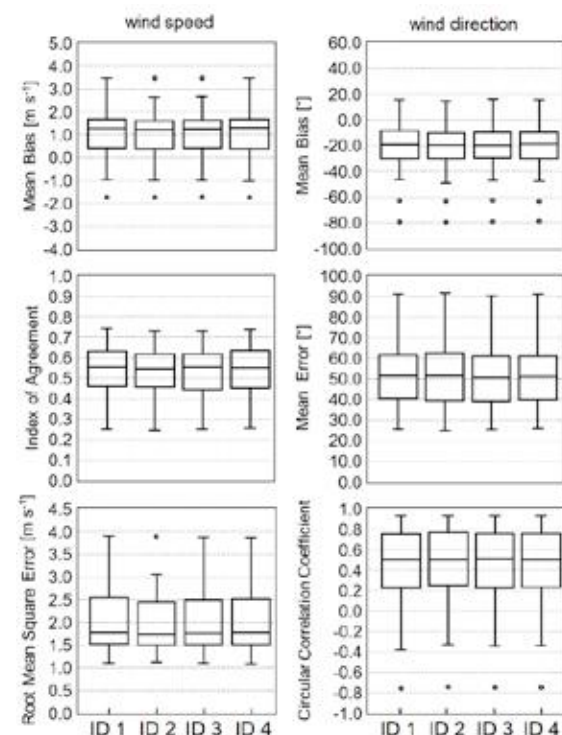


Figure 3 - Benchmarks for wind velocity (left side) and wind direction (right side) for non-segmentation (ID 1), 5.5-day (ID 2), 10.5-day (ID 3), and 15.5-day (ID 4) segments.

CONCLUSIONS

Meteorological spatially refined modeling is a critical requirement for air quality managers. The 5-km grid spacing used in this work proved to be adequate to represent the meteorological surface variables. Sensitivity simulations were conducted where run segmentations were evaluated. Our study demonstrates that breaking up a month simulation into small segments did not improve results. The Kruskal-Wallis test revealed that there is no significant difference between the continuous month simulation and those carried out in 5.5-day, 10.5-day, and 15.5-day overlapping segments. Furthermore, this test is shown as an important tool for applications in environmental data, when the objective is trying to identify significant differences among populations data.

ACKNOWLEDGEMENTS

Authors acknowledge CAPES.

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ASSESSMENT OF WRF URBAN SURFACE PARAMETERIZATION OVER A DENSELY OCCUPIED AREA

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Abstract: Urbanized regions have the potential to modify, locally or regionally, energy fluxes balance between the surface and the atmosphere by the land use changes. The urban boundary layer (UBL) features are the results of the fluxes of mass, energy and momentum exchange between the planetary boundary layer (PBL) air with the city structure, being, mainly affected by buildings disposition, presence of vegetation and anthropogenic activities. The Weather Research and Forecasting (WRF) model when coupled with urban canopy schemes such as the Building Effect Parameterization (BEP), can simulate more realistically the urban atmospheric processes, determining heat, moisture and momentum distribution, both horizontal and vertically. Thereby, this survey had as a main objective to evaluate the effect of BEP's urban canopy scheme coupling to WRF, denotated as uWRF, on the air temperature and surface energy fluxes of the Metropolitan Area of Belo Horizonte (MABH) - Brazil. To a better representation and differentiation of urban areas, were applied the Level 0 Local Climate Zones (LCZ) classification. Land use and land cover of uWRF were then updated and modeled results compared to the bulk configuration (control). The numerical simulations were performed for a period of five days in September of 2017 by WRF model version 3.9.1.1. It was seen that default model suppresses latent heat flux for the urban cells, resulting in a more pronounced nighttime temperatures, up to 1.1°C. In contrast, it was verified that the uWRF modeled higher temperatures for a high-rise area at midday (up to 2,9°C) than the bulk approach, possibly due to the radiation trapping and worsen ventilation conditions. Coupled model also proven its ability in differentiating urban classes from the LCZ classification, showing BEP is sensible to the urban canopy parameters adopted.

Keywords: Weather Research and Forecasting, Building Effect Parameterization, Local Climate Zones, Surface energy fluxes, Metropolitan Area of Belo Horizonte.

INTRODUCTION

In 2018, an estimated 55% of the world's population lived in urban settlements (UN, 2018). Population growth has intensified land use change by the expansion of urban areas. Variations in surface features are capable to interfere in the energy balance causing local meteorological changes (Oke et al., 2017).

The urban boundary layer (UBL) features are the results of the fluxes of mass, energy and momentum exchange between the planetary boundary layer (PBL) air with the city structure, being, mainly affected by buildings disposition, presence of vegetation and anthropogenic activities (Martilli, 2014). Capturing these effects on local meteorology using numerical models has been a growing area of study. The Weather Research and Forecasting (WRF) model when coupled with urban canopy models (UCM) such as the Building Effect Parameterization (BEP), can simulate more realistically the urban atmospheric processes. Developed by Martilli et al. (2002), the module BEP (Building Effect Parameterization) is a multi-layer UCM that recognizes the three-dimensional nature of urban surfaces and the fact that buildings vertically distribute heat, moisture and momentum

through the whole urban canopy layer, which allows for additional interaction of buildings (both the vertical and horizontal surfaces) with winds, temperature, turbulent kinetic energy (TKE), as well as the absorption, reflection, emission by building walls and roads (Chen et al., 2011).

Given human agglomeration in urban areas is a worldwide trend, it is imperative the need to test available tools for analyzing the urban coverage influence on the processes that dictate the meteorological conditions. Thereby, this survey had as main objectives to evaluate the effect of BEP's urban canopy scheme coupling to WRF, denotated as uWRF, and its application in the study of the Metropolitan Area of Belo Horizonte's (MABH) urban climate, the seventh most populated metropolis in South America with 5.3 million inhabitants, and for which temperature increases have been verified through the years, being, possibly, related to the changes on land cover.

METHODS

The meteorological simulations were performed for five (05) days of September of 2017, during a dry season, by the non-hydrostatic, mesoscale Weather Research and Forecasting model, version 3.9.1.1. Three nested domains,

centered at the same coordinate, have been set up (Fig. 1): a larger domain on 25 km spatial resolution, the second domain on 5 km resolution and the innermost domain on 1 km resolution. The initial and boundary conditions were provided by the National Centers for Environmental Prediction (NCEP) Global Forecast System (GFS) final analysis data on a $0.25^\circ \times 0.25^\circ$ horizontal resolution. It was considered a warm-up period of 24h. To take full advantage of the urban parameterizations, a vertical resolution of 44 eta levels was used, in which the first 16 levels are in the first 500 m, with the depth of the lowest level being approximately 10 m above the ground. The parameterizations chosen to simulate the meteorological conditions of the MABH were based on the best result obtained after twenty-two simulations. Physical schemes used were Lin (Purdue)(microphysics), RRTMG (short and longwave radiation), Eta (surface layer), Noah land-surface model (land surface model), BouLac (planetary boundary layer) and Betts-Miller-Janjic (cumulus).



Figure 1. Nested domains used on simulation by WRF and uWRF.

It was considered two surface parameterizations: default (MODIS + Noah LSM) and urban (Local Climate Zones + multi-layer Building Effect Parameterization). The Local Climate Zones (LCZ) represent a generic description of land use and occupation proposed by Stewart and Oke (2012). Such representation was applied in the classification of the urban areas and used to initialize BEP. The effect of BEP's urban canopy scheme activation in WRF, denoted here as uWRF, was observed from the modeled air temperature (at 2m) and surface energy fluxes of the Metropolitan Area of Belo Horizonte (MABH).

FINDINGS AND ARGUMENT

During the daytime period, it is observed that the differences produced in the urban area by the BEP activation presented smaller magnitude than at night (see Figure 2). Apparently during the day, the various classes of urban land use and occupation are not capable of causing different

patterns of temperature near the surface due to the instability conditions caused by solar irradiation, preventing the stratification of the atmosphere and the development of the urban climate. However, during midday it is possible to observe a heating core in the south-central region of Belo Horizonte, classified as LCZ 1. The higher temperatures may be related to the enhancement of radiation trapping due to the increase of building heights and density, and with worsen ventilation conditions. The observed differences presented a maximum value of 2.9°C . In the other regions of the RMBH, such effects were not observed since much of the region was classified as non-verticalized LCZs. For the night period, it is observed that, in general, the differences are negative, which indicates that the temperatures produced by the standard version (control) are higher than those modeled by the urban version. The greatest negative difference between the simulations was 1.1°C , at 18h (local time).

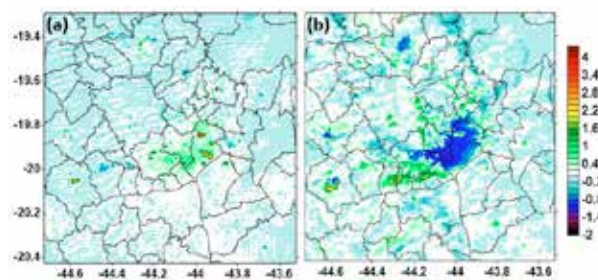


Figure 2. Mean air temperature (2m) difference ($^\circ\text{C}$) between uWRF and WRF for 12h (a) e 18h (b) (local time).

As the temperature can be influenced by other factors, the surface heat fluxes were also plotted in order to verify the impact of the activation of the BEP module in conjunction with the update of the urban area. Day and nighttime trends were represented by the fluxes of 15h and 21h, respectively (local time). In Figure 3 (day), are shown the results for latent (QE) and sensible (QH) fluxes modeled by WRF and uWRF. For the center of the domain, where the urban spot is located, the latent fluxes simulated by WRF were null, differently from what occurred in uWRF. Such behavior can be attributed to the different treatment given by BEP to cities. When working with the concept of urban fraction, the module allows the representation of urban vegetation in the cell while in the standard approach the whole area is considered exclusively urban and homogeneous. It is also observed that the BEP was able to differentiate the degree of occupancy of each LCZ. In the south-central region of Belo Horizonte, where the two regions of LCZs 1 are located, a lower latent heat flux was verified when compared to areas occupied by other classes.

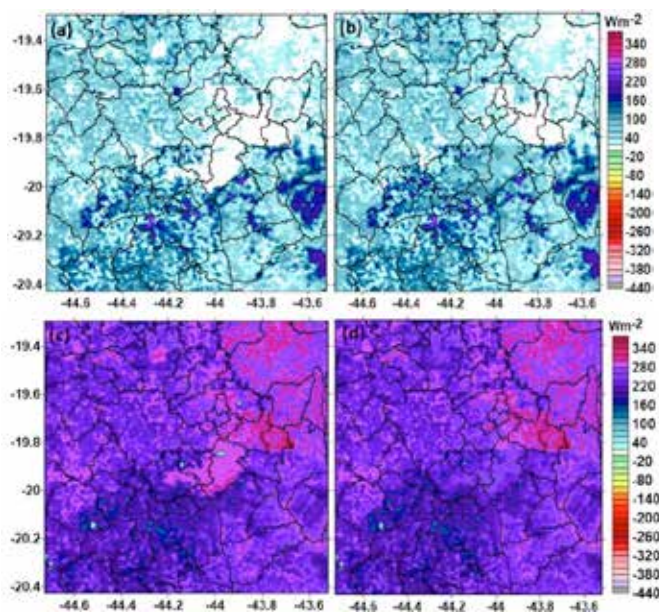


Figure 3. Mean latent heat flux modeled by WRF (a) and uWRF (b); and mean sensible heat flux modeled by WRF (c) and uWRF (d) - 15h (local time).

For the areas where latent heat was equal to zero, the highest sensible heat fluxes (b) were estimated, with a maximum of approximately 370 W.m^{-2} , in both cases. In a study for the city of Houston in the United States, Lee et al. (2011) found that for a low-density urban area where QE was suppressed, the Noah LSM model overestimated the sensible heat at a maximum of 200 W.m^{-2} during the day when compared to the observed data. In Figure 4, it is shown the results for the sensible heat flux during nighttime (21h) modeled by WRF (a) and uWRF (b).

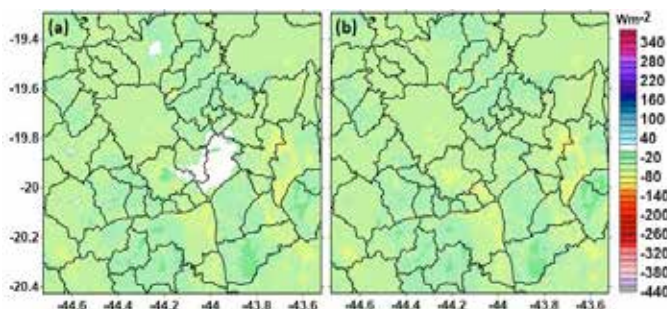


Figure 4. Mean sensible heat flux modeled by WRF (a) and uWRF (b) - 21h (local time).

It is possible to observe that fluxes are negative for most of the domain, where the exceptions are related to the urban spot in the center, for the standard simulation (a). In this case, the modeled fluxes are positive (maximum 22 W.m^{-2}), indicating that at 21h the surface is still able to increase air temperature, possibly due to the heat stored during the daytime period.

CONCLUSIONS

The present work had as general objective to analyse the modifications produced by coupling the urban scheme BEP in the meteorological model WRF, for purposes of evaluation of the tool. Regarding the effects produced by BEP's activation, it was observed that the results provoked in the study area were distinct and very dependent on the land use classification, being able to recognize different types of occupation and produce coherent results. Still within the scope of the differences between the standard and urban approaches, it is important surpass the common sense that the activation of an urban canopy scheme always results on temperature increase. The urban module is only more complex and realistic in representing the processes that take place in the cities.

It is recommended the analysis of the surface energy fluxes from others time periods.

ACKNOWLEDGMENTS

This research was supported by the following institutions, in alphabetical order: Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG).

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VALIDATION OF THE MODELING SYSTEM WRF / CALMET APPLIED TO THE DISPERSION OF PARTICULATE MATTER (PM₁₀) EMITTED BY THE BLASTING OPERATION IN ONE COAL OPENCAST MINE IN THE DEPARTMENT OF CESAR, COLOMBIA.

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Abstract: At present in the north of Colombia country there are many coal opencast mines operating on the Andes mountain feet. The topography in this zone is characterized by important peaks and large valleys and this allow the occurrence of micrometeorological phenomena that have influence in the air quality of the area. All the coal opencast mines produces approximately 80 ton of high quality coal per year, but the environmental impacts of this activity to the air quality are very serious.

The WRF / CALMET programs were applied in order to model the meteorologicals characteristics present in this area and to estimate the dispersion behavior of the particulate material (PM₁₀) generated by the coal opencast mine (PLJ). The results obtained in the meteorological modeling were validated with the data from weather stations of the air quality monitoring system of the area. In addition, in this job was studied the behavior of the dispersion of particulate material (PM₁₀) with the CALPUFF model and its impact on population centers closets to this mining project; with an analytical approach in one of the most important sources of particulate material in the coal opencast mining, "blasting". The runs of the programs were obtained in the laboratories of the PFA (Applied Physicochemical Processes research group) in the University of Antioquia (Medellín), It taking as study period the year 2014 (a year characterized by marked dry seasons and intense rains) One of the most accurate grids of the meteorological model WRF was used in the interest area (3 km) and the emission factors were calculated based on the amount of coal mined.

Keywords: coal opencast mining, blasting, WRF, CALMET, CALPUFF.

Resumen: En la zona carbonífera del departamento del Cesar, Colombia; se aplicaron los programas WRF/CALMET-CALPUFF con el fin de modelar la meteorología presente en la zona de estudio y realizar un diagnóstico del comportamiento de la dispersión del material particulado (PM₁₀) generado en el proyecto minero PLJ (ubicado en el área de la zona minera más cercana a la formación montañosa del Perijá). Se validaron los resultados obtenidos en la modelación meteorológica con los datos de las estaciones meteorológicas del sistema de vigilancia de calidad de aire de la zona. Además, se estudió el comportamiento de la dispersión del material particulado (PM₁₀) arrojado por el modelo CALPUFF y su impacto en los centros poblados cercanos a este proyecto minero; con un enfoque analítico en una de las fuentes de gran importancia dentro de las actividades de minería a cielo abierto, "la voladura". Las corridas se obtuvieron en los laboratorios del grupo de investigación Procesos Físicoquímicos Aplicados PFA de la Universidad de Antioquia (Medellín), tomando como periodo de estudio el año 2014 (un año caracterizado por épocas secas marcadas y lluvias intensas). Se usó una de las grillas de mayor precisión del modelo meteorológico WRF en la zona de interés (de 3 km) y los factores de emisión fueron calculados en base a la cantidad de carbón explotado en las minas de estudio.

Palabras claves: minería de carbón a cielo abierto, voladura, WRF, CALMET, CALPUFF

INTRODUCTION

Meteorology is the science on which the air quality models used today are based; although in the carboniferous zone of the department of Cesar there is a series of surface meteorological stations that can give us an idea of how the meteorology behaves in the zone. These do not have radiosonde campaigns for the measurement of meteorological variables in the vertical. It is for this reason that it is necessary to develop and/or apply modeling tools that adequately represent the meteorology of the study area and that make it possible to know the behavior of the dispersion of pollutants present in it. The mining zone of the department of Cesar currently has seven mining projects in operation, of which two are located closer to the mountainous formation of the Serranía del Perijá, which is considered the eastern strip of the mining zone, these are: La Jagua Project (PLJ) and Norcarbon.

The present work focused on studying the impact generated by the blasting operation of La Jagua Project (PLJ) on the surrounding populated centers. The meteorological model WRF (Weather Research and Forecasting) is a non-hydrostatic model of short-term atmospheric prediction that solves the dynamic equations of the atmosphere by the numerical methods and with a higher resolution than the global models using reanalysis information from the National Center for Atmospheric Research (NCAR). The formulation of a non-hydrostatic dynamic allows the model to be used effectively to represent phenomena with resolutions of very few kilometers (up to 3 and 1 km). It incorporates the most modern and realistic parameterization schemes of the physical processes related to: atmospheric radiation, microphysics of clouds and precipitation, convection by clusters, turbulence, energy flows and momentum over the earth's surface, and winds (NCAR, 2008). CALMET is a diagnostic meteorological model that takes as input information the meteorological information recorded at stations, both on the surface and at altitude, and from this data generates the output meteorological fields. This model uses objective methods of analysis that seek optimal interpolation and extrapolation of observations (Scire et al. 2000). It also has the ability to process the forecast data from the WRF program and convert them into diagnostic data. CALMET develops wind hour fields and three-dimensional temperature fields in a grid modelling domain (Scire et al, 2000). CALMET is designed to be executed with surface observations and meteorological observations of high tropospheric levels.

METHODOLOGY

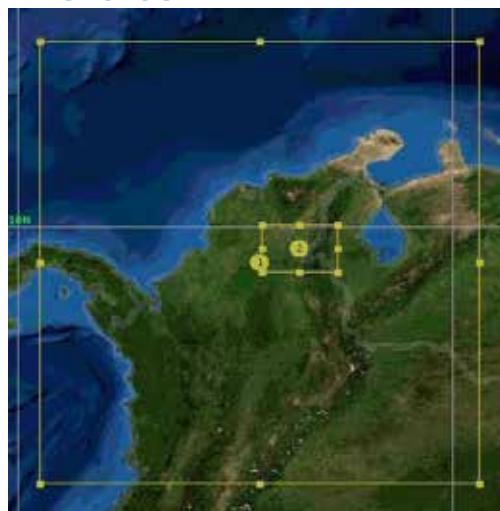


Figure 1. Location of the mining area of the department of Cesar, Colombia.

NCEP (National Centers for Environmental Prediction) CFSR (Climate Forecast System Reanalysis) data were used as initial and border conditions at a horizontal spatial resolution of 0.5 degrees (approximately 55Km), 37 levels of vertical resolution and a 6-hour output frequency (Saha, 2010; Saha et. al., 2010).

The basic physical parameterization that was used in the model is the same that IDEAM uses in an operative way to emit wind forecasts and predictions; taking advantage of the knowledge of the scope and limitations of its ability to represent the meteorological conditions at a national level. In particular, the WRF model (Skamarock et al 2001) was run non-hydrostatically. The planetary boundary layer parameterization used was the YSU (Yonsei University) scheme that explicitly resolves the planetary boundary layer on different atmospheric stability situations; this scheme exchanges information with soil physics based on the Monin-Obukov Similarity Theory as well as with the short wave (Radiative Fast Transfer Scheme) and long wave (Duhia Scheme) radiation schemes. A set of 2 nested domains was established, centered in the carboniferous zone of the department of Cesar. A large domain (2.098611, -79.783333); (16.453889 , -68.731111) covering a large part of Colombian territory (to take into account the influence of the Atlantic and Pacific oceans as well as the influence of the 3 mountain ranges) of 8 km spatial resolution and a second smaller domain of 3 km resolution (8.8881, -74.3882) ; (10.0412, -72,7181) which mainly covers the central part of the Perijá mountain range and the Cesar river valley, where the coal mining companies are currently operating.

WRF model runs were carried out in accordance with the particulate matter (PM₁₀) monitoring days of the air quality surveillance system of the department of Cesar, SVCADC, which are carried out every 3 days of the year, for a total of 10 runs for each month of the year. The year chosen for modeling was 2014. The results obtained by the WRF were used as an input to run the CALMET diagnostic meteorological model.

The validation of the superficial meteorological information existing in the study area was carried out, concerning the modeling period, for which the meteorological information used by the Air Quality Surveillance System of the Department of Cesar SVCADC for the year 2014. The validation was performed with daily average values of the variables: temperature, precipitation, wind speed, wind direction.

The modeling with CALMET program was performed in its initial wind field option implementing the WRF program. Land topography and land use data were processed by the subprograms, TERREL, CTGPROG, and MAKEGEO. Using geographic positioning, the points where the surface meteorological stations were located, with which the comparison and evaluation of modelled data would be carried out.

Through CALMET's wind diagramming and analysis function, the behaviour of the winds in the study area was studied, as well as the values of atmospheric stability and the height of the mixing layer.

After evaluating the CALMET model and knowing its correspondence with the study area, the pollutant dispersion study point was chosen (where no meteorological surface measurements were presented) and compared with data from the La Francia weather station -IDEAM. CALPUFF modeling was performed for the first half of 2014. Having two meteorological situations of the study region, a dry period comprising the months of January, February, March and a rainy period comprising the months of April, May and June. The modeling days in each month were chosen according to the established PM₁₀ monitoring calendar of the Zone. The sensitive receptors were located in the populated centers closest to the PLJ and Norcarbon mining projects. In this case, the municipal capital of the municipality of Jagua de Ibirico, where the PM₁₀ monitoring stations of the SVCADC, ZM2 and ZM9 are located; and the Victoria de San Isidro trail where the ZM21 station is located. All this was proposed in order to know the contribution of the blasting activity to the total concentration recorded by the SVCADC quality stations during the study period.

RESULTS

Most of scientific studies opt for an evaluation of qualitative results, and in those where the analysis is quantified they opt for the use of simple statistics with the quadratic mean error, the absolute mean error or the bias. Some works where different statisticians are proposed and used for the evaluation of forecasts. Willmott (1982), Pielke (1984), Willmott et al. (1985), Stauffer and Seaman (1990), Cox et al. (1998), Stenger (2000).

For the validation in the present study it was chosen to use the mean quadratic error (RMSE), the normalized mean absolute error (NMAE) and the bias (BIAS) defined by Peilke (1984) and Stauffer and Seama (1990). These statistics make it possible to measure the accuracy of the simulation.

Precision is the average of the degree of correspondence between individual pairs of predicted and observed values. Observed values are those obtained at meteorological measuring station.

The RSME indicates the average degree of correspondence between individual pairs of predicted and observed values. The RSME gives us the measure of the differences in average between the predicted and observed values. (Stauffer and Seaman, 1990). Another statistic that describes similar information is the mean absolute error defined as MAE, this is a measure of the closeness between predicted and observed values. To take into account the weight of the error with respect to the error of the measured variable, the absolute error, NMAE, is normalised, having the mean absolute error normalised (Stauffer and Seaman, 1990).

The BIAS provides information on the tendency of the model to forecast a variable, i.e., to overestimate or underestimate. It quantifies the systematic error of the Peilke model (1984).

Table 1. Evaluation statistics applied in modeling.

Estadístico	Fórmula	Interpretación
Bias medio, MB	$MB = \frac{1}{N} \sum_{i=1}^N (C_o - C_p)$	= 0 (OK) > 0 (subpredicción) < 0 (sobrepredicción)
Bias medio normalizado, NMB	$NMB = \frac{\sum_{i=1}^N (C_o - C_p)}{\sum_{i=1}^N C_o}$	= 0 (OK) > 0 (subpredicción) < 0 (sobrepredicción) > 1 (subpredicción muy importante) < -1 (sobrepredicción muy importante)
Error cuadrático medio, RMSE	$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (C_o - C_p)^2}$	= 0 (OK) Cuanto mayor sea, peor es la predicción.
Error cuadrático normalizado, NMSE	$NMSE = \frac{\sum_{i=1}^N (C_o - C_p)^2}{\sum_{i=1}^N C_o^2}$	= 0 (OK) Cuanto mayor sea, peor es la predicción.
Error normalizado, NME	$NME = \frac{\sum_{i=1}^N C_o - C_p }{\sum_{i=1}^N C_o}$	= 0 (OK) Cuanto mayor sea, peor es la predicción.

Co: data measured at the station. Cp: predicted data.
Designed by Ciemat 2009.



Figure 2. Validation of the surface temperature in (°C). (Autor).

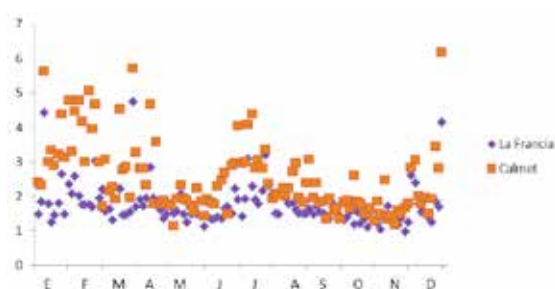


Figure 3. Validation of surface wind speed in (m/s). (Autor).

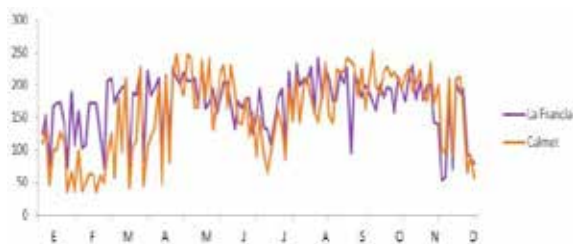


Figure 4. Validation of surface wind direction in sexagesimal degrees. (Autor),

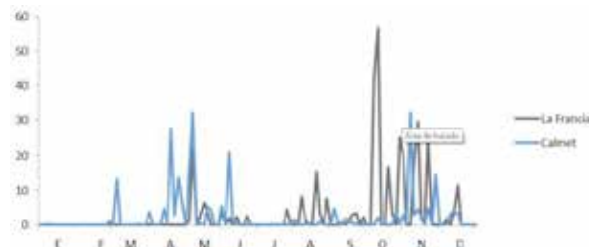


Figure 5. Validation of precipitation in (mm)

Table 2. Statistical evaluation results applied in modeling.

	NMAE	MBIAS	NBIAS	RSME	NMSE
Temperature	0.048	1.047	0.036	1.756	0.049
Wind speed	0.471	-0.747	-0.418	1.043	0.443
Wind direction	0.260	16.096	0.094	50.660	0.233
Precipitation	3.950	0.840	-0.579	9.506	1.795

Designed by autor.

CONCLUSIONS

With the WRF/CALMET system, it was found that better conditions are presented to forecast meteorological variables in the rainy season of the region; since characteristics are presented in the atmosphere of stability that facilitates this process.

The data from the WRF/CALMET meteorological modeling system displayed a behavior that corresponds to the behavior of the SVCDAC surface station data, achieving the lowest errors in the temperature variable and the highest errors in precipitation and wind direction. It was found that this modeling system has the tendency to over-predict the values of the variables studied, but with the assistance of real surface data that can be added to the system these errors would be reduced.

The CALMET results revealed that according to the Pasquill-Guifford classification (which takes into account incident solar radiation, cloudiness and wind speed), the study areas in the modeled period showed type E stability (slightly stable) with a tendency to neutrality in the hours of the day and type F stability (very stable) in the hours of night and early morning. We can say the type of stability F, does not propitiate a correct dispersion, allowing the pollutants to maintain their concentration for the period in which this stability is presented. It is worth mentioning that CALMET calculates atmospheric stability based on

the temperature variable (surface and vertical) and in the present research work the surface temperature variable was the variable where the model showed less error and greater correspondence with the data.

In the concentrations calculated by the CALPUFF dispersion model, it was observed that the impact caused by PM10 emitted by the "blasting" affects in considerable proportions the populations near the mining projects. During the months of January-February-March, when trade winds intensify over the northern part of the territory, PM10 particulate matter can become concentrated in the lower part of the atmosphere, and due to the strong speeds of trade winds, PM10 is dragged up to tens of kilometers below the source. During the months of April-May-June the intensity of the winds decreases so that the impact generated by PM10 is more local. The winds maintain predominant behaviors in a north-easter direction and propitiate a contribution of 14.33% in the station ZM2, affecting the municipal head of La Jagua de Ibirico. Otherwise, when the winds coming from the Southeast have influence on the zone of study, it is there when the sidewalk of La Victoria de San Isidro is affected with a contribution of 5.32% by the emissions of the blasting.

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DISPERSION OF SCALAR IN AN ALIGNED ARRAY OF RECTANGULAR BUILDINGS

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Abstract: The transport of a passive scalar within the canopy layer is investigated using a street network model (box model) and large-eddy simulation data (LES). Understanding the processes of transporting substances in the air is complicated, especially in urban areas in which the presence of buildings causes the flow to undergo disturbances, thus increasing the complexity of obtaining a dispersion pattern. The aim of this study is to investigate the behavior of the dispersion in an aligned array of rectangular and uniform high buildings. This configuration of the buildings gives rise to a long street resulting in an array more realistic to the cities. The domain size was $24H \times 24H \times 8H$ and the external flow is oblique (45°) to the building array in the test-case. Moreover, it was performed simulations considering different wind-directions to order to investigate the influence of wind direction on pollutant dispersion. For the simulations the ground source was located at a long street ($x/H=6$; $y/H=5$). The flux balance for a street box is performed partitioning the vertical flux into an advective and a turbulent component. The horizontal exchange between the streets and the intersection is considered predominantly advective while the vertical exchange occurring between the canopy and above the canopy is mainly turbulent. Comparisons between concentration data from the LES and the concentrations results obtained through the street network model were performed in terms of plume footprints and comparison of horizontal transects of volume-averaged concentration along x-axis (top) and along the y-axis (bottom) in the canopy layer. The results demonstrated the asymmetry of the plume and the strong channeling along the y-axis on the street where the source is located. This it was demonstrated both in the representation of LES data and in the results of the street network model. In numerical terms, the volume-averaged concentrations in the streets and intersections within the canopy layer showed very similar between both approaches. Concerning the simulations with different wind directions it was clear that in the array configuration evaluated and considering the source location in a long street was not a relevant factor to change the dispersion behavior. Therefore, for the 45° , 30° , 22° and 15° wind direction the spread of the contaminant is very similar for all evaluated cases. It has been demonstrated that the street network was able to represent adequately how the dispersion occurs in an array of rectangular and aligned buildings. Related to this, compliance with the LES data showed an advantage for the use of simplified models such as the street network model, with lower computational costs, faster and more accurate results.

Keywords: Street network model, Large-eddy simulation, Dispersion model, Urban dispersion.

INTRODUCTION

Air pollution can be a risk factor to the human health. According to the World Health Organization (WHO, 2018), nine out of 10 people breath air containing high concentrations of pollutants, and an estimated seven million deaths annually due to air pollution. These risks may be even more potential in the event of hazardous materials being release into the atmosphere, either by accident or intentionally, requiring rapid evacuation. In this context, it is necessary to have mechanisms capable of generating information that helps coordinates actions to avoid or mitigate the possible impacts on human health, such as the dispersion models of emergency response.

Simpler model formulations are being used to study the flow pattern and pollutant dispersion as fast simulation tools (GARBERO *et al.*, 2010; SOULHAC *et al.*, 2011; HERTWIG *et al.*, 2018).

In particular, street network dispersion models have been increasingly used and have demonstrated

accuracy in the results. Recently, the street network model developed by Belcher *et al.* (2015) and applied to the array of regular buildings presented satisfactory analytic solutions compared to DNS results and wind tunnel experiments, especially in the field near the source.

Goulart *et al.* (2017) used DNS data in an array of regular cubic buildings and employed these results in the street network model to treat the spread in an over the canopy layer. The authors verified that the street network model were able to capture the dispersion processes due to the presence of buildings from the parameterization of horizontal advection and vertical exchange processes.

The representation of the urban arrangement is another relevant point for the atmospheric flow studies whereas the effect of the geometry as well as the arrangement considerably affects the mechanism of field flow and mass exchange, resulting in extremely complex dispersion patterns (GARBERO *et al.*, 2010). Characteristics such as spacing between buildings, dimensions, shape and

linear or staggered layout of buildings, directly influence the behavior of turbulent flow and consequently the pollutants dispersion in urban environments. Therefore, in atmospheric flow studies, it is important to insert complexities into the urban arrangement in order to try to get closer to reality.

Against this background, this study was focused on evaluating the behavior of the flow in an aligned array of rectangular and uniform high buildings. Initially comparing the results obtained by the street network model and the large-eddy simulation (LES) data. Finally, it was evaluated the pollutant dispersion considering different wind direction.

METHODS

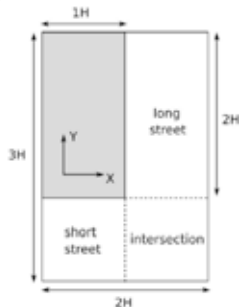
Urban Geometry

The representation of the urban geometry is a preponderant variable in studies about dispersion process. Features such as dimensions and shape of buildings, spacing between buildings, arrangement of obstacles, influence directly on the behavior of the turbulent flow and consequently on the dispersion in the urban environment. The dispersion patterns become extremely complex due to the urban setting that affect substantially the flow field and mass exchange mechanisms (GARBERO; SALIZZONI; SOULHAC, 2010).

Classical cube array has been extensively studied in recent years (BRANFORD *et al.*, 2011; CEZANA, 2015). Additionally, these layout is not always the one that best represents a city.

In this context, the study was developed in an aligned array of rectangular buildings of uniform high H and street width $W=H$ (Figure 1). This setting produce a geometrical asymmetry that is nearest to the actual street topology, more specifically a geometry representative of many European cities. Thus, the modelling process was performed in a domain size $24H \times 24H \times 8H$. Each building has a dimension of $1H \times 2H \times 1H$ in x , y and z .

The source is located in a long street whose coordinates are $x/H = 6$ and $y/H = 5$ (Figure 2). Furthermore, the wind direction focused in this study was 45° .



Reference: Hertwig *et al.*, 2018.

Figure 1. Plan-view of the repeating unit of the array. Building in grey shading.



Figure 2. Plan-view of the aligned array of rectangular buildings of uniform high.

Large-eddy simulation

LES data related to flow and dispersion of scalar were obtained in a study conducted by University of Southampton using the open-source CFD package OpenFOAM (v2.1). The study is part of DIPLOS project (DIspersion of LOcalised releases in Street networks; www.diplos.org) whose objective is to provide a high-quality data-set for development and implementation of parameterizations for dispersion processes in cities.

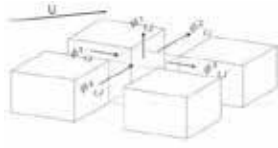
The DIPLOS test case was simulated in a computational domain of size $24H \times 24H \times 12H$ using Cartesian grid with resolution of $\Delta=H/16$. The dimensions of buildings are $1H \times 2H \times 1H$ in x , y and z . The no-slip boundary conditions were assumed on all solid surfaces. A stress-free condition was imposed at the top of the domain and periodic boundary conditions in horizontal directions. Finally, for the concentration fields, it was necessary to implement sponge layers at the outlet boundaries in order to prevent re-entry of materials into the domain through the input limits as part of the process of recycling the flow.

The friction velocity (u_*) obtained from LES had a value of $u_* = 0.305 \text{ m s}^{-1}$, resulting in $u_*/U_{2H} = 0.131$ and $u_*/U_e = 0.0828$, where $U_{2H} = 2.34 \text{ m s}^{-1}$ is the horizontal velocity magnitude at twice the building height and $U_e = 3.69 \text{ m s}^{-1}$ the free-stream velocity at $z/H = 12$. For consistency in the comparison of results from the LES and the street network model, it was used $H = 1 \text{ m}$.

Details of the LES DIPLOS test case are described by Hertwig *et al.* (2018) and Fuka *et al.* (2017).

Street-network model

Street network model or box model are based on the representation of the urban area through boxes interconnected boxes. In other words, the methodology is to represent streets and intersections by boxes where the flow will pass through the horizontal faces and the top. Therefore, it is possible to diagram the flux ($\phi_{i,j}^k$) that cross each box as shown in the Figure 3.



Reference: Goulart, 2012.

Figure 3. Scheme of scalar fluxes in a street intersection. Dashed lines represent the intersection box and U is the external flow.

Goulart (2012) and Belcher *et al.* (2015) described the street network model including scattering above the canopy. Both presenting results being confronted with DNS dispersion data for simulation in an array of cubic buildings.

Street network model approach is based in a flux balance equation that is a balance equation for the volume-averaged scalar concentration within a street or an intersection box in the canopy layer.

$$\begin{aligned} \frac{dC_{i,j}}{dt} + \frac{1}{V_{i,j}} \int_{\partial V_{i,j}} c \vec{u} \cdot d\vec{S} - \frac{\kappa}{V_{i,j}} \int_{\partial V_{i,j}} \nabla c \cdot d\vec{S} \\ = \frac{1}{V_{i,j}} \int_{\partial V_{i,j}} Q dV \end{aligned}$$

where $C_{i,j}$ is the concentration, $V_{i,j}$ is the volume of the $(i,j)^{th}$ cell of the network, c is the instantaneous concentration, $\vec{u}$ is the instantaneous velocity vector, κ is the molecular diffusivity coefficient, Q is the emission source term. The total area bounding the volume $V_{i,j}$ is $\partial V_{i,j}$ and $d\vec{S}$ is an area element on $\partial V_{i,j}$.

For an approach including a dispersion above the canopy, the following considerations were made:

- (a) The diffusive term is neglected because the flow is highly turbulent, so the molecular transport is very small compared to advective transport;
- (b) Transient regime is considered due to the coupling of the concentration within and above the canopy;
- (c) Constant rate for a point source

$$\frac{1}{V_{i,j}} \int_{\partial V_{i,j}} Q dV = q_{i,j}$$

where $q_{i,j}$ is the source emission rate.

- (d) The turbulent scalar fluxes were parameterized using the gradient diffusion model.

$$\overline{c' \vec{u}'} = -K \nabla \bar{c}$$

Where $\overline{c' \vec{u}'}$ is the turbulent scalar flux, K is the detrainment velocity.

Thus, the concentration can be written as:

$$V_{i,j} \frac{dC_{i,j}}{dt} + \int_{\partial V_{i,j}} \bar{c} \vec{u} \cdot d\vec{S} - K \int_{\partial V_{i,j}} \nabla \bar{c} \cdot d\vec{S} = q_{i,j}$$

The formulation of the network model including dispersion above the canopy can be written in discretized form as follows:

$$\Delta C_{i,j} = \frac{\Delta t}{V_{i,j}} \left(\sum_{k=1}^n \phi_{i,j}^k + \sum_{k=1}^n \phi_{i,j}^k + q_{i,j} \right)$$

where $\phi_{i,j}^k$ are the negative advective fluxes through the facets of the boxes, $\phi_{i,j}^k$ are the negative turbulent scalar fluxes through the facets of the boxes, k is the relevant facet number of the box and n is the total number of facets.

The scalar exchange between within and above the canopy can be modeled with a detrainment velocity, so

$$E = \frac{K}{\Delta r}$$

where E is detrainment velocity, K is the detrainment velocity and Δr is the distance between the center of two consecutive cells.

For the estimation of the concentration in the street, the flow balance is taken considering horizontally the advective transport of the scalar and in the vertical the turbulent transport of the scalar, as:

$$\begin{aligned} C_{i,j,k}^t = C_{i,j,k}^{t-1} + \frac{\Delta t}{V_{i,j}} [U^{st} A_x C_{i-1,j,k}^{t-1} - U^{int} A_x C_{i,j,k}^{t-1} \\ - E_s A_z (C_{i,j,k+1}^{t-1} - C_{i,j,k}^{t-1}) + q_{i,j}] \end{aligned}$$

where A_x and A_z are the area normal to the flux, U^{st} and U^{int} are the velocities at a street and an intersection, E_s is the detrainment velocity at a street, $C_{i,j,k}^{t-1}$ is the concentration at the previous time step and Δt is the time step.

The same principle is used to calculate the concentration at an intersection:

$$\begin{aligned} C_{i,j}^t = C_{i,j}^{t-1} + \frac{\Delta t}{V_{i,j}} [A_x U^{st} C_{i-1,j,k}^{t-1} - A_x U^{int} C_{i,j,k}^{t-1} \\ + A_y V^{st} C_{i,j-1,k}^{t-1} - A_y V^{int} C_{i,j,k}^{t-1} \\ - E_i A_z (C_{i,j,k+1}^{t-1} - C_{i,j,k}^{t-1}) + q_{i,j}] \end{aligned}$$

where A_y is the area normal to the flux and E_i is the detrainment velocity at an intersection.

These last two equations can be used to evaluate the concentration within the canopy.

Above the canopy the turbulent scalar transport cannot be neglected in the horizontal. Additionally it is necessary to consider that the vertical fluxes are only turbulent. In other words, the vertical component of the mean velocity is small. The last step is to include advection and turbulent scalar transport in the full transport equation. So, the concentration above the canopy can be written as:

$$C_{i,j,k}^t = C_{i,j,k}^{t-1} + \frac{\Delta t}{V_{i,j}} \left[A_x C_{i-1,j,k}^{t-1} - A_x U_{abv} C_{i,j,k}^{t-1} + A_y V_{abv} C_{i,j-1,k}^{t-1} - A_y V_{abv} C_{i,j,k}^{t-1} + K_x A_x \frac{(C_{i,j,k}^{t-1} - C_{i-1,j,k}^{t-1})}{\Delta x} - K_x A_x \frac{(C_{i+1,j,k}^{t-1} - C_{i,j,k}^{t-1})}{\Delta x} + K_y A_y \frac{(C_{i,j,k}^{t-1} - C_{i,j-1,k}^{t-1})}{\Delta y} - K_y A_y \frac{(C_{i,j+1,k}^{t-1} - C_{i,j,k}^{t-1})}{\Delta y} + K_z A_z \frac{(C_{i,j,k}^{t-1} - C_{i,j,k-1}^{t-1}) U_{abv}}{\Delta z} - K_z A_z \frac{(C_{i,j,k+1}^{t-1} - C_{i,j,k}^{t-1})}{\Delta z} \right]$$

where U_{abv} and V_{abv} are the velocities above the canopy, K_x , K_y and K_z are eddy diffusivity coefficients. The first four terms inside the square brackets are the advective transport and the last six terms are the diffusivity terms.

Input data

For this study it was used horizontal advection velocities and vertical exchange velocity from LES data obtained from DIPLOS project (Table 1). The diffusion coefficients are shown in the (Table 2).

Table 1. Horizontal advection velocities and vertical exchange velocities derived from LES.

Parameter	Description	Magnitude (m s ⁻¹)
U_i	Horizontal advection velocity of output in the y-direction	0.22
V_i	Horizontal advection velocity of output in the x-direction	0.71
U_s	Horizontal advection velocity of input in the y-direction	0.23
V_s	Horizontal advection velocity of input in the x-direction	0.77
E_i	Vertical exchange velocity in intersection	0.12
E_{sx}	Vertical exchange velocity on the x-axis	0.15
E_{sy}	Vertical exchange velocity on the y-axis	0.10

Initially, it was necessary to validate the street network model. So, the test case was developed with wind direction 45°. The results from the simulation in the street network model were compared with the LES data. For the test case the

velocities above the canopy layer were $U = V = 2.34 \text{ m s}^{-1}$.

Once validated, it was performed other three wind directions: 15°, 22° and 30°. These three wind directions were chosen with the aim to investigate the behavior of the plume and the dispersion in wind direction more near the 0° (15°), in the middle (22°) and more near the 45° (30°). The velocities above the canopy layer corresponding to each wind direction are shown in the Table 3.

Table 2. Horizontal and vertical diffusion coefficients applied to the street network model.

Parameter	Description	Magnitude (m ² s ⁻¹)
K_x	Horizontal diffusion coefficient on the x-axis	0.5
K_y	Horizontal diffusion coefficient on the y-axis	0.5
K_z	Vertical diffusion coefficient	0.3

Table 3. Velocities above the canopy layer in x-direction (U) and y-direction (V) according the wind direction.

Wind Direction	U (m s ⁻¹)	V (m s ⁻¹)
15°	0.85	3.19
22°	1.23	3.06
30°	1.66	2.87
45°	2.34	2.34

FINDINGS AND ARGUMENT

Street Network Model Evaluation

The qualitative inter-comparison between the LES reference data and the results from the street network model is presented in terms of footprints and the plume behavior in the x and y-direction in this section. The aim was to validate the street network model.

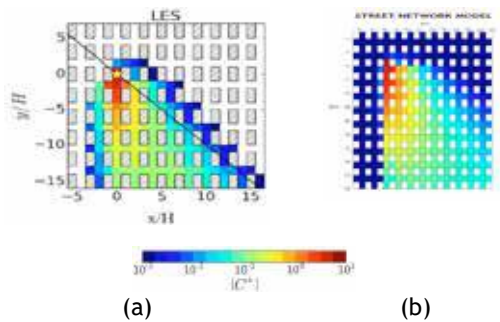
Figure 4 shows the volume-averaged concentrations within the canopy layer considering LES data (Figure 4a) and street network model results (Figure 4b).

As expected, the street network model represented satisfactorily the plume behavior. In both model results presented asymmetric plume shape. However, it is possible to note that the plume referring to the street network model was narrower than the plume referring to the LES. Furthermore, it is important to note a flow channeling along x/H corresponding to the source location in both approach.

In analyses quantitative the results also showed agreement between LES and street network model (Figure 5). The longitudinal and lateral concentrations profile presents a good correspondence with the LES data reference mainly

near the source ($x/H=6$ and $y/H=5$). As we move away from the source the differences are observed and the street network slightly underestimated (at lateral transect $x/H=6$, for example) or overestimated (at horizontal transect $y/H=8$, for example) the LES concentration. The largest deviations can be noted at the plume edges mainly at $x/H=4$ and $x/H=5$ in horizontal transects at $y/H=8$ and $y/H=14$.

For this test-case with the street network model it is concluded that the simple flux-balance methodology responds satisfactorily to demonstrate flux processes in the canopy layer considering an array with rectangular buildings. This is due to the street network model capture the topological dispersion effects like demonstrated the longitudinal concentrations profile ($x/H=6$ and $x/H=10$) especially the strong pollutant channeling in y -direction.



Reference: Hertwig et al., 2018.

Figure 4. Volume-averaged concentrations in streets and intersections within the canopy layer ($0 \leq z/H \leq 1$): (a) LES reference data; (b) Street Network Model.

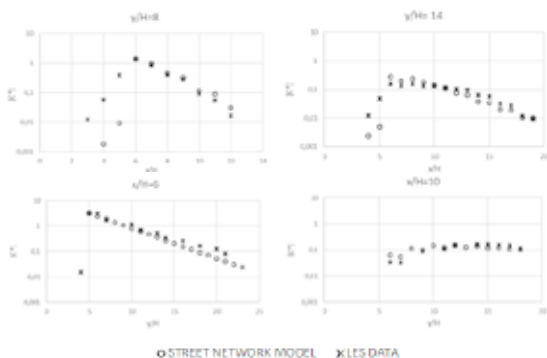


Figure 5. Comparison of horizontal transects of volume-averaged concentration between LES and Street Network Model along the x -axis (top) and the y -axis (bottom) in the canopy layer. The source position is $x/H = 6$ and $y/H = 5$.

Concentration profiles for different wind directions

Figure 6 presents a lateral concentrations profile considering 15° , 22° , 30° and 45° wind directions.

Horizontal transects were made at $x/H=6$ (source location), $x/H=10$, $x/H=17$ and $x/H=21$.

The lateral scattering was very similar for all wind directions analyzed in the regions closest to the source ($x/H=6$ and $x/H=10$). The largest differences can be seen as close to the edge of the pollutant plume. For $x/H = 21$, the concentrations into y -direction for the 45° wind direction have an order of magnitude ten times higher than when observing the results referring to 15° . This means that, as the wind direction approaches 0° , the plume is more diluted away from the source; therefore the spread of the plume is farther closed.

This became clear for $x/H = 17$, in which there is a largest spread between the concentrations presented for the different wind directions until $y/H=17$. From $y/H=17$ the results for all wind directions are very similar.

The difference becomes even greater when observed the horizontal transect $x/H=21$. In this case, the concentration decreases much less quickly in 45° wind direction along y -streets, so the plume is less diluted near the edge.

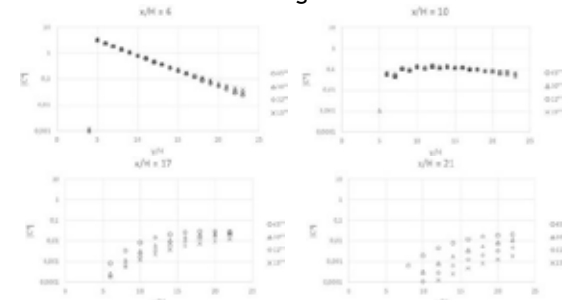


Figure 6. Comparison of lateral concentrations profile in horizontal transects within the canopy layer ($0 \leq z/H \leq 1$).

A comparison of longitudinal concentrations profiles was made for the different wind directions in the horizontal transects near the source ($y/H=6$, $y/H=8$) and away from the source ($y/H=14$, $y/H=22$). Figure 7 shows these profiles.

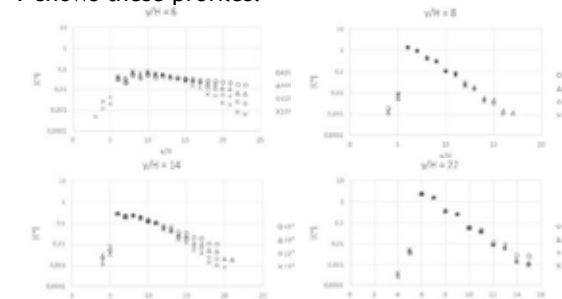


Figure 7. Comparison of longitudinal concentrations profile in horizontal transects within the canopy layer ($0 \leq z/H \leq 1$).

It is perceptible that the differences between the longitudinal concentrations profiles are very subtle as well as in lateral concentrations profiles.

These small oscillations may be due to the source location. The source was positioned in a long street which provides the pollutant channeling in y-direction. In addition, the building geometry is also a factor that induces this dispersion behavior in the array configuration. Thereby, for this arrangement of rectangular buildings and considering that the source is in a long street location, changes in wind direction do not influence considerably the lateral and longitudinal dispersion of the contaminant. Perhaps, in a different source location like in an intersection, the pollutant dispersion may be more influenced for the wind directions.

CONCLUSION

Street network model proved to be an adequate methodology for dispersion modeling considering in an array of rectangular and aligned buildings. From the comparison with the LES data it has been demonstrated that the main relevant dispersion processes are captured.

The plume behavior was described properly demonstrating that the advective transport mechanism and the vertical turbulent transfer of pollutants within and above the canopy layer were adequately represented in the street network model. It was possible to observe the channeling along y-street as well as the spread of the plume. So, the street network was able to represent adequately how the dispersion occurs in this situation.

When the simulations were performed in a street network model in that arrangement of buildings considering different wind directions it was possible to note that the concentrations profiles are very similar for all situations analyzed in the regions closest to the source. But, when concentrations profiles are drawn near the edges the largest differences appear. For wind directions approaching 0° the concentrations decay faster laterally.

It was observed that for the longitudinal spread in cases of various wind directions the results are very similar too. There are slight differences near the edges ($y/H=6$ and $y/H=14$) like happens in the lateral dispersion.

In general, the longitudinal and lateral concentrations profiles demonstrated that even when there are differences between the results from different wind directions, they are very subtle. That means that in an array with rectangular buildings, when the source is located in a long street the influence of the wind direction was demonstrated weak.

It is recommended to evaluate the street network model inputting other complexities into the urban arrangement like buildings of different heights, for example, with the view to try to get increasingly closer to the reality. In addition, further studies can be performed from the arrangement considered in

this study, but with the source location in an intersection or on a short street in order to investigate the influence of wind direction.

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DISPERSION OF SCALAR IN AN ALIGNED ARRAY OF RECTANGULAR BUILDINGS

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Abstract: The transport of a passive scalar within the canopy layer is investigated using a street network model (box model) and large-eddy simulation data (LES). Understanding the processes of transporting substances in the air is complicated, especially in urban areas in which the presence of buildings causes the flow to undergo disturbances, thus increasing the complexity of obtaining a dispersion pattern. The aim of this study is to investigate the behavior of the dispersion in an aligned array of rectangular and uniform high buildings. This configuration of the buildings gives rise to a long street resulting in an array more realistic to the cities. The domain size was $24H \times 24H \times 8H$ and the external flow is oblique (45°) to the building array in the test-case. Moreover, it was performed simulations considering different wind-directions to order to investigate the influence of wind direction on pollutant dispersion. For the simulations the ground source was located at a long street ($x/H=6$; $y/H=5$). The flux balance for a street box is performed partitioning the vertical flux into an advective and a turbulent component. The horizontal exchange between the streets and the intersection is considered predominantly advective while the vertical exchange occurring between the canopy and above the canopy is mainly turbulent. Comparisons between concentration data from the LES and the concentrations results obtained through the street network model were performed in terms of plume footprints and comparison of horizontal transects of volume-averaged concentration along x-axis (top) and along the y-axis (bottom) in the canopy layer. The results demonstrated the asymmetry of the plume and the strong channeling along the y-axis on the street where the source is located. This it was demonstrated both in the representation of LES data and in the results of the street network model. In numerical terms, the volume-averaged concentrations in the streets and intersections within the canopy layer showed very similar between both approaches. Concerning the simulations with different wind directions it was clear that in the array configuration evaluated and considering the source location in a long street was not a relevant factor to change the dispersion behavior. Therefore, for the 45° , 30° , 22° and 15° wind direction the spread of the contaminant is very similar for all evaluated cases. It has been demonstrated that the street network was able to represent adequately how the dispersion occurs in an array of rectangular and aligned buildings. Related to this, compliance with the LES data showed an advantage for the use of simplified models such as the street network model, with lower computational costs, faster and more accurate results.

Keywords: Street network model, Large-eddy simulation, Dispersion model, Urban dispersion.

INTRODUCTION

Air pollution can be a risk factor to the human health. According to the World Health Organization (WHO, 2018), nine out of 10 people breath air containing high concentrations of pollutants, and an estimated seven million deaths annually due to air pollution. These risks may be even more potential in the event of hazardous materials being release into the atmosphere, either by accident or intentionally, requiring rapid evacuation. In this context, it is necessary to have mechanisms capable of generating information that helps coordinates actions to avoid or mitigate the possible impacts on human health, such as the dispersion models of emergency response.

Simpler model formulations are being used to study the flow pattern and pollutant dispersion as fast simulation tools (GARBERO *et al.*, 2010; SOULHAC *et al.*, 2011; HERTWIG *et al.*, 2018).

In particular, street network dispersion models have been increasingly used and have demonstrated

accuracy in the results. Recently, the street network model developed by Belcher *et al.* (2015) and applied to the array of regular buildings presented satisfactory analytic solutions compared to DNS results and wind tunnel experiments, especially in the field near the source.

Goulart *et al.* (2017) used DNS data in an array of regular cubic buildings and employed these results in the street network model to treat the spread in an over the canopy layer. The authors verified that the street network model were able to capture the dispersion processes due to the presence of buildings from the parameterization of horizontal advection and vertical exchange processes.

The representation of the urban arrangement is another relevant point for the atmospheric flow studies whereas the effect of the geometry as well as the arrangement considerably affects the mechanism of field flow and mass exchange, resulting in extremely complex dispersion patterns (GARBERO *et al.*, 2010). Characteristics such as spacing between buildings, dimensions, shape and

linear or staggered layout of buildings, directly influence the behavior of turbulent flow and consequently the pollutants dispersion in urban environments. Therefore, in atmospheric flow studies, it is important to insert complexities into the urban arrangement in order to try to get closer to reality.

Against this background, this study was focused on evaluating the behavior of the flow in an aligned array of rectangular and uniform high buildings. Initially comparing the results obtained by the street network model and the large-eddy simulation (LES) data. Finally, it was evaluated the pollutant dispersion considering different wind direction.

METHODS

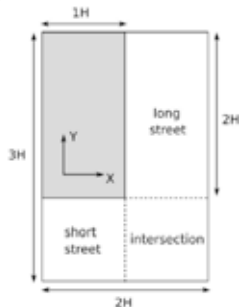
Urban Geometry

The representation of the urban geometry is a preponderant variable in studies about dispersion process. Features such as dimensions and shape of buildings, spacing between buildings, arrangement of obstacles, influence directly on the behavior of the turbulent flow and consequently on the dispersion in the urban environment. The dispersion patterns become extremely complex due to the urban setting that affect substantially the flow field and mass exchange mechanisms (GARBERO; SALIZZONI; SOULHAC, 2010).

Classical cube array has been extensively studied in recent years (BRANFORD *et al.*, 2011; CEZANA, 2015). Additionally, these layout is not always the one that best represents a city.

In this context, the study was developed in an aligned array of rectangular buildings of uniform high H and street width $W=H$ (Figure 1). This setting produce a geometrical asymmetry that is nearest to the actual street topology, more specifically a geometry representative of many European cities. Thus, the modelling process was performed in a domain size $24H \times 24H \times 8H$. Each building has a dimension of $1H \times 2H \times 1H$ in x , y and z .

The source is located in a long street whose coordinates are $x/H = 6$ and $y/H = 5$ (Figure 2). Furthermore, the wind direction focused in this study was 45° .



Reference: Hertwig *et al.*, 2018.

Figure 1. Plan-view of the repeating unit of the array. Building in grey shading.



Figure 2. Plan-view of the aligned array of rectangular buildings of uniform high.

Large-eddy simulation

LES data related to flow and dispersion of scalar were obtained in a study conducted by University of Southampton using the open-source CFD package OpenFOAM (v2.1). The study is part of DIPLOS project (DIspersion of LOcalised releases in Street networks; www.diplos.org) whose objective is to provide a high-quality data-set for development and implementation of parameterizations for dispersion processes in cities.

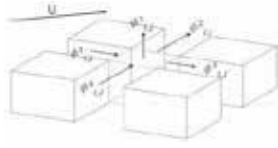
The DIPLOS test case was simulated in a computational domain of size $24H \times 24H \times 12H$ using Cartesian grid with resolution of $\Delta=H/16$. The dimensions of buildings are $1H \times 2H \times 1H$ in x , y and z . The no-slip boundary conditions were assumed on all solid surfaces. A stress-free condition was imposed at the top of the domain and periodic boundary conditions in horizontal directions. Finally, for the concentration fields, it was necessary to implement sponge layers at the outlet boundaries in order to prevent re-entry of materials into the domain through the input limits as part of the process of recycling the flow.

The friction velocity (u_*) obtained from LES had a value of $u_* = 0.305 \text{ m s}^{-1}$, resulting in $u_*/U_{2H} = 0.131$ and $u_*/U_e = 0.0828$, where $U_{2H} = 2.34 \text{ m s}^{-1}$ is the horizontal velocity magnitude at twice the building height and $U_e = 3.69 \text{ m s}^{-1}$ the free-stream velocity at $z/H = 12$. For consistency in the comparison of results from the LES and the street network model, it was used $H = 1 \text{ m}$.

Details of the LES DIPLOS test case are described by Hertwig *et al.* (2018) and Fuka *et al.* (2017).

Street-network model

Street network model or box model are based on the representation of the urban area through boxes interconnected boxes. In other words, the methodology is to represent streets and intersections by boxes where the flow will pass through the horizontal faces and the top. Therefore, it is possible to diagram the flux ($\phi_{i,j}^k$) that cross each box as shown in the Figure 3.



Reference: Goulart, 2012.

Figure 3. Scheme of scalar fluxes in a street intersection. Dashed lines represent the intersection box and U is the external flow.

Goulart (2012) and Belcher *et al.* (2015) described the street network model including scattering above the canopy. Both presenting results being confronted with DNS dispersion data for simulation in an array of cubic buildings.

Street network model approach is based in a flux balance equation that is a balance equation for the volume-averaged scalar concentration within a street or an intersection box in the canopy layer.

$$\begin{aligned} \frac{dC_{i,j}}{dt} + \frac{1}{V_{i,j}} \int_{\partial V_{i,j}} c \vec{u} \cdot d\vec{S} - \frac{\kappa}{V_{i,j}} \int_{\partial V_{i,j}} \nabla c \cdot d\vec{S} \\ = \frac{1}{V_{i,j}} \int_{\partial V_{i,j}} Q dV \end{aligned}$$

where $C_{i,j}$ is the concentration, $V_{i,j}$ is the volume of the $(i,j)^{th}$ cell of the network, c is the instantaneous concentration, $\vec{u}$ is the instantaneous velocity vector, κ is the molecular diffusivity coefficient, Q is the emission source term. The total area bounding the volume $V_{i,j}$ is $\partial V_{i,j}$ and $d\vec{S}$ is an area element on $\partial V_{i,j}$.

For an approach including a dispersion above the canopy, the following considerations were made:

- (a) The diffusive term is neglected because the flow is highly turbulent, so the molecular transport is very small compared to advective transport;
- (b) Transient regime is considered due to the coupling of the concentration within and above the canopy;
- (c) Constant rate for a point source

$$\frac{1}{V_{i,j}} \int_{\partial V_{i,j}} Q dV = q_{i,j}$$

where $q_{i,j}$ is the source emission rate.

- (d) The turbulent scalar fluxes were parameterized using the gradient diffusion model.

$$\overline{c' \vec{u}'} = -K \nabla \bar{c}$$

Where $\overline{c' \vec{u}'}$ is the turbulent scalar flux, K is the detrainment velocity.

Thus, the concentration can be written as:

$$V_{i,j} \frac{dC_{i,j}}{dt} + \int_{\partial V_{i,j}} \bar{c} \vec{u} \cdot d\vec{S} - K \int_{\partial V_{i,j}} \nabla \bar{c} \cdot d\vec{S} = q_{i,j}$$

The formulation of the network model including dispersion above the canopy can be written in discretized form as follows:

$$\Delta C_{i,j} = \frac{\Delta t}{V_{i,j}} \left(\sum_{k=1}^n \phi_{i,j}^k + \sum_{k=1}^n \varphi_{i,j}^k + q_{i,j} \right)$$

where $\phi_{i,j}^k$ are the negative advective fluxes through the facets of the boxes, $\varphi_{i,j}^k$ are the negative turbulent scalar fluxes through the facets of the boxes, k is the relevant facet number of the box and n is the total number of facets.

The scalar exchange between within and above the canopy can be modeled with a detrainment velocity, so

$$E = \frac{K}{\Delta r}$$

where E is detrainment velocity, K is the detrainment velocity and Δr is the distance between the center of two consecutive cells.

For the estimation of the concentration in the street, the flow balance is taken considering horizontally the advective transport of the scalar and in the vertical the turbulent transport of the scalar, as:

$$\begin{aligned} C_{i,j,k}^t = C_{i,j,k}^{t-1} + \frac{\Delta t}{V_{i,j}} [U^{st} A_x C_{i-1,j,k}^{t-1} - U^{int} A_x C_{i,j,k}^{t-1} \\ - E_s A_z (C_{i,j,k+1}^{t-1} - C_{i,j,k}^{t-1}) + q_{i,j}] \end{aligned}$$

where A_x and A_z are the area normal to the flux, U^{st} and U^{int} are the velocities at a street and an intersection, E_s is the detrainment velocity at a street, $C_{i,j,k}^{t-1}$ is the concentration at the previous time step and Δt is the time step.

The same principle is used to calculate the concentration at an intersection:

$$\begin{aligned} C_{i,j}^t = C_{i,j}^{t-1} + \frac{\Delta t}{V_{i,j}} [A_x U^{st} C_{i-1,j,k}^{t-1} - A_x U^{int} C_{i,j,k}^{t-1} \\ + A_y V^{st} C_{i,j-1,k}^{t-1} - A_y V^{int} C_{i,j,k}^{t-1} \\ - E_i A_z (C_{i,j,k+1}^{t-1} - C_{i,j,k}^{t-1}) + q_{i,j}] \end{aligned}$$

where A_y is the area normal to the flux and E_i is the detrainment velocity at an intersection.

These last two equations can be used to evaluate the concentration within the canopy.

Above the canopy the turbulent scalar transport cannot be neglected in the horizontal. Additionally it is necessary to consider that the vertical fluxes are only turbulent. In other words, the vertical component of the mean velocity is small. The last step is to include advection and turbulent scalar transport in the full transport equation. So, the concentration above the canopy can be written as:

$$C_{i,j,k}^t = C_{i,j,k}^{t-1} + \frac{\Delta t}{V_{i,j}} \left[A_x C_{i-1,j,k}^{t-1} - A_x U_{abv} C_{i,j,k}^{t-1} + A_y V_{abv} C_{i,j-1,k}^{t-1} - A_y V_{abv} C_{i,j,k}^{t-1} + K_x A_x \frac{(C_{i,j,k}^{t-1} - C_{i-1,j,k}^{t-1})}{\Delta x} - K_x A_x \frac{(C_{i+1,j,k}^{t-1} - C_{i,j,k}^{t-1})}{\Delta x} + K_y A_y \frac{(C_{i,j,k}^{t-1} - C_{i,j-1,k}^{t-1})}{\Delta y} - K_y A_y \frac{(C_{i,j+1,k}^{t-1} - C_{i,j,k}^{t-1})}{\Delta y} + K_z A_z \frac{(C_{i,j,k}^{t-1} - C_{i,j,k-1}^{t-1}) U_{abv}}{\Delta z} - K_z A_z \frac{(C_{i,j,k+1}^{t-1} - C_{i,j,k}^{t-1})}{\Delta z} \right]$$

where U_{abv} and V_{abv} are the velocities above the canopy, K_x , K_y and K_z are eddy diffusivity coefficients. The first four terms inside the square brackets are the advective transport and the last six terms are the diffusivity terms.

Input data

For this study it was used horizontal advection velocities and vertical exchange velocity from LES data obtained from DIPLOS project (Table 1). The diffusion coefficients are shown in the (Table 2).

Table 1. Horizontal advection velocities and vertical exchange velocities derived from LES.

Parameter	Description	Magnitude (m s ⁻¹)
U_i	Horizontal advection velocity of output in the y-direction	0.22
V_i	Horizontal advection velocity of output in the x-direction	0.71
U_s	Horizontal advection velocity of input in the y-direction	0.23
V_s	Horizontal advection velocity of input in the x-direction	0.77
E_i	Vertical exchange velocity in intersection	0.12
E_{sx}	Vertical exchange velocity on the x-axis	0.15
E_{sy}	Vertical exchange velocity on the y-axis	0.10

Initially, it was necessary to validate the street network model. So, the test case was developed with wind direction 45°. The results from the simulation in the street network model were compared with the LES data. For the test case the

velocities above the canopy layer were $U = V = 2.34 \text{ m s}^{-1}$.

Once validated, it was performed other three wind directions: 15°, 22° and 30°. These three wind directions were chosen with the aim to investigate the behavior of the plume and the dispersion in wind direction more near the 0° (15°), in the middle (22°) and more near the 45° (30°). The velocities above the canopy layer corresponding to each wind direction are shown in the Table 3.

Table 2. Horizontal and vertical diffusion coefficients applied to the street network model.

Parameter	Description	Magnitude (m ² s ⁻¹)
K_x	Horizontal diffusion coefficient on the x-axis	0.5
K_y	Horizontal diffusion coefficient on the y-axis	0.5
K_z	Vertical diffusion coefficient	0.3

Table 3. Velocities above the canopy layer in x-direction (U) and y-direction (V) according the wind direction.

Wind Direction	U (m s ⁻¹)	V (m s ⁻¹)
15°	0.85	3.19
22°	1.23	3.06
30°	1.66	2.87
45°	2.34	2.34

FINDINGS AND ARGUMENT

Street Network Model Evaluation

The qualitative inter-comparison between the LES reference data and the results from the street network model is presented in terms of footprints and the plume behavior in the x and y-direction in this section. The aim was to validate the street network model.

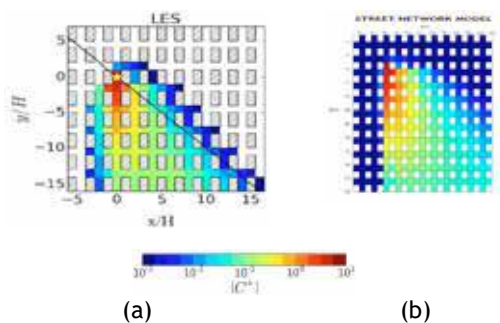
Figure 4 shows the volume-averaged concentrations within the canopy layer considering LES data (Figure 4a) and street network model results (Figure 4b).

As expected, the street network model represented satisfactorily the plume behavior. In both model results presented asymmetric plume shape. However, it is possible to note that the plume referring to the street network model was narrower than the plume referring to the LES. Furthermore, it is important to note a flow channeling along x/H corresponding to the source location in both approach.

In analyses quantitative the results also showed agreement between LES and street network model (Figure 5). The longitudinal and lateral concentrations profile presents a good correspondence with the LES data reference mainly

near the source ($x/H=6$ and $y/H=5$). As we move away from the source the differences are observed and the street network slightly underestimated (at lateral transect $x/H=6$, for example) or overestimated (at horizontal transect $y/H=8$, for example) the LES concentration. The largest deviations can be noted at the plume edges mainly at $x/H=4$ and $x/H=5$ in horizontal transects at $y/H=8$ and $y/H=14$.

For this test-case with the street network model it is concluded that the simple flux-balance methodology responds satisfactorily to demonstrate flux processes in the canopy layer considering an array with rectangular buildings. This is due to the street network model capture the topological dispersion effects like demonstrated the longitudinal concentrations profile ($x/H=6$ and $x/H=10$) especially the strong pollutant channeling in y -direction.



Reference: Hertwig et al., 2018.

Figure 4. Volume-averaged concentrations in streets and intersections within the canopy layer ($0 \leq z/H \leq 1$): (a) LES reference data; (b) Street Network Model.

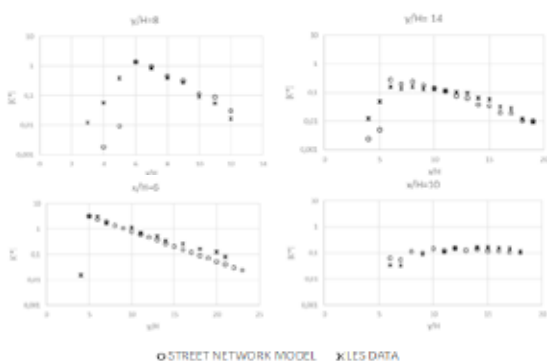


Figure 5. Comparison of horizontal transects of volume-averaged concentration between LES and Street Network Model along the x -axis (top) and the y -axis (bottom) in the canopy layer. The source position is $x/H = 6$ and $y/H = 5$.

Concentration profiles for different wind directions

Figure 6 presents a lateral concentrations profile considering 15° , 22° , 30° and 45° wind directions.

Horizontal transects were made at $x/H=6$ (source location), $x/H=10$, $x/H=17$ and $x/H=21$.

The lateral scattering was very similar for all wind directions analyzed in the regions closest to the source ($x/H=6$ and $x/H=10$). The largest differences can be seen as close to the edge of the pollutant plume. For $x/H = 21$, the concentrations into y -direction for the 45° wind direction have an order of magnitude ten times higher than when observing the results referring to 15° . This means that, as the wind direction approaches 0° , the plume is more diluted away from the source; therefore the spread of the plume is farther closed.

This became clear for $x/H = 17$, in which there is a largest spread between the concentrations presented for the different wind directions until $y/H=17$. From $y/H=17$ the results for all wind directions are very similar.

The difference becomes even greater when observed the horizontal transect $x/H=21$. In this case, the concentration decreases much less quickly in 45° wind direction along y -streets, so the plume is less diluted near the edge.

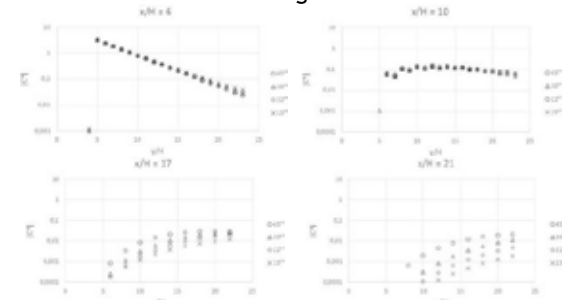


Figure 6. Comparison of lateral concentrations profile in horizontal transects within the canopy layer ($0 \leq z/H \leq 1$).

A comparison of longitudinal concentrations profiles was made for the different wind directions in the horizontal transects near the source ($y/H=6$, $y/H=8$) and away from the source ($y/H=14$, $y/H=22$). Figure 7 shows these profiles.

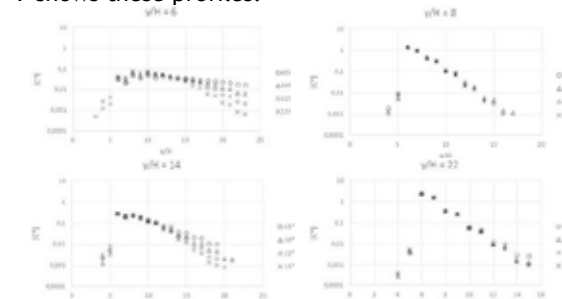


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It is perceptible that the differences between the longitudinal concentrations profiles are very subtle as well as in lateral concentrations profiles.

These small oscillations may be due to the source location. The source was positioned in a long street which provides the pollutant channeling in y-direction. In addition, the building geometry is also a factor that induces this dispersion behavior in the array configuration. Thereby, for this arrangement of rectangular buildings and considering that the source is in a long street location, changes in wind direction do not influence considerably the lateral and longitudinal dispersion of the contaminant. Perhaps, in a different source location like in an intersection, the pollutant dispersion may be more influenced for the wind directions.

CONCLUSION

Street network model proved to be an adequate methodology for dispersion modeling considering in an array of rectangular and aligned buildings. From the comparison with the LES data it has been demonstrated that the main relevant dispersion processes are captured.

The plume behavior was described properly demonstrating that the advective transport mechanism and the vertical turbulent transfer of pollutants within and above the canopy layer were adequately represented in the street network model. It was possible to observe the channeling along y-street as well as the spread of the plume. So, the street network was able to represent adequately how the dispersion occurs in this situation.

When the simulations were performed in a street network model in that arrangement of buildings considering different wind directions it was possible to note that the concentrations profiles are very similar for all situations analyzed in the regions closest to the source. But, when concentrations profiles are drawn near the edges the largest differences appear. For wind directions approaching 0° the concentrations decay faster laterally.

It was observed that for the longitudinal spread in cases of various wind directions the results are very similar too. There are slight differences near the edges ($y/H=6$ and $y/H=14$) like happens in the lateral dispersion.

In general, the longitudinal and lateral concentrations profiles demonstrated that even when there are differences between the results from different wind directions, they are very subtle. That means that in an array with rectangular buildings, when the source is located in a long street the influence of the wind direction was demonstrated weak.

It is recommended to evaluate the street network model inputting other complexities into the urban arrangement like buildings of different heights, for example, with the view to try to get increasingly closer to the reality. In addition, further studies can be performed from the arrangement considered in

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Early alert system of PM_{2.5} validation for Bogotá, Colombia through modeling software WRF-CHEM

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Abstract: Latin American cities such as Bogotá has environmental problems related to air quality mainly by PM_{2.5}. In addition, Bogotá does not have an efficient Early Alert System (SAT), in consequence the health of citizens has been seriously affected. The objective of this research is to model PM_{2.5} concentrations with the WRF-Chem model, the model was modified and validated for Bogotá conditions during dry and humid periods from 2018 - 2019. For this purpose, air quality data from RMCAB and EDGAR-HTAP were downloaded. For meteorological and terrestrial variables were used the values provided by the Global Forecasting System. In order to validate the results, the mean quadratic error (MSE), correlations, BIAS and Taylor diagrams were calculated by comparing the output data of the WRF-Chem with data of the RMCAB. The model output values were classified according to the ICA levels established in resolution 2254 of 2017 for 1 of 12 air quality stations (Carvajal) because of an alert emitted by the Bogotá government in this station. The best adjustment model to the observed data has a resolution of 1.666 meters, with a correlation of 0,18, MSE of 34,16 and a BIAS of 5,44. Additionally, this model was able to predict with an error of 8% the alert for atmospheric pollution generated on February 15th, 2019 in the city of Bogotá. This is the first step of a much larger investigation, that pretend to evaluate all the city.

Keywords: SAT, WRF-CHEM, PM_{2.5}, Bogotá, air quality modeling.

INTRODUCTION

The Weather Research and Forecasting (WRF) model is a weather forecasting system developed by NOAA (National Oceanic and Atmospheric Administration). The program has integrated the chemical component (WRF-Chem) which includes the transformation, transport, mobility, mixing and deposition of trace gases and aerosols simultaneously with meteorology (UCAR, 2018). The physical component predicts variables such as wind speed, turbulence, radiation, temperature, among others.

In Bogotá city, PM_{2.5} is measured by RMCAB (Bogotá air quality monitoring system). To estimate the daily concentration of PM_{2.5} (Particulate matter), each daily data is calculated from the arithmetic average of

hourly values, with a temporal representativeness of 75%. Bogotá has 11 air quality monitoring stations which by 2017 registered 84% of valid data (Secretaría Distrital de Ambiente, 2017). With these data and the maximum limits of PM regulated in resolution 2254 of 2017, it could be determined that some stations presented 21 µg/m³ above the threshold in the polluting load of the city from particulate matter. The Bogotá Air Quality Index (IBOCA) is designed to disseminate the data obtained from the RMCAB and classify them on a measurement scale that determines how favorable the air quality is in real time (IBOCA, 2016) according to the levels set in the resolution.

In the city, air pollution by particulate matter has posed a threat to human health (Mészáros, 1999). In 2007, models robust enough to evaluate the implementation and

effectiveness of strategies to reduce PM concentrations were established (e.g., Rojas et al. 2010; Rojas et al. 2006). Different types of studies have been developed to explain by means of models the atmospheric behaviour of the city (e.g., Kumar et al., 2016; Saavedra 2016; Ruíz, 2015).

This document presents the validation of a PM_{2.5} air quality early alert system for one station of the city of Bogotá, Colombia with the WRF-Chem model modified for the city's meteorological conditions. It was modeled and compared in two periods, one dry and one humid in 2018 - 2019 respectively.

METHODS

The initial conditions for the model were taken from the Global Forecast System (GFS) and the topographic and latitudinal data offered by the Geographical Institute Agustín Codazzi (IGAC) was modified to get a closer approximation to the real terrain, since this allows to reduce model errors.

The WRF-Chem model has a program or component in charge of data pre-processing (WPS, WRF Preprocessing System). The WPS has three subprograms, *geogrid.exe*, *metgrid.exe* and *ungrib.exe*. This process uses a file that specifies the days to model, the type of projection to use, the number of domain and the resolution.

We run the model four times with two different resolutions, these were carried out from 14th to 15th February 2019 (dry period) in order to simulate the Unhealthy alert generated in southwestern Bogotá and the Unhealthy sensitive groups alert in the rest of the city. The other two simulations were made from 22nd to 23rd November 2018 (humid period), the comparison between these two periods was made to determine the effectiveness of the model under different meteorological characteristics.

Two different settings were implemented for the parameterization of the WRF. In microphysics, WRF Single moment 3 class and 5 class Schemes and ETA Ferrier microphysics schemes were used, for the cumulus

Kain-FRITSCH and Grell 3D Ensemble Schemes. For the radiation the Dudhia Shortwave Scheme was used, finally, in the boundary layer the Revised MM5 Scheme was used for the resolution of 1.666m, while the 500m was turned off the parameterization.

For the design of the early alert, the air quality indexes established in resolution 2254 of 2017 (MADS, 2017) will be used. These indices, have a dimensionless value and are used to report the state of air quality according to a color code associated with effects that must be considered to reduce exposure of the population to high concentrations of PM_{2.5}. This index is also used in air quality forecasting.

Data from the WRF-Chem model were plotted using a Python algorithm that also calculates MSE, BIAS, correlation and Taylor diagrams. The validation was made taking as observations the concentrations reported by the RMCAB.

FINDINGS AND ARGUMENT

Analyzing the temporal variation of the hourly concentrations of PM_{2.5} for the simulations of the months of February and November a similar behavior is observed, on the other hand the model with the highest resolution does not recreate the trend of the observed data, while with a low resolution the trend is closer (Fig. 1, Fig. 2). Maybe this is because the program in a high resolution explicitly solves the equations for convection and also a parameterization was assigned, therefore this increase the values and creates an error.

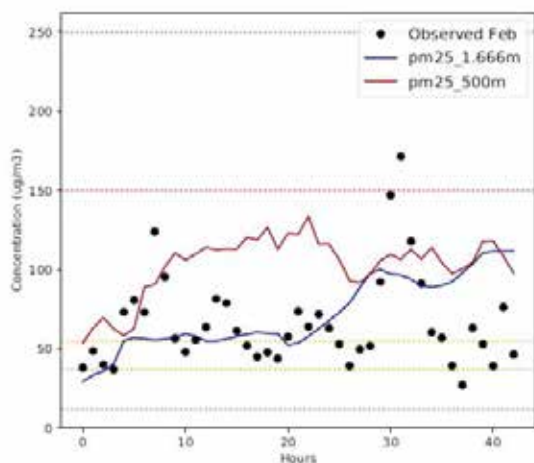


Fig 1. Concentrations of $PM_{2.5}$ for the 14th and 15th of February 2019 in the air quality station of Carvajal, Bogotá, Colombia. Continuous red line: model with resolution of 500m, continuous blue line: model with resolution of 1.666m, black points: data recorded dotted green: limit of the air quality index with good category, yellow dotted line: acceptable, dashed orange line : Harm to health for sensitive groups, Dotted red line: Harmful to health, Dotted purple line: very harmful to health, Brown line: dangerous.

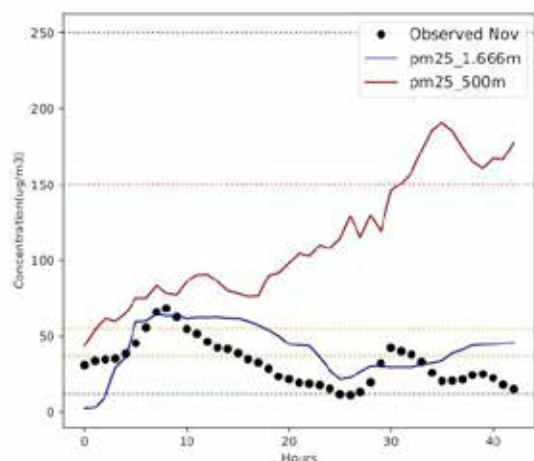


Fig 2. Concentrations of $PM_{2.5}$ for November 22nd and 23rd, 2018 in the air quality station of Carvajal, Bogotá, Colombia. Continuous red line: model with resolution of 500m, continuous blue line: model with resolution of 1.666m, black points: reported data, dotted green line: air quality index limit with good category, yellow dotted line: acceptable, line Dotted orange Harmful to health for sensitive groups, Dotted red line: Harmful to health, Dotted purple line: very harmful to health, Brown line: dangerous.

The Taylor diagram (Fig. 3) for the two models (1.666m and 500m) in February shows a correlation with values of 0,18 and 0,12 respectively and a standard deviation of 0,1 for the two models. The mean quadratic error (MSE) had values of 34,16 and 48,96, BIAS 5,44 and 36,32. It is analyzed that the models in a dry period have favorable results in the standard deviation, however the BIAS has high values in the resolution of 500m probably due to the explicit solving and parameterization of the convection explained previously. As a result, the BIAS increases.

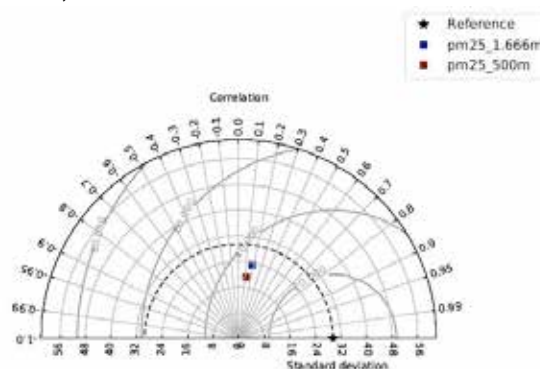


Fig 3. Taylor diagram of the 14th and 15th of February 2019. Blue dot: model with 1.666m resolution, Red dot: 500m resolution model, black dot: reference.

In the Taylor's diagram of November, only the model is observed at 1.667m (Fig. 4) because as shown in Fig. 2 at 30 hours, the model with high resolution (500m) loses the trend of the data and therefore the correlation is very low -0,47. However, for the resolution of 1.667m it shows a deviation of 10 and a correlation between the data of 0,52. The MSE for the 1,667m is 18,04 and 94,83 for the 500m model, while the BIAS had values of 9,56 and 80,36 respectively. The model with the lowest resolution in a humid period had a high data correlation and the lowest errors among the four simulations.

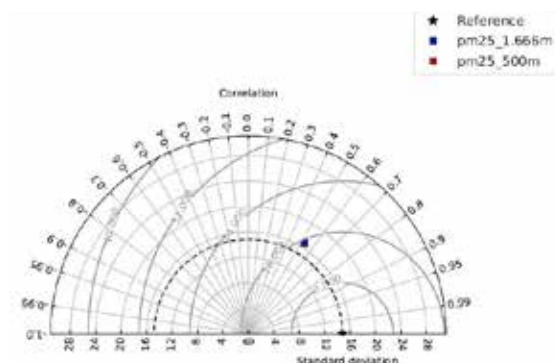


Fig 4. Taylor diagram of November 22nd and 23rd, 2018. Blue dot: model with 1.666m resolution, Black dot: reference.

The Air Quality Index (ICA) is determined for the observed and modelled concentrations for February and November respectively (Table 1). In addition, it is determined for each value whether the concentration reached a level of prevention, alert or emergency. For February 14th, the model with the highest resolution was able to predict the alert with an error of 12,07%. By February 15th, both models predicted the alert with an error of 12,67% for the highest resolution and 8% for the lowest. In November 22nd and 23rd, the model with the lowest resolution was able to predict the alert level with an error of 24,05% and 31,45% respectively for Carvajal station.

	Day	Observed data	Modeling 500 m	Modeling 1667 m
		ICA and Alert level	ICA and Alert level	ICA and Alert level
February 2019	14	154,67	173,34	145,71
	15	158,56	178,65	171,26
November 2018	22	101,8	161,85	130
	23	71,85	203,35	94,45

Table 1: ICA for $PM_{2.5}$ with the data observed and modeled for Carvajal air quality station on the 14th and 15th of February of 2019 and the 22nd and 23rd of November of 2018. The colors represent the level of the alert. Moderate: yellow. Unhealthy sensitive groups: orange. Unhealthy: red. Very Unhealthy: purple.

CONCLUSIONS

The model physics that best adapts to the observations was the ones used for February using a resolution of approximately 1.666m and integrating it with the topography offered by the IGAC. For this model the correlation was 0,18, MSE 34,16 and BIAS 5,44 for one

station data. The model managed to make the early alert prediction for poor air quality in Bogotá with an error of 8%, so the model is able to predict the alert, but overestimates the concentrations of particulate matter.

In the future it is expected to continue executing the model with different parameterizations to reduce errors. After this, it is expected to validate the model for all Bogotá air quality stations and generate an early alert that produce information for the early alert protocol of the city.

It is suggested for future research to develop studies that determine better parameterizations for models with high resolution in areas with complex topography. This would advance our understanding of atmospheric dynamics in regions similar to Bogotá.

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EVALUATION OF THE CHEMICAL TRANSPORT OF POLLUTANTS IN THE METROPOLITAN AREA OF SALVADOR, BRAZIL

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Abstract: This work presents an evaluation of the chemical transport of the ozone (O_3) over the Metropolitan Area of Salvador (MRS, which in Portuguese is “Região Metropolitana de Salvador”). The meteorological information required by the air quality modeling was driven by the Weather Research and Forecasting (WRF) model. For the emissions inventory, it was applied the Emissions Database for Global Atmospheric Research (EDGAR), in conjunction with an estimated emissions inventory of the major industrial complexes located at the RMS, in addition with the biogenic emissions estimated by the Model of Emissions of Gases and Aerosols from Nature (MEGAN). Then, for the process of these different emissions inventories, it was used the Sparse Matrix Operator Kernel Emission (SMOKE). Finally, the Community Multi-scale Air Quality (CMAQ) model was applied in order to simulate the dispersion, chemical transport and formation of the O_3 . The required boundary conditions were determined by applying the CMAQ model with the MEGAN and EDGAR global emissions inventory to a larger domain that incorporates the domain in which the RMS is represented. Due to the lack of air quality measurement data in the region, the results were analyzed in a qualitative way, and showed the importance of the application of these modeling tools in order to assess the air quality of the RMS. Thus, this work aims to be the first great effort for the RMS to study and simulate the chemical transport of pollutants based on a hybrid emissions inventory using the state of the art in the computational atmospheric modeling field.

Keywords: WRF-CMAQ, EDGAR, Salvador, air quality, air pollutants.

INTRODUCTION

The MRS is an urban-industrial area located at the State of Bahia, in the Brazilian Northeast region. It is composed by 13 municipalities, and although it is a very populated region, with around 4 million inhabitants and several enterprises of chemical segment, there is no official emissions inventory for the region, and consequently, there isn't any study with a proper diagnosis of the air quality status of the MRS.

Despite the lack of information of the atmosphere conditions, the land use and cover changes, and an emissions inventory of the MRS, which is also a worrisome situation in others Brazilian capital cities (Alonso et al, 2010), some efforts of our research group are being made in order to understand the chemical transport of air pollutants over the MRS.

A previous work evaluated qualitatively the dispersion of the atmospheric pollutants (NO_x and SO_2) over the RMS. The emission sources considered in that work were single stacks located at Camaçari Industrial Complex (CIC), and it was evident the need of the development of a proper emissions inventory for the region (Kitagawa et al, 2017).

Since the construction of a proper emissions inventory has not been carried out yet, we are trying to employ different approaches and methodologies to provide some kind of scientific background about the impact of air pollutant emissions over the MRS.

Then, a hybrid emissions inventory was build-up using information from EDGAR and MEGAN global dataset, and also from a local estimated emissions inventory based on point sources of the major industrial complexes, namely the Cristal factory, the Camaçari Industrial Complex (CIC), the Aratu Industrial Center (CIA), and the Landulpho Alves Refinery (RLAM) (see Figure 1).

Therefore, this work presents a qualitatively evaluation of the application of data from MEGAN, EDGAR and a local inventory on the formation and dispersion of the secondary pollutant ozone (O_3) over the MRS using the WRF (Skamarock et al, 2008), SMOKE (UNC, 2018), and CMAQ (Byun and Schere, 2006) modeling system.



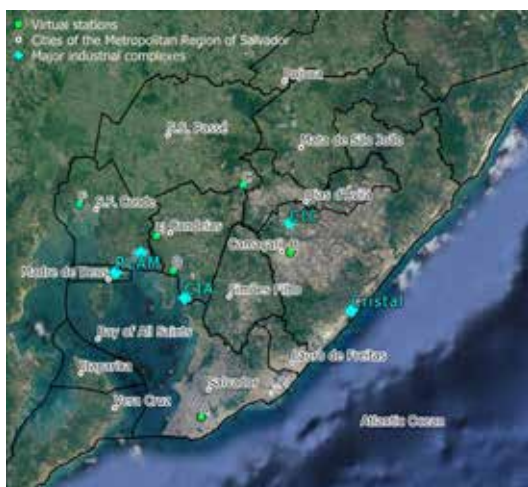


Figure 1: The location of Bahia state in Brazil (upper left), the domains used in the simulations (upper right), the major industrial complexes (cyan dots), and the virtual stations (green dots).

METHODS

As mentioned before, the study was carried out using the WRF (v. 3.9.1), SMOKE (v. 4.6), and CMAQ (v. 5.2.1) modeling system to simulate the meteorological fields, to process the emissions, and to simulate the chemical transport of ozone concentrations, respectively.

The WRF model was configured with 3 nested domains with grid resolutions of 9 km (D01), 3 km (D02), and 1 km (D03 - domain of interested). WRF meteorological input data came from National Centers for Environmental Prediction (NCEP) Final Analysis (FNL) at 0.25° resolution (NCEP, 2015) while the land use data were provided by United States Geological Survey (USGS) at 5 min, 2 min and 30 s resolutions. Simulations were performed during two episodes in order to evaluate possibly seasonal differences. Then, one period comprised the dry season (Jan. 16 - Feb. 15), and the other the rainy season (Jun. 23 - Jul. 23) of the year of 2015.

The MEGAN model (Guenther et al, 2012), version 2.04, used meteorology and land cover data from WRF to provide emissions in a suitable format for SMOKE processor. Emissions data of CO, NO_x, NMVOC, NH₃, SO₂, BC, OC, PM₁₀, PM_{2.5} from the EDGAR (Crippa et al, 2018), version 4.3.2, with spatial resolution of 0.1°, and base year of 2012 were also applied.

Both, MEGAN and EDGAR, were used in the simulations with the D01 and D03 domains. That was done in order to provide time-dependent boundary conditions (BC) to the D03. The default boundary conditions profile using the Carbon Bond 05 (CB05) gas-phase chemical mechanism, with the sixth-generation aerosol and aqueous modules (AERO6), for the boundary conditions pre-processor

BCON, also was applied in the D01 to evaluate its impacts to the simulations for ozone in the D03. A simulation using BC with all concentrations set to zero values was also tested. The features of boundary conditions and emissions data used in each simulation is summarized in Table 1.

The local inventory used information of Lyra's work (2008) who estimated the emission rates of SO₂, NO_x, CO based on the data of consumption, the fuel composition, the type of boiler/furnace, the hours of operation per year and the oil/gas density. Thus, 42 companies were listed and 203 point sources were computed only in the runs with the domain D03.

Table 1. Settings of the CMAQ simulations.

Simulation ID	BC	Inventory for D03		
		EDGAR	MEGAN	Local
00	Zero-values	x	x	x
01	EDGAR-MEGAN from D01	x	x	x
02	Default	x	x	x
03	EDGAR-MEGAN from D01		x	x
04	Default			x
05	EDGAR-MEGAN from D01			x

To assessing the ozone concentrations, the time series were analyzed by creating virtual air quality stations in the MRS (Figure 1). The stations were placed in sites where either had already been reported the annoyance caused by air pollution; or sites nearby the industrial complexes. Although they are virtual stations, their locations (latitude and longitude) were determined by the physical presence of air quality monitoring stations in the region, but that still do not have concentration data measured for model validation. The location of virtual stations is listed in Table 2.

Table 2. Location of the virtual air quality stations in the MRS.

Virtual Station	Description	Lat.	Lon.
A	Salvador city (nearby a heavy-traffic road)	-12.98	-38.47
B	Camaçari city (nearby CIC)	-12.71	-38.32
C	Lamarão (in São Sebastião do Passé, nearby CIC)	-12.60	-38.40
D	Gamboa (in Candeias, nearby CIA and RLAM)	-12.74	-38.52
E	Malembá (in Candeias, nearby RLAM)	-12.68	-38.55
F	SFC (São Francisco do Conde city, nearby RLAM)	-12.63	-38.68

The CMAQ plots are presented at local time and were made using the Python packages with the Google Earth program. They are shown in the next section.

FINDINGS AND ARGUMENT

Ozone is considered the major product of tropospheric chemistry, and its production can occur in the presence of various substances, which are considered its precursors, and mainly are: nitrogen oxides (NO_x), volatile organic compounds (VOCs), carbon monoxide (CO), and methane (CH_4) (Seinfeld and Pandis, 2006).

Figure 2 presents the variation of maximum mean hourly O_3 for the dry (solid lines - upper) and rainy (dashed lines - lower) season for each performed simulation, interchanging the MEGAN, EDGAR and local inventories, and also the boundary conditions.

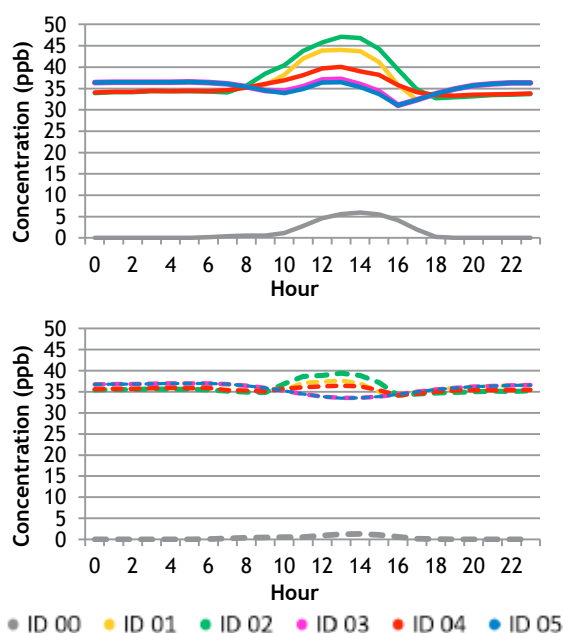


Figure 2: The maximum mean hourly O_3 variation during the dry (upper) and rainy (lower) season, comparing the application of the different inventories and BC.

It can be observed that the ozone in the MRS follows a typical secondary photochemical pollutant profile, with minima occurring in the dawn, increasing during the day with peaks occurred at 1 p.m. in both seasons, and decreasing again at night. The exception was the simulation ID 03 (magenta lines) and 05 (blue lines) in the rainy season, which showed an inversely behavior and were performed by the BC provided by a previous run for D01 with MEGAN and EDGAR inventories, however they differ in the inventories used in the D03.

By the way, the simulation ID 03 and 05 presented almost the same behavior in the dry season, and an identical behavior in the rainy season, meaning that the MEGAN input data may not influence the ozone simulations in CMAQ model.

It also can be noted that the amplitude in the dry season was greater than during the rainy season. The simulations performed for the dry period reached concentration values around 47 ppb, while the rainy season the maximum concentrations were less than 40 ppb.

Comparing the ID 01 (green lines) and 02 (yellow lines), which the unique difference is the BCs applied; the CB05 mechanism had the highest concentrations values in both seasons. The same behavior occurred when it is compared the ID 04 (red lines) and ID 05 (blue lines), which the only difference again was the BCs applied, however only applying the local inventory in the D03 domain.

The greatest difference between all simulations was when the boundary conditions were set to zero values (the ID 00 - grey lines), showing clearly the impact of applying BC in the ozone simulations.

Figure 3 shows the mean hourly O_3 concentrations for each simulation, for both seasons, and at the point where virtual stations are located at, namely Salvador (a), Camaçari (b), Lamarão (c), Gamboa (d), Malemba (e), and SFC (f).

As mentioned before, the simulations ID 01 and 02 (which applied the “full inventory” - EDGAR, MEGAN and local) presented almost the same behavior for all virtual stations, even using different BC. Similarly, the simulations ID 03 and 05 had identical behavior with very slightly variation, however the reason for this behavior was the non-influence of MEGAN.

Although the mean hourly O_3 concentrations presented similar values for both seasons and for all simulations tested (except when the BC were set to zero), the highest O_3 concentrations were noted mostly during dry season.

To Salvador (a) and Camaçari (b), the daily variation was not so prominent when compared with the other sites, which means that O_3 concentrations virtually remain constant throughout the day. The areas that presented the highest values was Lamarão (c), Malembá (e), and São Francisco do Conde (f), which are approximately 10-15 km downstream from the industrial sources of CIC, and RLAM, respectively.

If we would evaluate in terms of the air quality standards established by the Brazilian Environmental Council, the O_3 concentrations would

not exceed the limit, which is 50 ppb. However, according to Neves (2009), who evaluated observed O_3 concentrations in CIC and RLAM refinery and their surroundings, he reported several peaks with values around 70 ppb, in the south of CIC, and records in Camaçari city center reached 100 ppb (virtual station 'B'). In the northwest of CIC (virtual station 'C'), it was registered even worse hourly O_3 concentrations, with peaks between 100 and 200 ppb. To the RLAM refinery, the maximum hourly O_3 concentrations values were around 40 and 70 ppb (virtual station 'E').

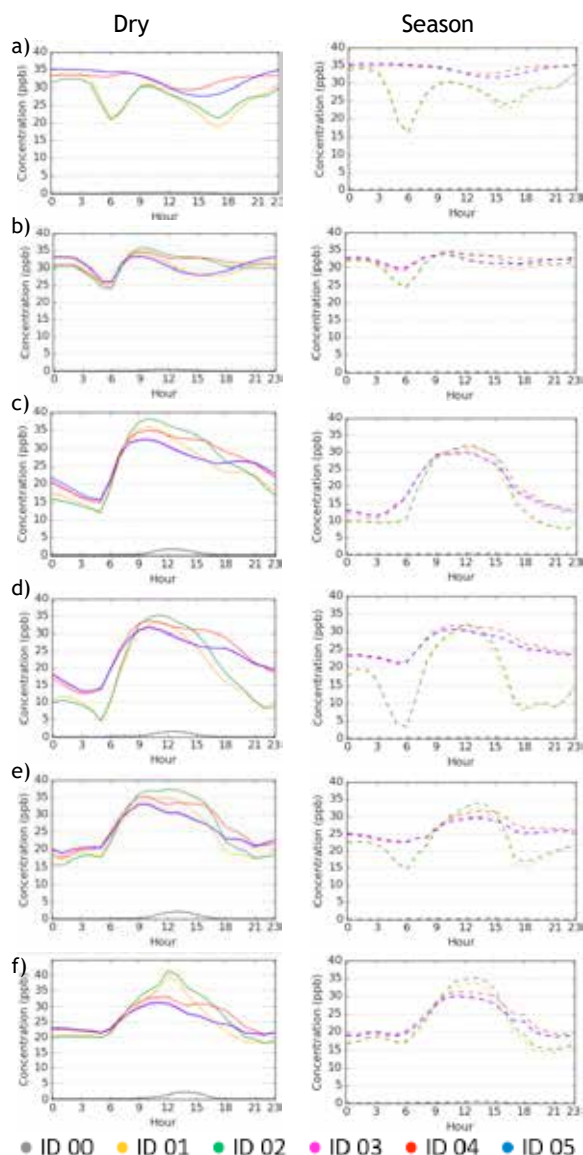


Figure 3: The mean hourly O_3 variation at the virtual stations, at local time, for dry (left) and rainy (right) season, comparing the application of the different inventories and BC.

CONCLUSIONS

The main purpose of this work was to assess qualitatively the dispersion of the secondary pollutant, ozone, from a hybrid inventory build-up with information from EDGAR, MEGAN and a local estimated inventory by using the WRF-SMOKE-CMAQ modeling system. The assessment was performed by combining, in different ways, the input data described above and the boundary conditions. Seasonal differences of observed data between dry and rainy seasons were quite difficult to be noted, however the daily variation were captured by the CMAQ model. The MEGAN data seemed not significantly to contribute to the production and consumption of O_3 . Local inventory only has counted with industrial point sources, missing the representation of others types of sources, such as the vehicular emissions, which for sure would influence on the production of O_3 . The use of the default BC produced the highest O_3 values. It was evident that the BC influenced the CMAQ results as well as the different combinations of inventories used in the D03 domain. For future works it is recommended to analyze in more detail the BC applied to the MRS, including the usage of global photochemical models like GEOS-Chem (Bey et al, 2001) model to provide BCs to the regional photochemical modeling.

ACKNOWLEDGMENTS

The authors thank the CIMATEC Supercomputing Center for Industrial Innovation (Yemoja), the Fundação de Amparo à Pesquisa do Estado da Bahia (FAPESB), the NQualiAr research group of UFES, and also to the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for granting the PhD scholarship to the first author.

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MODELING GAS-PHASE POLLUTANTS IN PARIS CITY USING STREET-IN-GRID MODEL

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Abstract: Nowadays air pollution is a serious problem in many big cities, causing harmful effects on human health and environment. Air-quality models are often used to simulate pollutant concentrations to which the population is exposed. Regional scale air-quality models have coarse spatial resolution, and thus are adapted only to simulate background concentrations. They fail to simulate the high concentrations observed close to roads and in streets, i.e. where a large part of the urban population lives. Local scale models may be used to simulate concentrations in streets. They often assume that background concentrations are constant and/or use simplified chemistry. Recently developed, the multi-scale Street-in-Grid (SinG) model is capable to estimate gaseous pollutant concentrations simultaneously at local and regional scales, coupling them dynamically. This coupling combines the chemistry-transport model Polair3D, with a comprehensive treatment of atmospheric transport and chemistry at regional scales, and the street network model MUNICH (Model of Urban Network of Intersecting Canyons and Highway), which estimates pollutant concentrations in the streets. MUNICH models explicitly street canyons and intersections, and it is coupled at the first vertical level of the chemical-transport model, enabling the transfer of pollutants mass between the street canyon roof and the atmosphere. The original versions of SinG and MUNICH adopt a stationary hypothesis to estimate pollutant concentrations in the streets. This study presents a dynamic approach to calculate pollutant concentrations in streets. Because the stationary hypothesis is not made, it is more appropriate to represent secondary pollutants formation. Air quality simulations of gaseous pollutants are run with Polair3D, SinG and MUNICH over Paris city to (i) estimate the impact of the stationnary hypothesis on pollutants concentrations in streets, (ii) estimate the added value of a dynamic multi-scale modeling approach for these pollutants. Concentrations obtained with the different simulations are compared to observations at traffic and urban air quality stations. As expected, the regional chemical-transport model Polair3D underestimates pollutant concentrations in the streets. With the street models MUNICH and SinG and the stationnary hypothesis, NO_x concentrations are well modelled, but the partitioning between NO and NO₂ is highly sensitive to time step. However, in both MUNICH and SinG, the dynamic approach is numerically stable, with a relatively good agreement between measurements of NO and NO₂ and the simulated concentrations. Streets aspect-ratio (ratio of street height and width) is an important parameter to indicate the importance of multi-scale modeling, especially for NO₂.

Keywords: Air quality models, multi-scale coupling, gaseous pollutants, numerical parameters, street-network.

INTRODUCTION

Air pollution is a serious problem in many cities due to its considerable impacts on human health and environment, as reported in WHO (2000), Katoto *et al.* (2019), De Marco *et al.* (2019), Wang *et al.* (2019). These impacts motivated the development of air-quality models, which estimate pollutants dispersion at a determined spatial scale. These models are largely employed to calculate the population exposure and they can support public strategies for pollution control.

Regional scale air-quality models, as three-dimension gridded Eulerian models (e.g. Polair3D (Boutahar *et al.*, (2004), Mallet *et al.*, (2007), Sartelet *et al.*, (2007)), CHIMERE (Menut *et al.*, (2014)) and CMAQ (Community Multi-scale Air Quality Modelling System) (Byun and Ching (1999)) solve a chemistry-transport equation for divers chemical species. The calculated concentration for each grid cell is averaged over the whole grid surface, in general with a coarse resolution. They are employed to simulate background

concentrations, but they are not capable to represent the variations observed between near-traffic areas and background urban concentrations. Therefore, many street-network air-quality models were developed to estimate pollutants concentration at the local scale more accurately and with a relatively low computational cost. A limitation of street-network models is the assumption that background concentrations are constant and/or calculated with simplified chemistry. Expanding the interactions between regional and local scales, Street-In-Grid (SinG) is a new multi-scale model (Kim *et al.*, 2018) capable to estimate gaseous pollutant concentrations simultaneously, coupling dynamically the regional and local scales. SinG associates the regional scale model Polair3D (Mallet *et al.*, 2007) and the street-network model MUNICH (Kim *et al.*, 2018). Although the coupling between Polair3D and MUNICH is dynamic, SinG and MUNICH originally adopt a stationary hypothesis to calculate pollutants concentrations in the streets. These models are available in the Polyphemus platform.

This study presents a dynamic rather than stationary approach to calculate pollutant concentrations in the streets using both MUNICH and SinG. This dynamic approach is more appropriate to represent secondary pollutants formation in the streets. Air quality simulations of gaseous pollutants are run with Polair3D, SinG and MUNICH over Paris city to estimate the impact of the stationary hypothesis on pollutants concentrations in streets, and estimate the added value of a dynamic multi-scale modeling approach for these pollutants. Model validation at local and regional scales is based on comparisons with observations at traffic and urban air quality stations.

METHODS

Different numerical simulations were performed with SinG, MUNICH and Polair3d separately, considering or not the stationary hypothesis at the local scale. A robust treatment of three databases was performed in order to determine streets dimensions for the whole Paris city: BD-TOPO and OpenParis data for street width, APUR and OpenParis data for street height. Emission data were obtained from Aiparif inventory, meteorological data were calculated by a two-way nesting WRF simulation, with a nudging technique in Paris domain. For MUNICH simulations, background concentrations were obtained from a Polair3d simulation. The simulation period is 1st May to 25th May 2014.

FINDINGS AND ARGUMENT

As observed in Figure 1(a), concentrations of NO_x are independent of stationary/non-stationary hypothesis.

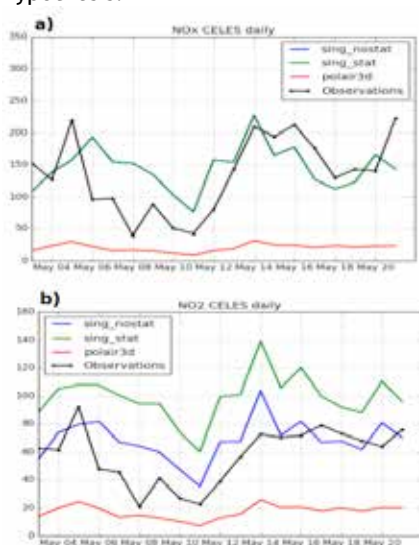


Figure 1. Temporal evolution (daily average) of NO_x (a) and NO₂ (b) concentrations at traffic station CELES.

On the other hand, NO₂/NO partition presented a considerable improvement with the non-stationary hypothesis, proving the importance of a fine coupling between transport and chemistry for these pollutants. As expected, Polair3d underestimates pollutants concentrations in streets.

Comparing the concentrations calculated by SinG and MUNICH, it is noted that streets with an intermediate aspect ratio α (ratio of streets height and width) can be more influenced by dynamic coupling between regional and local scales, especially for NO₂, as represented in Figure 2. The aspect ratio is directly connected to turbulent vertical transfer between the canopy and the atmosphere.

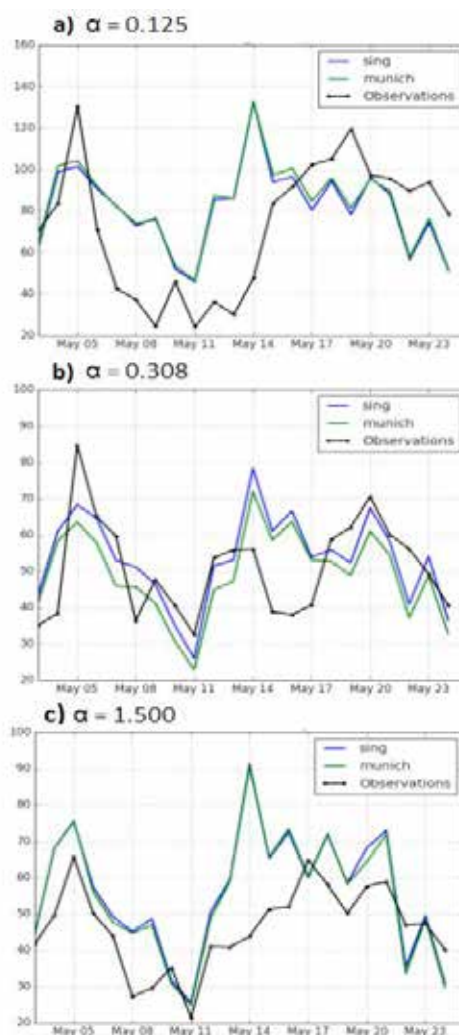


Figure 2. Temporal evolution (daily average) of NO_x (a) and NO₂ (b) observations and concentrations calculated by SinG and MUNICH in three streets with different aspect ratios.

CONCLUSIONS

In this study a multi-scale simulation was performed over Paris city to represent NO₂, NO and NO_x concentrations with a robust street model to estimate the added value of a dynamic multi-scale modelling. A treatment of different databases was performed to determinate street dimensions in the whole city.

Comparisons between stationary/non-stationary results demonstrate that a fine coupling between chemistry and transport is important for NO₂ and NO, but not for NO_x. Multi-scale and local scale simulations indicate that street aspect ratio is an important factor to determine the added value of dynamic multi-scale simulations.

A new version of SinG is in development to evaluate the added value of multi-scale simulations of particle-phase pollutants.

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USING COMPUTATIONAL FLUID DYNAMICS COUPLED WITH MESOSCALE WRF-CMAQ MODELLING TO PREDICT WIND FIELD AND AIR POLLUTANT CONCENTRATION IN A REAL URBAN AREA

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Abstract:

The Weather Research and Forecasting (WRF) and the Community Multiscale Air Quality (CMAQ) modeling systems are able to predict respectively meteorological variables and pollutant dispersion for large areas. However, these models are not able to accurately evaluate airflow or dispersion of pollutants inside the complex features of a real urban array, such as street canyons or intersections. The microscale CFD models, on the other hand, can account for the effect of complex building arrays on the urban wind field, as well as the dispersion of contaminants from different sources. In this sense, the use of mesoscale models coupled with microscale CFD models have the potential of presenting valuable information about street-level concentrations inside the urban canopy and the effects of building arrangements and layouts. In this work, WRF and CMAQ modeling systems are off-line coupled with a microscale CFD model based on ANSYS FLUENT. A 2 km x 3 km densely populated neighborhood in the Metropolitan Area of Vitória in Brazil is studied in the present work. WRF and CMAQ hourly outputs are used as time-varying boundary conditions for CFD simulations. An ANSYS FLUENT transient 3D simulation with 20 million tetrahedral elements was set up by solving the conservation equations for mass, momentum and chemical species. A standard κ - ϵ turbulence model was used to deal with turbulence effects in the fluid flow and chemical species transport. The simulations were performed using 64 processing cores of a Linux cluster based on Intel I7 processor. Data from a fixed meteorological and air quality monitoring station is used to validate the simulated wind and concentration fields obtained by numerical simulations. Overall, the microscale model results show a good improvement in relation to the prediction capability of mesoscale models. Nonetheless, it is important to note that the accuracy of the emission inventory and mesoscale prediction have a very significant impact on the CFD results.

Keywords: Urban air quality, CFD modeling, WRF model, CMAQ model, Modelling scale coupling.

INTRODUCTION

Urban air quality is a major concern worldwide, due to the fast growing urban population and increased volume of motorized traffic in cities. The evaluation of the airflow and pollutant dispersion in real urban areas has been a major challenge considering the size of the areas and all the physical phenomena involved.

The wind flow over urban environments is affected by the geometrical features of buildings which in turn influence the vertical and horizontal fluxes of pollutants within the urban canopy and above. Many works on this topic have been using field measurements, wind tunnel models and computational models to study characteristics of the wind field and dispersion over idealized and real urban scenarios (TOPARLAR et al., 2015, CUI et al., 2016, SANCHEZ et al., 2017).

In the last decade the use of photochemical air quality models has become significantly important for air quality management in urban regions, due to the potential for generating detailed information about the air pollution chemistry and meteorology of a region. The mesoscale modeling systems, such as Weather Research and Forecasting (WRF-CHEM) and Community Multiscale Air Quality (CMAQ), are able to predict respectively meteorological

variables and pollutant dispersion for regional areas, encompassing hundreds of kilometers with resolutions in the order of 1 to 10 kilometers.

However, these models are not able to accurately evaluate airflow or dispersion of pollutants inside the complex features of a real urban array, such as street canyons or intersections. The interaction between the wind flow over the urban canopy and the urban morphology induces complex flow patterns. Therefore, in order to obtain street level concentration data; the use of microscale models is necessary. Parameterized microscale models such as OSPM (Berkowicz, 2000), SIRANE (Soulhac et al., 2011) or ADMS-URBAN (Di Sabatino et al., 2008) have been applied to simulate urban air quality. Although this class of model is quite useful for several city morphologies, the empirical assumptions about the relation between the flow and dispersion of pollutants are significantly based on idealized urban patterns, such as squared geometries of uniform height buildings.

The microscale CFD models, on the other hand, can account for the effect of complex building arrays on the urban wind field, as well as the dispersion of contaminants from different sources. The use of microscale CFD models has the potential of presenting valuable information about street-level concentrations inside the urban canopy and the

effects of building arrangements and layouts. The main limitation of CFD modelling for urban environments is the computational effort required to simulate large urban areas with a sufficient level of detail, since urban areas may extend for several dozen kilometers and complex geometrical features of the urban morphology (such as buildings or road intersections) may require resolutions in the order of a few meters.

In this sense, the use of mesoscale models coupled with microscale CFD models may provide sufficient level of detail for critical areas of interest, while mesoscale models provide the general flow pattern and dispersion over the complete urban region.

Recently, many authors have used of mesoscale models coupled with microscale CFD models, such as Kwat et al. (2015), Liu et al. (2017) and Sanchez et al (2017). However, the computational effort is still a considerable challenge since air pollution applications usually require the calculations long averaging times for practical or regulatory applications. A cost-effective method is required to simulate the air flow and pollutant dispersion in a whole neighborhood at the building-resolving scale with hourly time resolution. Thus, a few authors have used different numerical approaches to deal with computational effort required. For instance, Berchet et al. (2017) relied on the pre-computation of a discrete set of possible weather situations and corresponding steady-state flow and dispersion patterns to meteorological observation in and around the city; and the most suitable situation for any given hour is then selected by matching the simulated wind patterns to meteorological observations in and around the city. Sanchez et al (2017) used a methodology based on weighted average of CFD simulations is applied computing the time evolution of NO_x dispersion as a sequence of steady-state scenarios taking into account the actual atmospheric conditions, by using a 8.3×10^6 grid point to model a neighborhood in Madrid with 1300m x 1300m.

In this work, a quasi-steady approach is used for the simulations coupling WRF-CMAQ mesoscale simulations, using 1 km resolution, with ANSYS-Fluent microscale simulation using 1.5m resolution of a neighborhood of 2000m x 3000m. A fully implicitly time integration with 1 hour time step is used deal with the time evolution of the microscale fluid field and NO_x, SO₂ and PM₁₀ concentrations over 1 month.

METHODS

The area selected to the study is a neighborhood called Jardim Camburi located in the city of Vitória, Brazil. It is an urbanized area that has 12 km² surrounded by the city's airport, industrial areas, other urban areas and also a coastal limit. This area

was selected considering the location of an air quality monitoring station operated by the State Institute of Environment (IEMA) installed inside the neighborhood, and the availability of data provided by the municipality used to build the computational geometry.

For the mesoscale simulations, both Weather Research and Forecast (WRF) and Community Multiscale Air Quality (CMAQ) models were used to provide the wind velocity, direction, and pollutant concentrations used as boundary conditions for the microscale simulation. WRF/CMAQ and FLUENT are coupled in an off-line way. The wind flow and concentration data for the grid cells near the lateral and the top boundaries of the CFD domain are extracted from WRF/CMAQ output files. Figure 1 presents a schematic representation of the solution procedure.

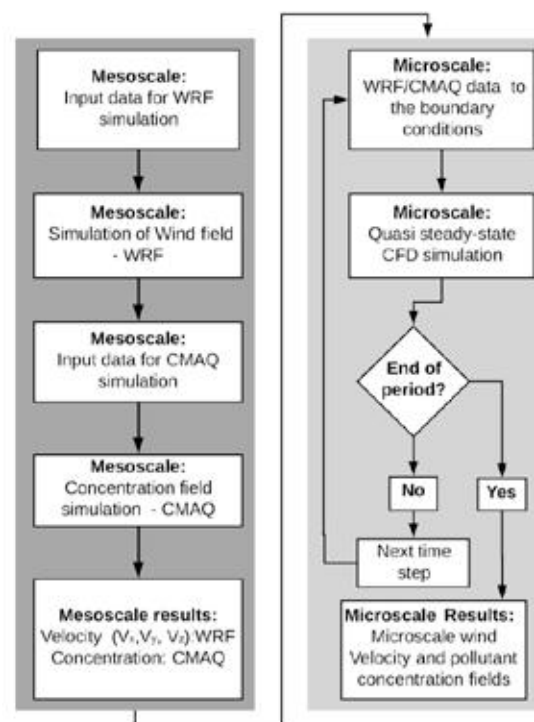


Figure 1. Schematic representation of the off-line coupling between WRF/CMAQ data to the CFD microscale model.

Figure 2a presents the nested computational domains used for the mesoscale simulations. The outer domain, D01, covers a great portion of the southeast region of Brazil, has 70 x 70 grid cells with horizontal resolution of 27 km. The innermost domain D04 is the more refined domain with grid cells of 1 km x 1km resolution, and 120 x120 grid cells.



Figure 2. (a) Mesoscale model domains and (b) details of the domain D04 and the points that delimit the neighborhood.

Figure 2b presents the region of study comprised by 14 WRF-CMAQ simulation cells, where data of wind velocity direction and concentration are hourly taken to be used as input data for microscale simulations.

The CFD simulations domain has a 3D grid with approximately 19×10^6 cells with a resolution inside the urban canopy of 1.5×1.5 m near the buildings and streets. The ANSYS FLUENT 19.2 is used to solve the governing equations conservation of mass, momentum, and chemical species, as shown respectively bellow, using a quasi-steady state approach (SCHLÜNZEN et al., 2011). To treat turbulence, it is used the Reynolds Averaged Navier Stokes (RANS), the k-ε standard model.

The CFD boundaries were divided in 110 regions corresponding to the faces of WRF/CMAQ computational cells (4 cells in the y direction, 3 cells in x direction and 7 cells in the z direction). Figure 3 shows the computational domain with the lateral and top divisions. The coupling of the mesoscale data to the microscale CFD simulation, a user-defined function (UDF) used to customize the boundary condition was applied to the CFD solver. Hourly data of wind components from WRF and concentrations from CMAQ are dynamically loaded by the UDF and assigned to each point of the domain.

CFD boundary cell faces with flow entering the computational domain are set as Inlet, with prescribed velocity obtained from the WRF computation. CFD boundary cell faces with flow exiting the computational domain are set as Outlets, with zero velocity gradients.

To evaluate the wind field, one of the cases designated CFD-Aero, was conducted using velocity components input from a weather station located at the airport.

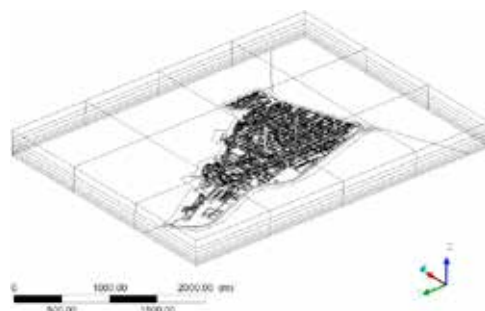


Figure 3. CFD computational domain showing the boundary regions derived from WRF/CMAQ simulation.

For the concentration field, data from the State's Official Emission Inventory was considered accordingly for the primary and secondary streets of the neighborhood. Figure 4 presents a schematic representation of the streets distributions as well as the indication of primary and secondary streets. Three main streets are considered primary streets (P1, P2, and P3) and the remaining are all secondary streets. Table 1 present the average emission considered.



Figure 4. Upper view of Jardim Camburi neighborhood, with the sources input: Red ways are the primary streets and blue ways, are the secondary streets.

Table 1. Emission rates for each street type.

	SO ₂ (µg/m ² s)	NO _x (µg/m ² s)	PM10 (µg/m ² s)
P1 Ave. Carlos Martins	0.7	14.4	34.8
P2 Ave. Dante Michelini	0.5	8.6	7.5
P3 Ave. Norte-Sul	1.2	18.6	17.8
Secondary streets	0.2	5.3	6.8

FINDINGS AND ARGUMENTS

Figure 5 presents a comparison between the results obtained by WRF-CMAQ mesoscale simulation, CFD coupled with the mesoscale model and the monitoring station for SO₂, NO_x and PM10. It is possible to note that there is a considerable

difference between the measurements and the results predicted by WRF-CMAQ mesoscale simulation, CFD coupled with the mesoscale model. In fact, the results obtained by CFD coupled with the mesoscale model are closer to the measurements, but since the WRF-CMAQ mesoscale simulation are used as boundary conditions for the CFD runs, the CFD results present significant level of over prediction as observed in the WRF-CMAQ mesoscale simulation.

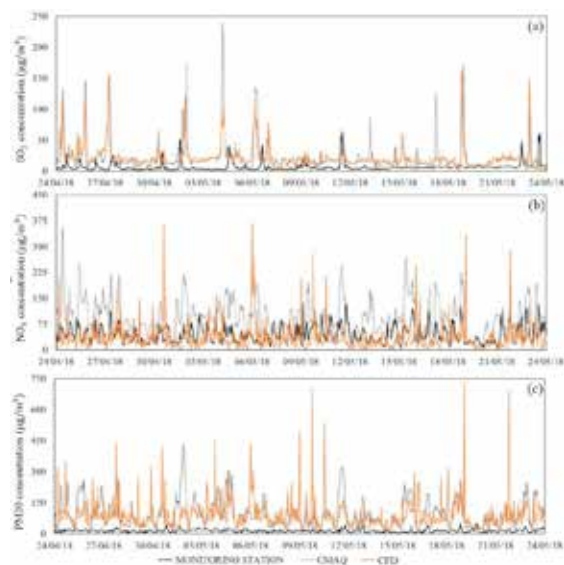


Figure 5. Time series of pollutant concentrations obtained by WRF-CMAQ mesoscale simulation, CFD coupled with the mesoscale model and the monitoring station for (a) SO₂, (b) NO_x and (c) PM₁₀.

On the other hand, Figure 6 presents a comparison between the results obtained by WRF-CMAQ mesoscale simulation, the monitoring station and CFD coupled with the mesoscale model without using WRF-CMAQ concentrations as boundary conditions. In this case, CFD coupled with the mesoscale model only uses the wind field derived from the WRF-CMAQ simulations. It is possible to note the results obtained by CFD coupled with the mesoscale model are significantly better than WRF-CMAQ mesoscale simulation in comparison with measured data.

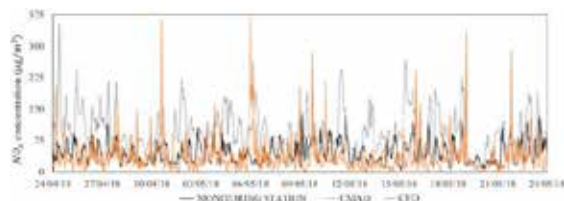


Figure 6. Time series of NO_x concentrations obtained by WRF-CMAQ mesoscale simulation, the monitoring station and CFD coupled with the mesoscale model without using WRF-CMAQ concentrations as boundary conditions.

This trend suggests that over-prediction obtained in the CMAQ runs causes a negative effect on the ability of the CFD code to predict the concentration dynamics. When the boundary condition over-prediction is removed, the results tend to present a much better agreement. This trend also suggests that air quality in the region is affected by local sources than regional or more distance sources of pollutant.

A similar trend can be observed by using bugle plot for NO_x considering statistical metrics with acceptance criteria proposed by Boylan and Russel (2006) - Figure 7. Values delimited by the green lines indicate a good prediction of the model, and those delimited by the red line indicate the minimum limit of acceptance of the results. The points outside the boundaries between the lines indicate bad results with great variability comparing measured and simulated. It is possible to note that results obtained by WRF-CMAQ mesoscale simulation tend to be positioned outside the limits of the green lines, while the CFD coupled with the mesoscale model without using WRF-CMAQ concentrations as boundary conditions presents results well within the green lines limits, which indicates a considerable improvement of the solution.

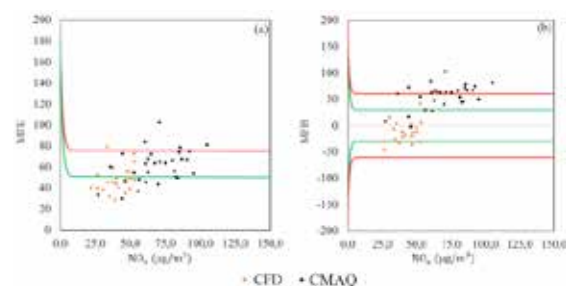


Figure 7. Bugle Plots of the daily average of NO_x concentration obtained by WRF-CMAQ mesoscale simulation and CFD coupled with the mesoscale model without using WRF-CMAQ concentrations as boundary conditions.

CONCLUSIONS

The accuracy or the coupling of mesoscale and microscale CFD modelling was evaluated against field measurements, and using some statistical metrics with proper acceptance criteria.

Overall, it is possible to conclude that the microscale model results have improvements in the prediction capability when using mesoscale data. The modelling shows to be robust, with results reproducing trends and peaks observed on the input data. It is as an advantage of the coupling to study, with acceptable accuracy, the wind flow and dispersion in urban areas that lack monitoring stations. Nonetheless, it is important to note that

the accuracy of the emission inventory and mesoscale prediction have a very significant impact on the CFD results. Improvements in the mesoscale precision could certainly increase the accuracy of the results from the simulations.

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AIR QUALITY FORECAST MODELS APPLIED IN THE METROPOLITAN REGION OF SALVADOR

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Abstract: The present work shows the pollutants dispersion of the anthropogenic emissions from the main fixed sources located in the Metropolitan Region of Salvador (MRS), the most populous state of the Brazilian Northeast. In this sense, the main objective of this study was to *evaluation of the online regional model WRF-Chem* (Weather Research and Forecasting Model with CHEMistry) e *CMAQ* (Community Multiscale Air Quality) over MRS with a focus of the concentration of atmospheric pollutants sulphur dioxide (SO₂), nitrogen oxides (NOX) and ammonia (NH₃) from the inventory of emissions of the Emissions Database for Global Atmospheric Research (EDGAR). Simulations were carried out using the CMAQ model and the WRF-Chem model. Due to the lack of measured ground level concentrations data, only a qualitative verification of the dispersion process was obtained. Despite this, the results show the relevance of the application of the state of the art in computational atmospheric modeling in order to verify the air quality in the MRS.

Keywords: MRS, WRF-Chem, CMAQ, air quality.

INTRODUCTION

Air pollution, especially in large cities, can pose risks to human health, as well as cause impacts on climate and the environment (Loriato et al., 2018). According to the World Health Organization (WHO), air pollution levels remain dangerously high in many parts of the world, new data shows that nine out of 10 people breathe air containing high levels of pollutants (WHO, 2018).

There are several pollutants that are released into the atmosphere, either by natural or anthropogenic sources, among them are carbon monoxide, nitrogen oxides, sulfur oxides, volatile organic compounds and particulate matter. The degradation of air quality is due to the presence of these pollutants and also factors such as location and concentration of sources, emission rates and

characteristics of the pollutants emitted, as well as their dispersion in the atmosphere and the chemical reactions that occur between them, which are strongly influenced by the meteorological conditions (IEMA, 2014). To address this problem, it is necessary to adopt air quality management systems that incorporate environmental management instruments to provide a measure both in space and time for concentrations of pollutants in the atmosphere, and thus to increase integrated actions to reduce concentration levels of primary and secondary pollutants in Metropolitan Regions and Megacities.

As an example of these instruments, it is possible to mention, besides air quality monitoring data, the Air Quality Models (MQAr). The MQAr promote more accurate studies and a complete assessment of air

quality in a region these models are divided into two broad categories: non-coupled models, in which the meteorology is calculated separately from the chemical model and models (on-line), in which meteorology and chemistry are coupled (Zhang, 2008). Air quality models are widely used in research and are able to predict concentrations and provide information on population exposure to air pollutants. Among the several existing models, it was chosen to work in this study with two MQAr, the Weather Research and Forecasting (WRF) model, integrating an on-line model called WRF-Chem (Weather Research and Forecasting Model with CHEMISTRY) used for air quality research on a regional scale, which includes a specific module for calculating the dispersion of air pollutants representing the physical phenomena and the photochemical reactions that affect the chemical species present in the atmosphere and condition the spatial and temporal distribution of concentrations. The second model is the Community Multiscale Air Quality (CMAQ), which represents the state of the art in air quality modeling and is widely used and recommended by the US Environmental Protection Agency (EPA) capable of modeling multiple air pollutants. Both are open source programs and have been supported by a scientific community that develops constant evolutions to reduce the uncertainties in the simulations (Nascimento et al., 2016).

WRF-Chem and CMAQ have been used in several studies on air quality. For example, Iriart and Fisch (2016) uses the WRF-Chem model to verify the CO dissipation in the region of the Launch Center in Alcântara, identifying intense winds as a responsible for a faster dissipation of pollutants. Also, in Andrade and Junior (2013) they used the model to evaluate the efficiency of the model in simulating the photochemical pollutants CO and O₃ on the Metropolitan region of São Paulo. Most recent in Kitagawa et al. (2018) and Pedruzzi (2016) used the Multiscale Community Air Quality (CMAQ) model to qualitatively evaluate the dispersion of atmospheric pollutants in Metropolitan Regions, all having good results.

Considering the need to better evaluate the pollutant dispersion (SO₂, NO_x and NH₃) of the anthropogenic emissions of the main fixed sources located in the Metropolitan Region of Salvador (MRS), the most populous state in the Brazilian Northeast, the main objective of this study was to evaluate the efficiency of the WRF-Chem and CMAQ models in simulating the photochemical pollutants for RMS, using as parameters the inclusion of emissions inventory of the Emissions Database for Global Atmospheric Research (EDGAR), in order to provide some scientific evidence that guides the relative decision making to the environmental risks

in which the population has been constantly exposed.

METHODS

The area under study is the Metropolitan Region of Salvador (MRS) located in the state of Bahia, between latitudes 12 ° 20'S and 13 ° 10'S and longitudes 37 ° 50'W and 38 ° 50'W, composed of thirteen cities and is occupied approximately 3.6 million inhabitants distributed in an area of 4375 km² (Brazilian Institute of Geography and Statistics, 2010). MRS is an urban-industrial area with a peninsular configuration and consists of a Bay located in the southwest of the region and east of the Atlantic Ocean. The Bay of All Saints (BTS) is a reentrance of the Brazilian coast where the sea penetrates the continent from a narrowing between the city of Salvador that is the capital of the state of Bahia and the island of Itaparica. Its presence adds local humidity due to evaporation, forming a humid tropical climate in the region. The period with the highest rainfall is the months of April-May-June-July, while the least rainy season is September-October-November-December. The mean annual temperature and humidity are 26 ° C and 80% respectively in Salvador, with higher values of the mean hourly wind speed in the afternoon and lower values during dawn and early morning hours (Silva, 2014).

With this in mind the scenario that encompasses several industrial activities such as chemical, petrochemical and automobile factories, whose industrial sources contribute to the total emissions in the region without counting the motor vehicles that according to the National Transit Agency, MRS owns a fleet of vehicles which represents 30% of the state of Bahia, the determinant factor for the choice of this region was due to the increasing industrialization, population and urbanization, in addition to the fact that there have been few previous studies evaluating air quality using modeling of photochemical pollutants in this region. The modeling was divided into two parts (one atmospheric and one chemical). To perform the meteorological simulations, the WRF Version 3.9.1 model was developed by NOAA, NCAR and other research institutes. The WRF model responsible for simulating the meteorological fields for a better understanding of the atmospheric, physical and atmospheric dynamics was configured as follows: three nested domains with grid resolutions of 9 km, 3 km and 1 km, shown in (Fig. 1a and 1b) An overview of the physical options adopted is listed in Table 1. The domain of interest has horizontal resolution of 1 km and twenty-one vertical levels with the top model set at 50 hPa. Previous work eg (Kitagawa et al., 2018) has already validated previously modeled data with the same configuration for this region.

In order to initialize the WRF model, the data of the global model of the National Centers for Environmental Prediction (NCEP), represented by the global operational model Global Forecast System - Final (GFS-FNL) with data of analysis of spatial resolution $0,25^\circ \times 0,25^\circ$ degrees and temporal every 6 hours, as initial and border conditions. Topography and vegetation cover data were obtained from the United States Geological Survey (USGS) at resolutions of 5 min, 2 min and 30s. The time period analyzed was March 19-27, 2016, with a spin-up of 24 hours to obtain realistic initial conditions. In the second and third domains that were run at 3 km and 1 km of spatial resolution, respectively, the simulations were performed using explicit convection.

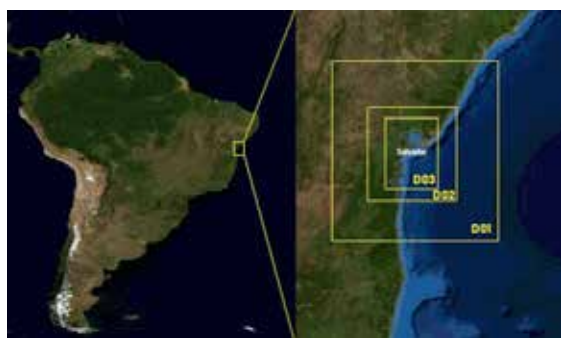


Figure 1a. The location of the MRS in Brazil (left) and Location of the three nested domains with grid resolutions of 9 km (D01), 3 km (D02) and 1 km (D03) (right).



Figure 1b. The location of the MRS in Brazil.

Table 1. settings of the WRF model for the simulation.

Physics parameterization	Schemes selected	Reference
Microphysics	Kessler	Kessler (1969)
Cumulus	Kain-Fritsch	Kain (2004)
Shortwave radiation	Dudhia	Dudhia (1989)
Longwave radiation	Rapid Radiative Transfer Model (RRTM)	Mlawer et al. (1997)
Surface layer	MM5 similarity	(Fairall et al. 2003)
Planetary boundary layer	Mellor-Yamada, Nakanishi and Niino 2.5	Nakanishi and Niino (2006)
Land surface model	Noah land surface scheme	

As an online model, WRF-Chem engages meteorological simulations with chemistry. After simulating the meteorological fields as described in the previous paragraph and obtaining intermediate files necessary for the processing of chemical data, the anthropogenic emissions are prepared through the anthro_emiss chemical emission preprocessor. Anthro_emiss is a Fortran program to create compatible anthropogenic emissions files (wrfchemi files) for a WRF-Chem simulation and is based on global emission inventory data with a latitude/longitude projection for initiating the chemical part of the model. In this work, the Emission Database for Global Atmospheric Research (EDGAR) with $0.5^\circ \times 0.5^\circ$ resolution was used to generate the wrfchemi initialization files to run the WRF-Chem.

The WRF-Chem simulation was performed for the period from March 19 to 27, 2016. The initial and boundary conditions for chemical fields in WRF-Chem were used data from the Model for Ozone and Related Chemical Tracers, version 4 (MOZART-4) (Emmons et al., 2010) coupled with the simple mechanism of GOCART aerosols.

The dispersion of pollutants (SO_2 , NO_x and NH_3) was also evaluated through simulations with the Community Multiscale Air Quality (CMAQ) model. 5.0.2. The domain used in the CMAQ, the terrain characteristics and meteorological conditions for the period were extracted from the D03 domain ($132 \times 132 \text{ km}^2$) of the simulation with the WRF model. The meteorological data obtained from the WRF model were preprocessed in order to obtain information necessary for the simulations with

CMAQ. The emission inventory used was the Emission Database for Global Atmospheric Research (EDGAR), even used with WRF-Chem and the chemical mechanism used was the CB-05.

FINDINGS AND ARGUMENT

The results of the air quality simulations are directly related to the performance of the WRF, thus, changes in concentrations over time result from local weather conditions.

To evaluate the chemical transport of SO₂, NO_x and NH₃, the height of the planetary boundary layer (PBLH), temperature in the PBL and the length of Monin-Obukhov were checked in order to observe the hourly variation generated by the atmospheric turbulence, which is responsible by the diffusion of pollutants.

To analyze the hourly evolution of the simulated meteorological variables, time series graphs were used. Figures 2 and 3 represent the hourly mean variation of the PBLH and temperature respectively simulated for the analyzed period, which was late summer and early autumn, characterized by high temperatures and dry weather conditions.

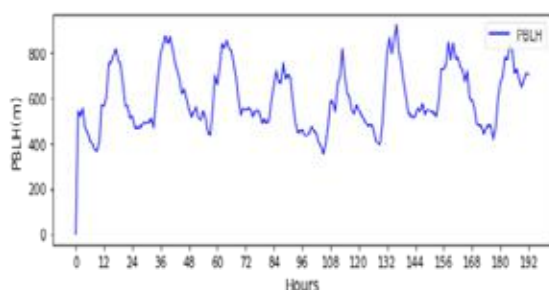


Figure 2. Mean hourly variation of simulated PBLH with WRF model.

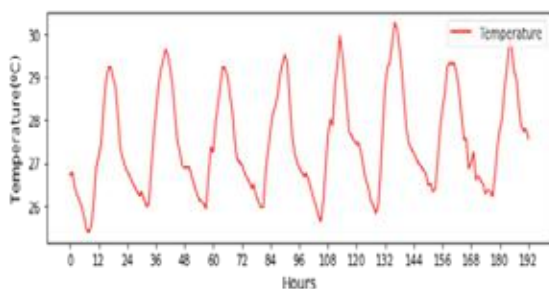


Figure 3. Mean hourly variation of simulated temperature with WRF model.

After evaluation of the temperature and height of the PBLH, the U10 and V10 directions (vertical and horizontal respectively, collected approximately 10 meters high) and the wind speed from these variables were evaluated. pink winds for simulated data. Through the roses of the winds it is observed that the simulated data presented prevailing easterly winds.

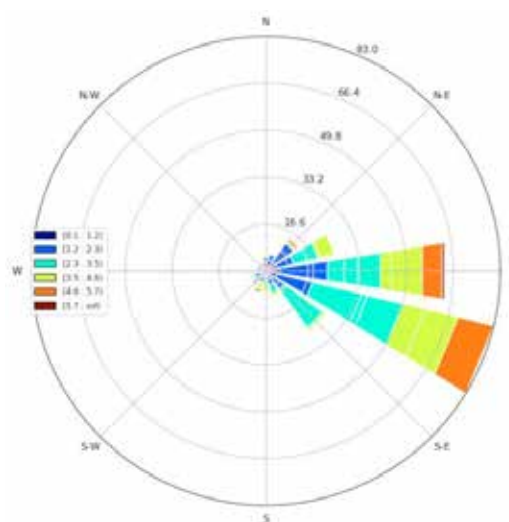


Figure 4. Wind roses of the simulated date with WRF model.

After the meteorological analysis, the performance of the WRF-Chem and CMAQ models (left to WRF-Chem and right of CMAQ images) were verified, shown in figures 5, 6 and 7 below.

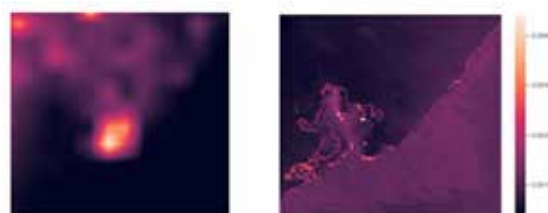


Figure 5. The average of the NH₃ concentration in the RMS simulated by the WRF-Chem model (on the left) and simulated with the CMAQ model (on the right).

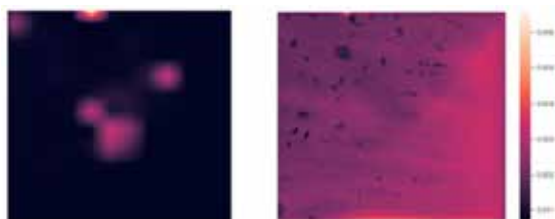


Figure 6. The average of NO concentration in RMS simulated by the WRF-Chem model (on the left) and simulated with the CMAQ model (on the right).

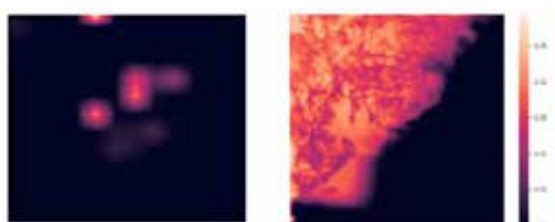


Figure 7. The average of the SO₂ concentration in the RMS simulated by the WRF-Chem model (on the left) and simulated with the CMAQ model (on the right).

The analysis of the average concentrations in ppmV of the NH₃, NO and SO₂ components were simulated by the chemical models, on March 22, 23, 24 and 25. The WRF-Chem model presents good results regarding the concentration of pollutants as shown in Figures 5, 6 and 7 on the left. On the other hand, the CMAQ model demonstrates good results regarding concentration and visualization in the investigated domain. In addition, when concentrations of pollutants reach values above the primary air quality standards set by the US-EPA, it may be detrimental to the health of the population.

CONCLUSIONS

The main objective of this study was to compare the performance of the atmospheric models WRF-CMAQ and WRF-Chem by qualitatively evaluating the dispersion of atmospheric pollutants (NH₃, NO_x and SO₂) in the Metropolitan Region of Salvador (MRS).

This work was an important step in contributing to further studies on the impact of local anthropogenic emissions on MRS air quality, as some difficulties were encountered due to a lack of information on the region's emissions sources.

For future work it is proposed to validate the regional photochemical modeling of air quality with the WRF-CMAQ, WRF-Chem and WRF-CHIMERE using monitoring data, in order to allow an analysis of the

local air quality, and to correlate air pollution with adverse health events in the population.

ACKNOWLEDGEMENT

The authors thank the Supercomputing Center for Industrial Innovation (CIMATEC) for providing the computational infrastructure needed to run the models, and the Fundação de Amparo à Pesquisa do Estado da Bahia (FAPESB) for the financial support.

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Long-range transport of air pollutants over Brazilian Southeastern: Meteorology modeling and emissions processing

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Abstract: Air pollution is an issue which have been on spotlight because of its negative impacts on human health and environment. Air quality over a certain region is affect meteorological conditions, topography, chemical process in atmosphere and emissions. Another atmospheric process which also affects air quality is the Long-range transport of air pollutants (LRTAP). The Brazilian Southeastern is a region which have been suffering with bad air quality, especially on the metropolitan, which requires an understanding of this issue. Since monitoring air quality over all area of interest requires a lot of resources, studies rely on the air quality modeling, however there are more local than regional air quality studies. Local studies are good to understand most of local air pollution, but the regional and even the global scales have their share on the air quality, especially because of LRTAP. Thus, the goal of this work is to develop a regional air quality modeling domain to cover all metropolitan areas in Brazil Southeastern and to understand the interaction between the metropolitan areas regarding their emissions. WRF-SMOKE-CMAQ system was used to develop the meteorological conditions, emissions and air quality modeling, respectively. WRF modeling will rely on one domain with 9km grid spacing and 190 columns and 160 rows. This domain will be applied into SMOKE and CMAQ to generate the base cases for the all sensitivity analysis and source apportionment analysis.

Keywords: WRF-SMOKE-CMAQ, Emissions, Long range transport, AQM.

INTRODUCTION

Long-range transport of air pollutants (LRTAP) refers to the atmospheric transport of air pollutants within a moving air mass for a distance greater than 100 kilometers. Therefore, the air pollution in each area is caused by local emissions and emissions from another areas, which were transported and transformed by atmospheric dynamic (OECD, 2007).

According to Borge et al. (2007), there are evidences that air quality over urban areas are affected by long-range transport of natural and/or anthropogenic air pollutants. Studies such as Qu et al. (2016), Shimadera, Kojima, and Kondo (2016b), Chen et al. (2017b), and Sun et al. (2017) have shown the effects of LRTAP in local air pollutants concentrations in Asia, North America and Europe, for particulate matter, nitrogen oxides, sulfur dioxides and ozone. In Brazil, the researches of Alonso et al., (2010); Andrade et al., (2015); Miranda et al., (2016); de Miranda et al., (2018); Ribeiro et al., (2018) and Pedruzzi et al., (2019) have highlighted the existence and influence of LRTAP on national and regional air quality.

The Brazilian Southeastern was one region addressed by the cited works; however, they did not point out the influence of LRTAP over the metropolitan areas and how these regions pollutions interacts with each other. Thus, there is this lack on the research that needs to be fill.

Therefore, to understand the interactions between the metropolitan areas using WRF-SMOKE-CMAQ, the first steps are to perform the WRF modeling and

emissions processing with SMOKE, which are the goal of this work. The period of interest is August, September and October of 2015.

METHODS

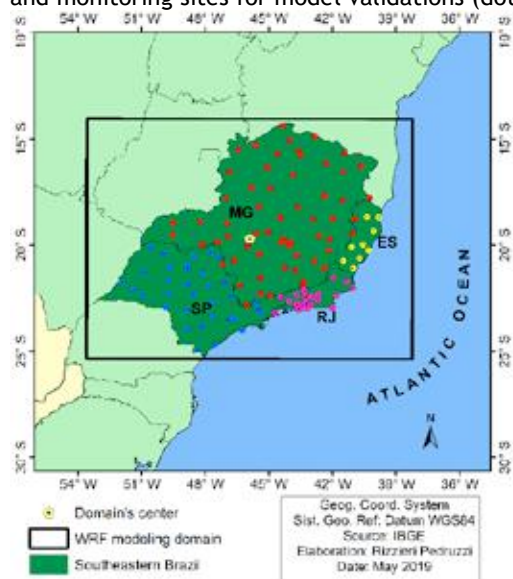
Meteorological conditions were modeled by Weather Research and Forecasting model (WRF) version v4.1 with a domain covering the entire Southeastern Brazil. The domain has 190 columns and 160 rows with 9km of grid spacing. Physical options for August and September were: WRF Single-Moment 5-class for microphysics, RRTM for long-wave and New Goddard for short-wave radiation, Noah Surface Model for Land-Surface, Revised Monin-Obukahov for Surface Layer and Yonsei University scheme for Planetary boundary layer. For October the physics options were the same, except for microphysics, long and short radiation, which WRF Single-Moment 3-class, CAM and Dudhia were used, respectively. The initial and boundary conditions were provided by the National Center for Environmental Prediction (NCEP) Global Forecast System (GFS) final (FNL) with a horizontal grid spacing of 0.25×0.25 degrees (ds083.3). The modeling validation was made according (LADCO - Lake Michigan Air Directors Consortium, 2016) and Emery *et al.*, (2017). The Figure 1 show the modeling domain and the meteorological monitoring stations used for the validation.

The emissions were processed by using Sparse Matrix Kernel Operator (SMOKE) version 4.6. The global emissions from EDGAR Hemispheric Transport of Air Pollution v2 (EDGAR HTAPv2) were used, because only few areas over Southeastern have

emissions inventory, bringing the necessity to rely on global inventories. All sector of EDGAR-HTAP v2 were used, Agriculture; Aircrafts; Energy; Industry; Residential; and Transport. In addition, fire emissions from Fire Inventory from NCAR (FINN v1.5) (Wiedinmyer *et al.*, 2011) and biogenic emissions by Model of Emissions of Gases and Aerosols from Nature (MEGAN v3.0) (Guenther *et al.*, 2012) have been processed to inserted into baseline emissions.

The source apportionment and source sensitivity analysis cases using CMAQ are under development.

Figure 1 - WRF modeling domain (black rectangle) and monitoring sites for model validations (dots).



FINDINGS AND ARGUMENT

According to the WRF validation, temperature and humidity had a good representation by WRF, among all modeled months. For humidity, the acceptable benchmark for mean bias is from -1 to 1 [g·kg⁻¹] and the worst benchmark was 2.37. For temperature, the bias benchmark ranges from -2 to 2 [K] and the worst benchmark was -6.85, however, only 17% observed sites are out of the benchmark.

Wind speed and direction are the hardest variable to get a good agreement, achieved moderate results. For Wind Speed, the worst bias was 5.85, and the benchmark varies from -1.5 to 1.5 [m·s⁻¹]. Wind direction, which is the hardest parameter to achieve the benchmark, reach the worst bias of 177, and the benchmark range from -10 to 10 [degrees],

besides, 53% of monitoring stations achieved the benchmark.

The EDGAR-HTAPv2 emissions have shown that the Industry and Transport sector have greatest contribution on emissions for the Southeastern modeling domain for all pollutants, as shown at Table 1. From Figure 2 and Figure 3 show the average emissions for PM_{2.5} and CO, respectively. For PM_{2.5} the highest emissions are localized over metropolitan areas, in exception of the emissions on column 72 x row 38m which is the maximum value of 69.148 g/s. This emissions peak is from industrial sector. Similar to PM_{2.5}, CO emissions are most concentrated over metropolitan areas with transport industrial being responsible by 89.63% of emissions, on average.

Figure 2 - PM_{2.5} average emissions over Southeastern modeling domain

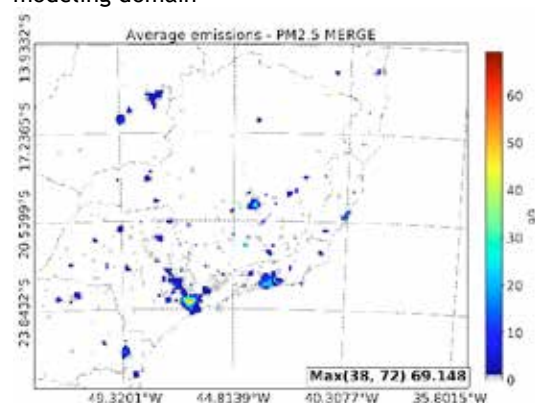


Figure 3 - CO average emissions over Southeastern modeling domain

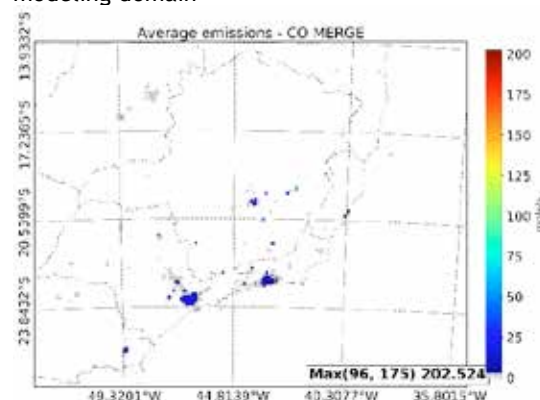


Table 1 - Average emissions of Southeastern modeling domain.

	Total [ton/day]	Transport	Residential	Industry	Aircraft	Energy	Ships
PM _{2.5}	279.26	3.47%	25.12%	69.28%	0.01%	0.37%	1.74%
PM ₁₀	501.52	6.74%	23.88%	68.11%	0.01%	0.29%	0.97%
CO	6251.04	42.67%	10.03%	46.96%	0.04%	0.22%	0.07%
SO ₂	481.69	1.75%	6.82%	70.06%	0.05%	15.31%	6.00%
NO _x	600.91	56.88%	2.48%	34.67%	0.28%	0.24%	5.44%
VOC	3650.58	27.31%	8.52%	57.23%	0.00%	6.79%	0.14%

CONCLUSIONS

The main goal of this work is to apply WRF-SMOKE-CMAQ over Southeastern Brazil aiming to accomplish source apportionment and source sensitivity. WRF results were satisfactory for the modeled period, especially for temperature and humidity. The emissions preliminary results have shown that the transport and industry sectors are the responsible for the major part of emissions, followed by residential, energy, ships and aircraft.

As expected, the highest emissions were observed over the metropolitan areas, especially of São Paulo and Rio de Janeiro metropolitan areas.

This amount of emissions can be transported by LRTAP and reach each other, causing interactions between their emissions, impacting the air quality. This means that air pollution over Southeastern Brazil should be addressed as regional problem with regional policies. The step that will answer this question is under development, which is the source apportionment and source sensitivity analysis.

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New geographical data for WRF: an updated input for Brazil

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Abstract: Geographical data is mandatory to perform weather modeling with WRF, like land use, topography and soil type. By default, these data are available for all globe in WRF, however, the better and well representative data is for United States. This means that the default data may have discrepancies or outdated data for areas outside United States, like Brazil. These input data impact the albedo, heat flux, energy balance, moist and friction velocity, which directly affects meteorological variables, such as radiation, specific humidity, ambient temperature, planetary boundary layer (PBL), and wind speed and direction. Aiming to avoid errors on these variables, a good and realistic input data for the modeling area is required. Thus, the goal of this work is to process geographical data for Brazil to insert it into WRF and to compare the WRF results for heat flux, moist and PBL using the default geographical data and the updated Brazilian data. The updated data for Brazil is from: GMTED2010 with 250 meters of resolution for Topography, MapBiomass data for Land Use/Land cover with 250 resolution and for soil type the Harmonized World Soil Database (HWSD) were used, with 1 kilometer of resolution. It were observed differences between the default and the three updated data, which may impact the WRF final results..

Keywords: WRF-SMOKE-CMAQ, Emissions, Long range transport, AQM.

INTRODUCTION

Geographical data, such as topography, land use/land cover (LULC), soil textures, etc., is provided by WRF community for the entire world. However, the data which covers the South America are outdated, such as United States Geological Service (USGS) and Moderate Resolution Imaging Spectroradiometer (MODIS) land use, which are from 1992 and 2007-2011, respectively, or are in a low-medium resolution, which is the case of default topography data from Global Multi-resolution Terrain Elevation (GMTED) 2010, with approximately 990 meters of grid spacing. These inputs can play a critical role in modeling results, affecting wind pattern, heat flux, radiations process, moisture and evolution of planetary boundary layer (Cheng et al., 2013; Dy and Fung, 2016; Li et al., 2017, 2018), so it is important to have a higher resolution and up to date dataset to apply in WRF simulations.

Besides the WRF default input data, there are alternative sources which are newer and/or have a higher resolution than the default, such as Land Use from Brazilian Annual Land Use and Land Cover Mapping Project (MAPBIOMAS), which was prepared based on satellite and observed data for Brazil with 30 meters of grid spacing. The data is free download at <http://mapbiomas.org/>. For topography, there is the higher resolution GMTED 2010 product with 250 meters of grid spacing, and for soil texture the Soil Grids (Hengl et al., 2017) data, with 1 km or 250m of grid spacing.

METHODS

Land use/Land cover data from MAPBIOMAS collection 3.1 was used. The MAPBIOMAS was reclassified to to MODIS 21 classes.

For topography, the GMTED 2010 data has 7.5 arc-seconds of grid spacing, approximately 250 meters and it was used as topography input in WRF. This data is available at <https://lta.cr.usgs.gov/GMTED2010> website on geotiff format.

Another input data requested by WRF is the soil texture (mix of sand, clay, and silt). To create a new input data for soil, the data from Soils Grid (<https://soilgrids.org>) was used. After the aggregation by layers, a combination of the three soil content were compared to the soil triangle (García-Gaines and Frankenstein, 2015), which classify the soil into 16 classes, used by WRF, generating a single tiff file with soil texture classification for soil top and bottom.

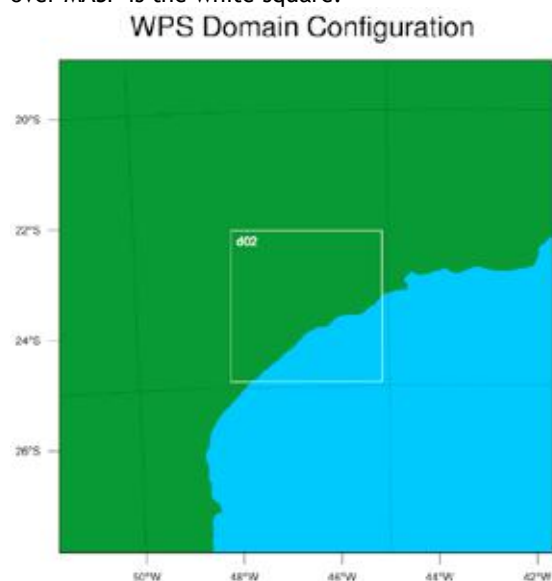
To WRF reading the prepared files, it was necessary to convert the data to binary format to make it available to WRF. This step was performed using the free tool `convert_geotiff` (https://github.com/openwfm/convert_geotiff).

To test the new geographical data in WRF, two cases was developed. The first one using only default data (W1) and the second with the updated data (W2). The WRF simulations were with two nested domains. The mother domain has 200 columns and 200 rows with 5 km of grid spacing. The inner domain is centered over Metropolitan area of São Paulo and it

has 305 columns and 305 rows with 1 km of grid spacing. Figure 1 shows the domains configuration.

The initial and boundary conditions were provided by the National Center for Environmental Prediction (NCEP) Global Forecast System (GFS) final (FNL) with a horizontal grid spacing of 0.25×0.25 degrees (ds083.3).

Figure 1 - WRF modeling domains. The greater square in the mother domain. The inner domain over MASP is the white square.



FINDINGS AND ARGUMENT

The Figure 2, Figure 3, Figure 4 and Figure 5 are the differences between the W1 and W2 (default minus updated) for the topography, land use/land cover and soil top model inputs, respectively. Great differences are noticed between the cases. W1 topography, in general, have higher altitudes than W2. LULC have shown great differences in the major part of domain, having the differences ranging from -19 to 14. Soil Top and Soil bottom are similar to the other data sets, with great differences between W1 and W2, having values ranging from -10 to 10, meaning that some grid cell have completely different classification.

The Figure 6 is showing the differences on modeled temperature at 2 meters in Kelvin. Since the analysis is default simulation minus the updated, it possible to say that the W1 case reached higher modeled temperatures than W2. Even over the ocean the W1 temperature was higher. Only few areas did not have a null or small variation.

This differences in temperature can lead variation in moisture, planetary boundary layer and heat flux, variables which have to be investigated in future.

Figure 2 - Difference on Topography

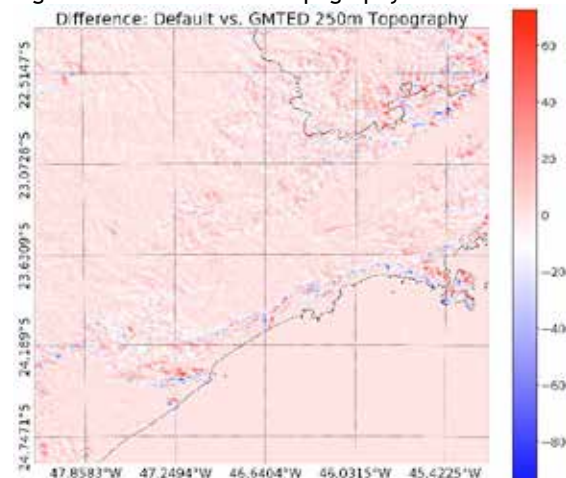


Figure 3 - Differences on LULC

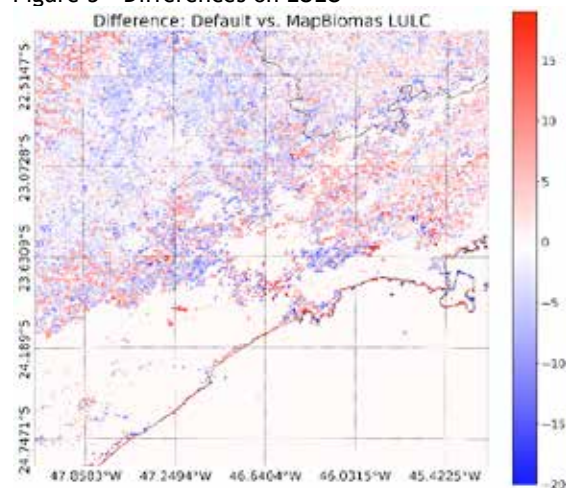


Figure 4 - Differences on Soil Top

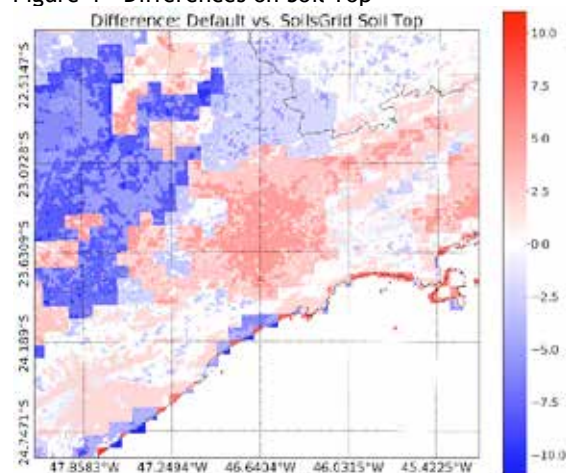
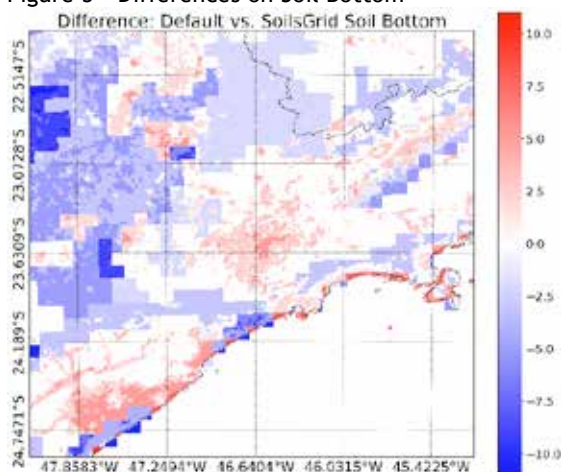


Figure 5 - Differences on Soil Bottom



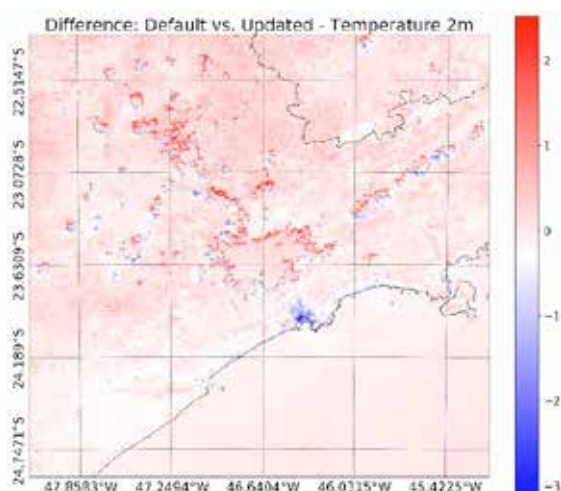
García-Gaines, R. A. and Frankenstein, S. (2015) *ERDC/CRREL TR-15-4 - USCS and the USDA Soil Classification System: Development of a Mapping Scheme*. Available at: www.erd.usace.army.mil. (Accessed: May 21, 2019).

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Figure 6 - Differences on Temperature [K]



CONCLUSIONS

This work goal was to develop an update version for WRF's geographical data like topography, land use land cover and soil texture. In conclusion, the new data have great differences when compared to the default data for data sets, which lead to variation in temperature. This variation, probably is not only on temperature, so more variables should be evaluated and analyzed in future works.

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ANALYSIS OF THE NEW CONAMA 491/19 RESOLUTION ESTABLISHING AIR QUALITY STANDARDS: ITS IMPLICATIONS FOR LARGER SIZED COMPANIES

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Abstract: This article provides a critical analysis essay of the recently published Conama Resolution 491/18 on air quality standards recommended by the World Health Organization (WHO). According to the Brazilian Institute for the Environment and Renewable Natural Resources (IBAMA), the implementation of the new resolution will raise many environmental benefits and improvements to human health, since the expectations are to eliminate about 99% of the pollutant emissions in Brazil. This paper wants to discuss the interferences and implications of this new Resolution in meeting air quality standards for projects with high atmospheric emission potential, such as mining and steelmaking, since emission values are very high. Its much more restrictive than the former Resolution 03/90. Given more than a decade waiting for a modern and updated Resolution on air quality considering countries like Brazil, where serious problems on high rates of respiratory diseases and deaths are already accounted and those WHO-Standards should've been implemented since back to 2005. Although Conama Resolution 491/18 mentions that it is guided by WHO-Standards, this was not actually applied in practice regarding the so-called intermediate standards. The intermediate patterns with no goal and time to reach can stimulate the inertia of any attempt to reach the limits, as in São Paulo where the legislation follows practically the same mechanisms. After all, the reason for the existence of the intermediate patterns were based on temporary goals, leading in a staggered way to the achievement of final standards. This would require mechanisms and deadlines that could effectively stimulate progression to the most restrictive standards over time, and this has not been aimed in this new legislation. In addition to these issues it is observed that large companies, especially those related to the mining and steel industry, are those that have the most potential for being subjected to infractions through subjective and "conflictual" aspects of Conama Resolution 491/18 not very well enlightened.

Keywords: Resolution Conama 491/18, air quality, mining and steel, environment and World Health Organization - WHO, Attorney General of the Republic.

INTRODUCTION

The recently published CONAMA Resolution No. 491/18, which sets the new air quality standards, taking as reference those recommended by the World Health Organization (WHO) in 2005, revoked CONAMA Resolution No. 03/90 and the standards of primary and secondary quality, established by CONAMA Resolution No. 05/89. The amendment was adopted by the Council plenary, keeping the basic text on air quality standards much more restrictive than the previous resolution, very close to WHO-Standards. According to the Brazilian Institute for the Environment and Renewable Natural Resources (IBAMA), the implementation of the new phase of the Program on Vehicle Emissions Control will bring many environmental benefits, as well as human health features, since the expectation through this measure is to eliminate about 99% of the Brazilian pollutants emissions.

The benefits to human health include reducing heart disease, lung disease and stroke. However, the Attorney General filed an action of unconstitutionality to the Superior Court based on the argument that although it uses as reference the guide values on air quality recommended by the World Health Organization (WHO) in 2005, the

resolution does not treat the air quality standards adequately. It's too permissive on starting values, failing to set decisive deadlines for reaching successive stages of air quality standards and presenting a vague decision-making procedure.

According to the Attorney General of the Republic the resolution doesn't grant the availability of clear and accessible information on air quality to the population. In this new resolution the elaboration of the Control of Atmospheric Emissions Plan is under responsibility of the state environmental organs.

The deadline is up to three years after the resolution becomes effective, ie until 2021. The plan should contain which regions will be involved, the identification of the main sources of pollutants and what they are, as well as the establishment of goals and deadlines for the implementation of so-called Intermediate Standards. Each federal entity should still be responsible for issuing an Air Quality Assessment Report annually.

OBJECTIVES

The objective of this article is to discuss the interferences and implications of the new

resolution to meet the indicated standards against projects with great potential for atmospheric emission, such as steel and mining, since the emission values are much more restrictive than the values of the former Resolution 03/90.

This article presents an analysis of the interactions of the new Conama Resolution 491/18 with the atmospheric dispersion modeling studies. What should be the analyzes to be worked out, how should modeling reports be worked out in the face of the new resolution?

Finally, to take an approach on the recent challenge of the PGR with the STF regarding the action of unconstitutionality of the new resolution.

METHODOLOGY

The methodology used will be review and critical analysis of current legislation, using the authors' experience to deal with legal issues through the scenario of interaction with large enterprises with high potential for atmospheric emission, as well as a research of issues in the post-resolution debate.

In addition, an analysis of the Attorney General opinion regarding the unconstitutionality of the respective resolution. Future scenarios of mining and steel enterprises will be evaluated in the light of the new legislation, comparing their emissions by means of available data with the guidelines of the new legislation.

RESULTS

The first stage of the new resolution came into effect as of publication on November 21, 2018 and comprises Air Quality Standards called Intermediaries - PI-1 and Final Standards - PF, which are:

II - air quality standard: one of the air quality management instruments, determined as the concentration value of a specific pollutant in the atmosphere, associated with a time interval of exposure, in order for the environment and the health of the population to be preserved in relation to the risks of damage caused by air pollution;

III - intermediate air quality standards - IP: standards established as temporary values to be met in stages;

IV - final air quality standard - PF: guideline values defined by the World Health Organization - WHO in 2005; V - critical episode of air pollution: situation characterized by the presence of high concentrations of pollutants in the atmosphere in a short period of time,

resulting from the occurrence of meteorological conditions unfavorable to the dispersion of the same;

The Intermediate and Final Air Quality Standards shall be adopted, each subsequently, taking into account the Air Emission Control Plans (PCEA) and the Air Quality Assessment Reports (RAQA), prepared by the state bodies and district environment. The state bodies must prepare the PCEAs within three years from the entry of the normative act on. In addition, the plans should take into account the standards defined in the new resolution, as well as the guidelines contained in the PRONAR - Air Quality Control Program.

The Air Quality Assessment Reports shall be prepared annually and contain the monitoring data and air quality evolution with the minimum content set forth in Annex II of the Resolution. The new resolution also provides for the elaboration of Plans for Critical Air Pollution Episodes, based on levels of attention, alert and emergency, which should provide for preventive measures with the aim of avoiding serious and imminent risks to the health of the pollution.

Finally, the new legislation grants the state environmental agencies the power to define criteria in air quality standards for licensing purposes.

According to the PGR (Attorney General of the Republic) when it comes to air quality standards, the new resolution deliberates on concepts, establishes parameters, makes decisions and creates attributions to state and district environmental agencies, even to the Public Ministry.

In this way, the Attorney General's understanding is that the resolution does not adopt a typical regulatory nature and it is within its competence, as it innovates in the legal system with articles endowed with legal autonomy, abstraction, generality and impersonality.

In this way the PGR (Attorney General of the Republic) understands by the direct action of unconstitutional action against resolution that contains serious errors of primary normative content. Based on the criteria defined by the current legislation on air quality, Conama Resolution 491/18 has:

Art. 9 The Ministry of the Environment shall prepare an annual monitoring report and will present it at the last regular meeting of CONAMA.

Art. 10. The state and district environmental agencies shall elaborate,

based on levels of attention, alert and emergency, a Plan for Critical Air Pollution Episodes, to be submitted to the competent authority of the state or the Federal District, aiming at preventive measures with the aim of avoiding serious and imminent health risks to the population according to the pollutants and concentrations listed in Annex III. Single paragraph. The Plan mentioned in the caput should indicate those responsible for the declaration of the various levels of criticality, and should be disclosed in any of the mass media.

Art. 11. The levels of attention, alert and emergency referred to in art. 10 shall be declared when the emissions are expected to be maintained as well as conditions.

Art. 12. The Ministry of the Environment and the state and district environmental agencies shall disclose on their web page monitoring data and information related to the management of the air quality.

Art. 13. The state and district environmental agencies shall disclose Air Quality Index - IQAR as defined in Annex IV.

Art. 14. The CONAMA Resolution No. 03/1990 and items 2.2.1 and 2.3 of CONAMA Resolution No. 5/1989 are revoked.

In 2005 the World Health Organization (WHO) released an update of its known air quality "guidelines" for air quality guidelines, based on recognized international studies. They are guides with concentration values set for certain atmospheric pollutants, considered as the limit to indicate the lowest health risk, and serve as a parameter for the countries in the elaboration of their standards of air quality measurement. The EU was one of the first to use these figures as a reference.

In this way, the values recommended in Conama Resolution 03 of 1990 were already far behind the international references when, in 2010, civil society environmental organizations provoked the process of revision of the Resolution, that is, 5 years later. Taking into account the values reviewed by the WHO in 2005, it has been 13 years without our resolution on air quality being revised.

Recently, in May 2018, WHO released alarming estimates of the risks and epidemic of deaths from air pollution. According to the organization about 7 million people as a result of exposure to airborne microparticles suspended in the air. In Brazil, an estimated 50,000 annual deaths are due to air pollution. In this way, it was to be expected that air quality standards, in turn, would already begin

with the definitions established by the WHO, since the 13-year gap has been established. Although Conama Resolution 491 mentions that it is guided by WHO standards, this does not actually happen in establishing the so-called intermediate standards Pls. See below in the comparative table between WHO and Conama Resolution 491.

Pollutant	Sample concentration time	Conama Resolution 491. Intermediate Standard	OMS 2005
Particles inhalation (MP10)	24 hour	120	50
	Annual average	40	20
Particles inhalation (MP2,5)	24 hour	60	25
	Annual average	20	10
Ozone (O3)	8 hour	140	100

Source: Conama Resolution 491 and World Health Organization (WHO).

In fact, the values adopted by air quality standards assume the goal function to be achieved, stimulating states, municipalities, productive sector and organized civil society to guide their agendas in accordance with the reach of this protective north, in spite of state environmental authorities they can set their own goals, provided they are more restrictive (stricter and more secure).

Although CONAMA Resolution No. 491/2018 aims to achieve, in the final standard, although after 13 years after the WHO reports, it does not establish peremptory periods between the intermediate stages (PI-1, PI-2 and PI- 3) and the final step (PF), stimulating the inertia of any attempt to reach the limits, as in the São Paulo legislation that has practically the same mechanisms. After all, the reason for the existence of intermediate patterns is that they effectively function as temporary goals, leading in a staggered way to the achievement of final standards. This would require mechanisms and deadlines that could effectively stimulate progression to the most restrictive standards over time.

The mechanism of pattern progression can still stagnate in the initial pattern, not only due to the absence of peremptory time between stages, but also through the writing of art. 4, paragraph 4 of the CONAMA Resolution No. 491/2018, which provides that "if migration to the subsequent standard is not possible, the standard already adopted" prevails. According to the PGR, the device, too generic, allows the perpetuity of high levels of atmospheric contamination.

The question being asked is whether, in fact, states will actually advance their policies for setting final standards as outlined in Resolution

491? In what time and periodicity will this evolution take place? Is there a risk of not moving towards final standards? In addition to all these issues there are still many questions and uncertainties that put the productive sector in a situation of discomfort.

Initial analyzes indicate that medium- and large-sized mining ventures with extensive exposed areas such as tailings dams, sterile and ore piles will not meet the air quality standards for particulate matter emissions in the face of higher values new legislation.

For steel mills, the risks are also non-attendant, especially for large ones, which were built more than three decades ago, whose emission controls were scaled in the face of less restrictive legislation or absent any definition. Let us see how Resolution Conama 491 deals with environmental issues in a broad way, placing levels of concentration and human pollution in the same conditions of pollution for fauna, flora and materials.

Article 2. For the purpose of this resolution, the following definitions are adopted:

I - atmospheric pollutant: any form of matter in quantity, concentration, time or other characteristics which render or may render air unfit or harmful to health, inconvenient to public welfare, harmful to the environment, fauna or flora or harmful to security, the use and enjoyment of property or the normal activities of the community;

In face of this scenario of definition of pollutant and human standards also become references for fauna, flora and materials. The questions are based on the fact that these values were determined based on studies to human health by the WHO and not for fauna, flora and materials, depending on the species or material being more or less restrictive. As it is known each species is whether the fauna and flora are more or less resistant to air pollution, some, for example, very sensitive like mosses and lichens. The question of materials also in fact refers to innumerable doubts and questions in the face of the resistance of each one of them and their importance.

Atmospheric dispersion models are important tools to predict these realities and indicate the effects of emissions on the new legislation. Early analyzes for mining and steel mills indicated that concentrations of particulate matter and gases as expected were high within the operational area, and concentrations outside the company

boundaries tended to decline. In addition, large mining companies are located outside urban centers and in green areas.

However, the new legislation does not distinguish between what is operational area and external area and what concentrations are limits for the operational areas. For the green areas without population should be adopted the maximum concentration values? In this way, they impose an important legal fragility that the internal values (within the operational areas) are in fact violating the legislation since the legislation does not distinguish between operating environments and external environments, nor regions absent from population, where only fauna and flora.

Another issue that draws attention to the concepts indicated by the new Conama Resolution 491/18, especially with regard to the impacts on "public welfare, harmful materials, fauna and flora or harmful to use and enjoyment of property or the normal activities of the community, "which are in principle questionable.

Taking the term "harmful to materials" as an example, one can understand that the concentrations of a given enterprise that are above the maximum allowed standard value, even if there is no associated community or fauna and flora, may be in violation of "harmful to materials"? Another term that raises important doubts about the obligation to attend refers to the term harmful to security. What, in fact, will this question of air quality be detrimental to safety?

CONCLUSIONS

Given more than a decade waiting for a new resolution on modern and up-to-dated air quality standards, despite of countries like Brazil having serious problems and high rates of respiratory diseases and deaths and a poor public support on health offered to its population, it was about to expect at least the air quality standards given WHO back to 2005.

Although Conama Resolution 491 mentions that it is guided by WHO standards, this is not actually the case in establishing the so-called intermediate standards. The intermediate patterns with no goal and time to reach can stimulate the inertia of any attempt to reach the limits.

After all the reason for the existence of intermediate patterns is that they effectively function as temporary goals, leading in a staggered way to the achievement of final standards. This would require mechanisms and deadlines that could effectively stimulate progression to the most restrictive standards over time. This has

unfortunately didn't happened in this new legislation.

Large companies, especially those related to the mining and steel industry, have the greatest potential to be subjected to infractions by the new legislation. Many of them that fail to comply can be closed or receive high fines from environmental agencies for non-compliance. The situation is further aggravated from a legal point of view if it takes into account the subjective and "conflicting" aspects of Conama Resolution 491/18, such as protection against damage to materials and safety.

Addressing these subjective issues of the new legislation, it is important to note that in fact the more restrictive standards will oblige productive sectors to adapt and present better operational practices in their systems. It remains to be seen whether the air quality, especially of the more urbanized regions, will improve since the emissions of motor vehicles, fires and deforestation are important sources of air pollutants, which in turn depend on governmental actions and policies.

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4th CMAS SOUTH AMERICA

COMMUNITY MODELING AND ANALYSIS SYSTEM

**PROCEEDINGS OF THE
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Session 05
**Modeling to Support Exposure
and Health Studies and
Community-scale Applications**

AIR POLLUTION EXPOSURE DURING CYCLING IN SÃO PAULO

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Abstract: Cyclists usually pedal extremely close or on streets and, therefore, experience direct exposure to traffic emissions coming from vehicles, usually the main source of air pollutants in the city. Fine particulate matter (PM_{2.5}) is an air pollutant that has strong association with health problems, such as respiratory and cardiovascular diseases, because it can penetrate deep into the respiratory system. This work aims to differentiate by route and period of the day the cyclists' exposure to PM_{2.5} and identify areas with enhanced pollution levels in the city of São Paulo. Exposure to PM_{2.5} was measured during peak (morning and evening) and off-peak (afternoon) hours while cycling in six different routes using an aerosol monitor (TSI DustTrak 8530). Two routes were selected, one main (route A) and one alternative (route B), from three different origin-destination pairs (origins: Anhangabaú, Ibirapuera and Faria Lima, common destination: Av. Paulista), giving a total of six routes. The routes covered different urban regions and had distinct characteristics regarding the traffic and type of cycling infrastructure. The main routes included street segments with high traffic and street-canyons, and the alternative routes included roads with reduced traffic and, where possible, the presence of green/open areas (squares, parks, and urban forests). The results showed that PM_{2.5} concentrations were higher during the morning-peak hours than during evening-peak hours. In most cases, the cyclists using alternative routes were substantially less exposed to PM_{2.5} when compared to the main routes. Also, there were indications that the presence of green/open areas helped to decrease air pollution levels on cyclists, and, on the contrary, proximity to traffic intersections helped to increase pollution levels. The route running the Consolação Street cyclelane presented the highest average concentrations, almost three-times higher than those on the route running inside the Ibirapuera Park. It was concluded that cyclists' exposure is highly related to route choice, period of the day and proximity to on-road vehicles. These findings suggest that cyclists should avoid high trafficked streets. Furthermore, urban planners should consider to increase, as much as possible, the distance between the road and the cycleways when establishing new cycle networks. In existing cycle infrastructure, it is suggested to plan Green Barriers (trees and hedges) between the road and cycleway to reduce the exposure of cyclists.

Keywords: Exposure assessment, Cyclist exposure, Particulate Matter, Mobile measurements.

INTRODUCTION

Over the past years, cycling as a choice of commute has increased in many urban areas, as in Ireland, United Kingdom and in the United States cities. Public policies are extremely important to encourage and strengthen cycling activities. Segregated cycling facilities, priority cycle traffic signals, safe and convenient parking spots, and integration of cycling with public transport (Pucher and Buehler, 2008) are a few examples of public policies that can be implemented. In São Paulo, cycles represent 2% of the commuting choice as the main transport mode (CEBRAP, 2018), and the city has almost 500 km of cycle infrastructure.

Although cycling brings benefits to human health like reducing risks of chronic diseases, and reduction of air pollution emissions, cycling is frequently related with health and safety hazards due to the direct exposure to traffic emissions (Hartog et al., 2010; Tainio et al., 2016) and because of the short distance between the cyclist

and the on-road vehicles. Fine particulate matter (PM_{2.5}) is an example of an air pollutant that have strong association with health problems, such as total and cardiovascular mortality, blood pressure and respiratory diseases (Geng et al., 2013; Jansen et al., 2005; Mordukhovich et al., 2009), because it can penetrate deep into the respiratory system.

In São Paulo, a projection of the number of deaths, hospitalizations and amount of money spent on public hospital admissions from 2012 to 2030 showed that if air pollution continues at its current level, it will cause more than 246 thousand deaths from all causes between 2011 and 2030, as well as 953 thousand hospital admissions and public health expenses estimated in R\$ 1.6 billion due to hospitalizations (Rodrigues et al., 2015).

Therefore, the goal of this work is to assess the air pollution concentration in the daily cycling commutes in São Paulo. There are limited studies quantifying the exposure to air pollutants in

cyclists' in the city. There is only a pilot study conducted by Targino et al. (2018) and a comparative assessment among three cities, London, Rotterdam and São Paulo, performed by Brand et al. (2019). Both studies assessed black carbon concentrations only. Therefore, this work aims to distinguish by route and period of the day the cyclists' exposure to $PM_{2.5}$, and identify areas with enhanced pollution levels in the city of São Paulo.

METHODS

Exposure to $PM_{2.5}$ was measured while cycling during morning (MP) and evening (EP) rush hours (7:00 - 9:00 and 17:00 - 19:00, local time) and during afternoon (AP) hours (12:00 - 14:00, local time) in six different routes. To do so, we used an aerosol monitor (TSI DustTrak 8530) with an $PM_{2.5}$ inlet and a time resolution of 10 seconds. The routes were chosen to cover different urban regions and distinct traffic conditions. We selected three origin-destination (O-D) pairs (origins: S1 - Anhangabaú, S2 - Ibirapuera, and S3 - Faria Lima, with a common destination: Paulista). In each O-D two routes were selected, one main (route A) and one alternative (route B) (Figure 1). The main routes included street segments with higher traffic conditions when compared to the alternative routes. The cycleways were present predominantly on the main routes while the alternative routes included presence of green/wooded streets (Republica square in S1B route, Ibirapuera park in S2B route, and street trees in S3B route). Additional meteorological data was used from the meteorological station of the Institute of Astronomy, Geophysics and Atmospheric Sciences.

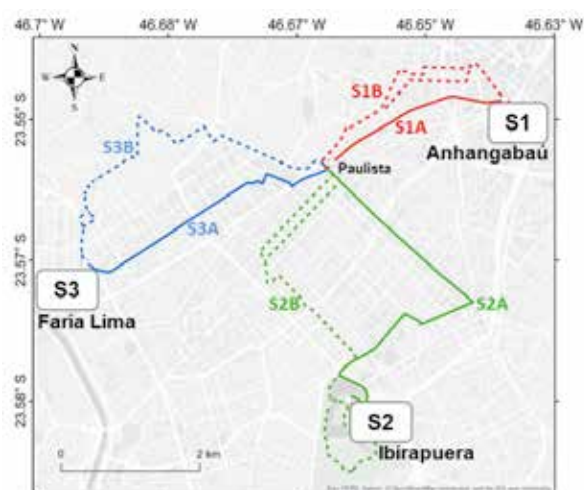


Figure 1. Cycle routes in the city of São Paulo. The full lines represent the main routes and the dotted lines the alternative routes.

Data processing and statistical analysis were performed with the statistical software R (v 3.4.3, R Core Team, 2016). ArcGIS (Esri Inc.) was used for generating the maps and calculating the Kernel density.

FINDINGS AND ARGUMENT

The results showed that the average $PM_{2.5}$ concentration in all routes and periods was $14 \mu g/m^3$. Higher concentrations were found in London by Kaur et al. (2005), where they measured an average concentration of $33.5 \mu g/m^3$ of $PM_{2.5}$, and in Barcelona, de Nazelle et al. (2012) measured $29 \mu g/m^3$ $PM_{2.5}$ average concentration. Similarly to São Paulo, Boogaard et al. (2009) found $13 \mu g/m^3$ average $PM_{2.5}$ concentration in Groningen and $11 \mu g/m^3$ in Apeldoorn.

The results also showed that average $PM_{2.5}$ concentrations were higher during the morning-peak hours than during evening-peak hours and afternoon hours (Figure 2), what can be associate to the high relative humidity during morning hours. Higher concentrations during morning hours were also observed by Hankey and Marshall (2015) and Quiros et al. (2013) in Santa Monica and Minneapolis respectively in the United States.

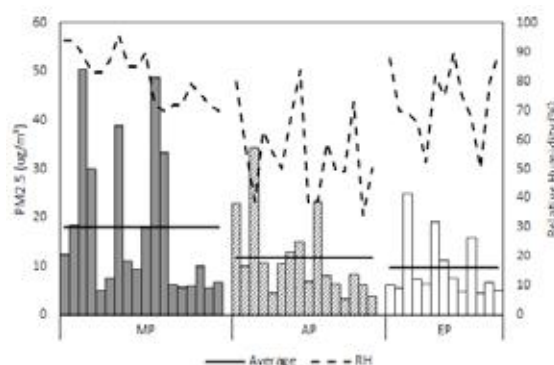


Figure 2. Average $PM_{2.5}$ concentrations ($\mu g/m^3$) by run by period of the day in all routes in São Paulo and hourly relative humidity (RH - %).

Besides that, in most cases, the cyclists using alternative routes were less exposed to $PM_{2.5}$ when compared to the main routes (Figure 3). The variability of the average concentrations was higher during morning rush hours and in the main routes (S1A, S2A and S3A) represented by the larger boxes in Figure 3. This high variability can be explained by the traffic, wind speed, period of the day and by the characteristics of the route.

The presence of green/wooden streets helped to decrease air pollution levels on cyclists, and, on the contrary, proximity to traffic intersections helped to increase pollution levels (Figure 3 and 4). The route in the Consolação Street cyclelane (S1A) presented the highest average concentrations,

almost three-times higher than those on the route inside the Ibirapuera Park (S2B).

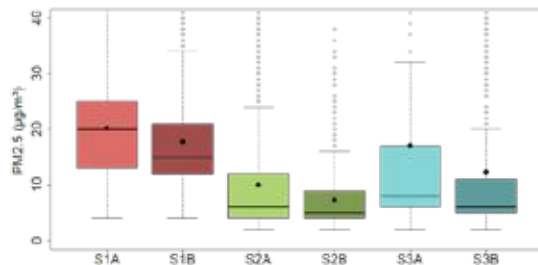


Figure 3. Boxplot of $PM_{2.5}$ concentrations ($\mu\text{g}/\text{m}^3$) measured in the six routes in São Paulo.

In Figure 4 we can see the enhanced pollution levels spots, or hotspots, in all six routes in São Paulo calculated with the Kernel density tool. The scale is different for each O-D pair due to differences in measured concentrations. These hotspots occur notably in big intersections where the cyclist wait longer for the signal before continuing to pedal. Also, the number and intensity of these hotspots are higher in the main routes.

CONCLUSIONS

An air pollution exposure assessment study focusing on the cyclists was performed in São Paulo. The findings indicate that cyclists' exposure to $PM_{2.5}$ is highly related to route choice, period of the day and proximity to on-road vehicles. Therefore, cyclists are advised to avoid high trafficked streets, especially during morning rush hours, giving preference to alternative routes with less traffic. Furthermore, urban planners should consider increasing, as much as possible, the distance between the road and the cycleways when establishing new cycle networks. In the existing ones, we recommend the implementation of green barriers, like trees and hedges, between the road and cycleway to reduce the exposure of cyclists.

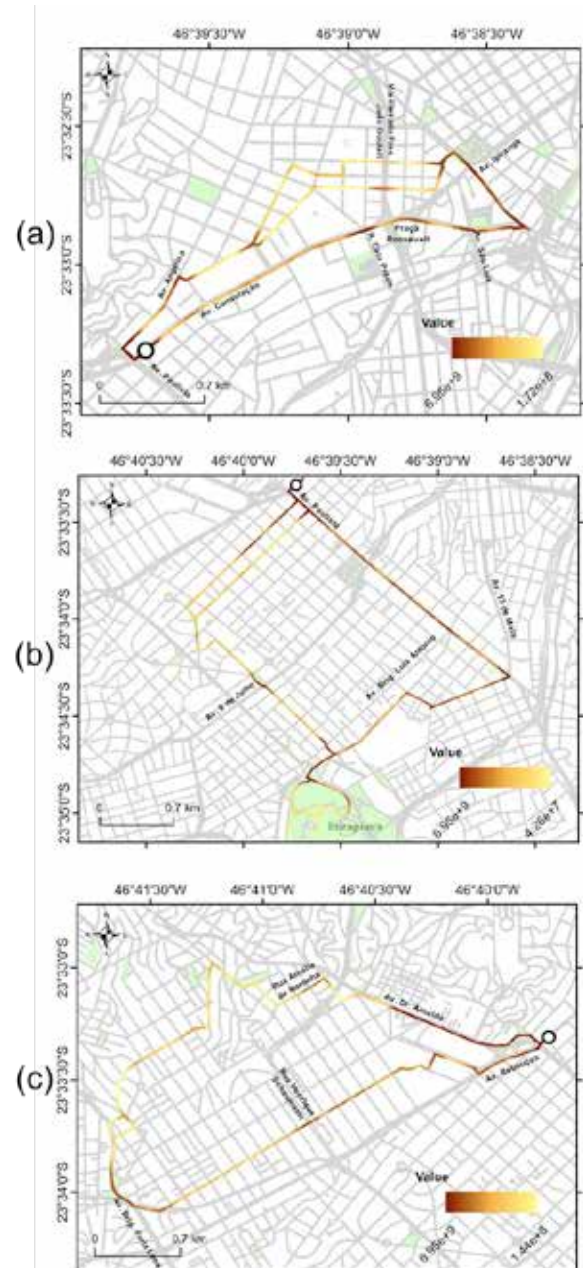


Figure 4. Kernel Density of $PM_{2.5}$ concentrations [points . ($\mu\text{g}/\text{m}^3$)/area] measured in (a) S1, (b) S2 and (c) S3 O-D pairs.

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GENERALIZED ADDITIVE MODEL FOR COUNT TIME SERIES: AN APPLICATION TO STUDY THE IMPACT OF AIR POLLUTANTS ON HUMAN HEALTH

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Abstract: The Generalized Additive Model (GAM) has been used in many epidemiological studies where frequently the response variable is a nonnegative integer-valued time series. However, GAM assumes that the observations are independent, which is generally not the case in time series. Therefore, in this paper we propose the Generalized Additive Autoregressive Moving Average (GAM-ARMA) model, which is an extension of GAM with an autoregressive moving average component. The GAM-ARMA is based on the Generalized Linear Autoregressive Moving Average Model (GLARMA), with some linear components of GLARMA being replaced by natural splines. Here we focused on the estimation either for the parametric elements, as well for the non-parametric components. In order to evaluate the performance of the GAM-ARMA we performed two simulation studies which showed that, although the estimates present small bias and mean squared error, the autoregressive and moving average components influence the estimation. In general, we found better estimates when these components assume small values. In a real data analysis of the effects of air pollution on respiratory disease in the metropolitan area of Belo Horizonte, Brazil, we observed that the proposed model presented a better fit when compared to the widely used GAM approach, that do not take into account the autocorrelation of the data.

Keywords: Autocorrelation, ARIMA models, Semiparametric Models, Respiratory diseases, Principal component analysis.

INTRODUCTION

Many epidemiological studies have been carried out to investigate the impact of atmospheric pollution and meteorological conditions on human health. Dockery and Pope (1996), Villeneuve et al. (2003) and other authors indicated a positive association between mortality and particulate matter (PM₁₀). Ostro et al. (1999) and Schwartz (2000) found a significant association between daily pollutant concentration levels and hospital admission for respiratory and cardiovascular diseases. Studies such as these provide support for health departments in resource allocation and stakeholders in prevention. In this work we proposed a methodology called GAM-ARMA (Generalized Additive Autoregressive Moving Average), which is based on the GLARMA model proposed by Davis et al. (2003), allowing the fit of semiparametrical models which includes both linear and nonlinear components in the mean of the process.

METHODS

The methodology is based on GLARMA (Davis et al., 2003) and GAM (Hastie and Tibshirani, 1990) model. For this an autoregressive moving average term is added on GAM structure.

As in the GLARMA model the observations y_t given the past information, possess any distribution belonging to the exponential family.

$$y_t | F_{t-1} \sim EF(\mu_t),$$

where μ_t is the mean of the process.

The predictor in a GAM-ARMA(p, q) model is written with the addition of an autoregressive moving average of order p and q to the general form of a GAM predictor. Considering semiparametric form, the predictor η_t combines k variables ($x_1, \dots, x_k$) related linearly with the response variable and r variables ($w_1, \dots, w_r$) related with the response variable through some smooth function, in the following way:

$$\eta_t = \beta_0 + \beta_1 x_{t,1} + \dots + \beta_k x_{t,k} + s_1(w_{t,1}) + \dots + s_r(w_{t,r}) + \sum_{i=1}^{\infty} \tau_i \varepsilon_{t-i},$$

where s is a smooth function. The structure of component $\sum_{i=1}^{\infty} \tau_i \varepsilon_{t-i}$ is defined similarly to the GLARMA model.

The function s is approached with B-splines or Basis splines (De Boor, 1978), given their simplicity to obtain flexible smoothing. B-splines are constructed from polynomial pieces, jointed at control points called knots. By definition the B-splines $B_{j,d}$ depends on the knots $t_j, \dots, t_{j+1+d}$, where d is the order polynomial piece. A linear

combination of B-splines is called spline function and is given by

$$s = \sum_{j=1}^m \alpha_j B_{j,d},$$

where $\alpha = (\alpha_j)_{j=1}^m$ are m real numbers called the B-spline coefficients or control points of s .

The analysis of the goodness-of-fit of the GAM-ARMA can be performed through the Akaike Information Criterion (AIC) and by the Bayesian Information Criterion (BIC), which is most used in time series models.

FINDINGS AND ARGUMENT

In order to evaluate the performance of the proposed model with respect to the parameters estimation, some simulation studies were developed. The simulation study revealed that the values of autoregressive and moving average components can influence the accuracy of estimates. In general as the values of these components increases, we have the worst estimates.

Besides that, the GAM-ARMA was applied in an epidemiological dataset. In this analysis was studied the impact of air pollutants and meteorological factors in the monthly numbers of Chronic Obstructive Pulmonary Disease (COPD) cases in Belo Horizonte, Brazil, between the years of 2007 and 2013 ($n = 84$). Here were evaluated the concentrations of the following pollutants: Particulate Matter (PM10), Nitrogen Monoxide (NO), Nitrogen Dioxide (NO2), Carbon Monoxide (CO) and Ozone (O3). Besides that, meteorological information, as temperature and relative humidity of the air, were investigated. Table 1 presents some descriptive statistics.

Table 1. Comparison of the Relative Risk and 95% confidence interval

	Mean	Standard Deviation	Minimum	Percentile			Maximum
				25	50	75	
CO	0.44	0.19	0.02	0.35	0.41	0.51	1.50
PM10	30.97	9.51	16.16	25.21	29.88	35.32	70.83
NO	12.97	5.80	0.57	9.05	12.01	15.52	33.11
NO2	16.59	4.18	0.52	13.74	16.07	19.76	27.90
O3	15.038	5.33	5.994	11.49	13.77	17.44	32.10
Temp	17.89	1.90	13.87	16.43	18.27	19.62	21.15
Hum	61.00	7.48	45.83	56.17	61.69	67.55	77.53
Cases	54.03	42.3	10.00	27.00	41.00	60.00	196.00

In the analysis were proposed two approaches: first, following previous studies we adjusted a model with a single air pollutant as covariate, once the pollutants presented correlation among them, and this may imply identification problems and multicollinearity. In the second approach, we adjusted a model with more than one pollutant, based on the methodology proposed by Souza *et al.* (2018), the GAM-PCA-VAR.

In the approach with a single pollutant Nitrogen Monoxide (NO) as covariate, were adjusted a GAM

and GAM-ARMA model to compare the effects of the autocorrelation structure in the modelling. The results revealed that the GAM-AR(1), with all coefficients significant including the coefficient of order 1 in the autoregressive polynomial, presented the best fit. This model presented smaller BIC (1297.514) and white noise residuals, which was not observed in the GAM model.

Table 2. Results of parameter estimates of GAM-AR (1) model

Variable	Estimates	Standard Error	p-value
NO	0.0515	0.0029	0.0000
sen12	0.3271	0.0499	0.0000
cos12	-0.5221	0.0615	0.0000
cos6	-0.2324	0.0362	0.0000
trend	0.0127	0.0010	0.0000
ϕ_1	0.0700	0.0053	0.0000

Besides that, we calculate relative risks (RR) and 95% confidence intervals for an interquartile variation of the pollutants concentrations. The RR analysis revealed that the NO contributed significantly to the increase of COPD cases in Belo Horizonte. Moreover, the RR value decreased when the autoregressive term was added.

Table 3. Comparison of the Relative Risk and 95% confidence interval

NO	Relative Risk	CI
GAM	1.0627	[1.0553;1.0702]
GAM-AR(1)	1.0591	[1.0524;1.0658]

In Figure 1 we present the comparison among adjustments of GAM and GAM-AR(1) models, revealing that the fitting of GAM-AR(1) described better the number of COPD cases.

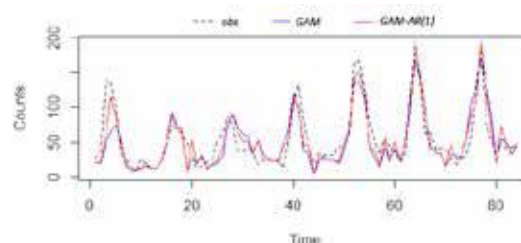


Figure 1. Comparing the fit of GAM and GAM-AR(1) models

The second approach considered the following pollutants: PM10, NO, NO2, CO and O3.

The autocorrelation and multicollinearity present in the pollutants were modelled using PCA and VAR methodologies.

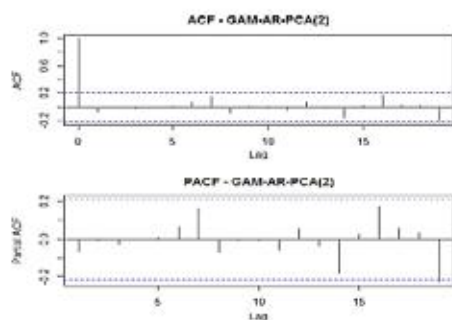


Figure 2. ACF and PACF of residuals - GAM-AR-PCA(2) model

The best fit was obtained with the GAM-PCA-AR(2) with the coefficients of order 1 and 2 in the autoregressive polynomials significant. Table 4 reveals that all coefficients were significant (p -value < 0.05). This model presented white noise residuals (Figure 2) and smaller BIC (1155.059) in comparison with the model that did not include the autocorrelation structure of the response variable.

Table 4. Results of parameter estimates of GAM-AR-PCA(2) model

Variable	Estimates	Standard Error	p-value
PC1	-0.0758	0.0131	0.0000
PC2	0.0400	0.0183	0.0287
PC3	-0.1699	0.0199	0.0000
sen12	0.1626	0.0544	0.0028
cos12	-0.9668	0.0595	0.0000
sen6	-0.2339	0.0347	0.0000
cos6	-0.1927	0.0398	0.0000
trend	0.0162	0.0020	0.0000
ϕ_1	0.0724	0.0077	0.0000
ϕ_2	0.0351	0.0095	0.0000

The Relative Risk (RR) analysis revealed that the PM₁₀, NO, NO₂ and O₃ contributed significantly to the increase of COPD cases, and once again the addition of the autoregressive component contributed to decreasing the relative risks (Table 5). This suggests that without this component, the RR can be overestimated.

Table 5. Comparison of the Relative Risk and 95% confidence interval

	$\widehat{RR}$	$\widehat{RR}^*$
CO	0.9235 (0.8986;0.9492)	0.8995 (0.8724;0.9275)
PM ₁₀	1.1386 (1.1113;1.1667)	1.1914 (1.1604;1.2231)
NO	1.0383 (1.0131;1.0640)	1.0811 (1.0532;1.1097)
NO ₂	1.0302 (1.0076;1.0533)	1.0647 (1.0419;1.0881)
O ₃	1.1007 (1.0649;1.1376)	1.1108 (1.0699;1.1532)

Figure 3 presents the comparison among adjustments of GAM-PCA-VAR proposed by Souza *et al.* (2018) and GAM-AR-PCA(2) models, revealing

that the fitting of GAM-AR-PCA(2) described better the number of COPD cases.

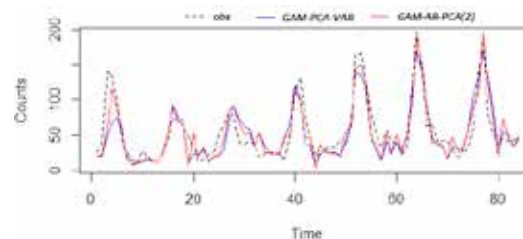


Figure 3. Comparing the fit of GAM-AR-PCA(2) and GAM-PCA-VAR models

CONCLUSIONS

In this work, we proposed a new class of models, called GAM-ARMA, which is an extension of the GAM based on GLARMA methodology. The structure of GAM-ARMA allows the fitting of non-parametric and semiparametric models, accommodating covariates with non-linear and linear relation with the response variable in count data with time dependence.

The time structure is modelled by an autoregressive and moving average component. We presented the estimation procedure both the parametric and non-parametric components. Here we focused on the estimation either for the parametric elements, as well for the non-parametric components. To evaluate the performance of the GAM-ARMA we performed two simulation studies which showed that, although the estimates present small bias and mean squared error, the autoregressive and moving average components influence the estimation. In general, we found better estimates when these components assume small values. In a real data analysis of the effects of air pollution on respiratory disease in the metropolitan area of Belo Horizonte, Brazil, we observed that the proposed model presented a better fit when compared to the widely used GAM approach, that do not take into account the autocorrelation of the data. The results revealed that the proposed model provides better adjustments than the conventional models applied in count time series.

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ESTIMATION OF HEALTH BENEFITS ASSOCIATED WITH REDUCTION OF PM₁₀ IN SURROUNDINGS AREAS OF A COLOMBIAN UNIVERSITY, THROUGH BENMAP SOFTWARE

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Abstract: Particulate material is the main pollutant of urban air in Colombia and can affect air quality, health, economy and society. The aim of this work was to estimate health benefits and costs of people belonging to Sergio Arboleda University, from measurements of PM₁₀ concentrations, performed for 3 hours in 37 points of the 252,000 m² surroundings areas of university. BenMAP response concentration function was adjusted to estimate respiratory diseases cases (RDC) and the cost include consultation, laboratory tests, images, medicines, materials, supplies and hospital stay due to a respiratory disease. The analysis demonstrates that 51 RDC were presented with an approximate cost of \$ 14,487 USD for all the cases and that the most promising scenario was the one that meets the indications of the WHO, presenting 33 RDC with a cost of \$ 9,445 USD.

Keywords: Estimates for cost-benefit, Air quality, Respiratory Disease Cases.

INTRODUCTION

In Colombia, the capital cities have the highest air pollution, in Bogota vehicles contribute 78% and in Medellin 81% of emissions are from mobiles sources (CONPES, 2018). For 2008, Bogota was ranked as sixth most polluted city in Latin America for particulate matter (Krzyzanowski, 2008), which is the main pollutant of urban countries (CONPES, 2018). For 2017 Bogota was the fifth of Latin American capital cities most polluted by PM₁₀ (PM of size between 2.5 and 10 µm) (Mead, 2017), which comes up to 80% of mobile sources of vehicles that use diesel as fuel (CONPES, 2018).

Mapping and Analysis of Environmental Benefits (BenMAP) software was designed by Environmental Protection Agency (EPA), to calculate cost benefits of changes in pollution concentrations (EPA, 2017). Software use inputs as shapefile, population, pollution concentrations, incidence, concentration-response function and the economic value. The results obtained allow us to analyze scenarios that reduce atmospheric pollutants, or determine a standard.

Estimates for cost-benefit in Bogota using BenMAP, described that reducing 5 µg/m³ the PM₁₀ in the zonal planning units, from 2010 to 2020, would lead to economic and health benefits in the capital city that are estimated at USD 6 trillion, for the reduction of respiratory diseases and morbidity (Ortiz, 2013).

For more information of an atmospheric pollution in Bogota, the city counts with the Bogota Air Quality Monitoring Stations, which register the pollution concentrations in order to know, regulate and understand his air quality problems (García & Rojas, 2017). In Bogota, Chapinero is the locality with the largest number of cases treated for respiratory diseases (OSAB, 2016) and the mobile station lacks of a representative sample of the data for 2015. It is important to use information from the locality because private stations located in Chapinero, detect measurements that exceed the Colombian daily emission standards (AMB, 2012).

The Sergio Arboleda University is one of the universities located in the locality of Chapinero (Fig. 1) and presents an estimated population of 9,576 among administrators, teachers and students who

use the facilities to develop their work and academic activities. Previous monitoring of this PM_{10} at the university reported concentrations above the permissible limit, evidencing the vulnerability of the community to high exposures of PM_{10} .



Figure 1. Location of study area in Chapinero, Bogotá, Colombia.

Based on the determination of PM_{10} concentration during the second semester of 2017, data were analyzed through BenMAP with the aim to estimate possible respiratory diseases cases (RDC) and the cost to pay for them at that time, for university community. Additionally, we estimate health benefit and the cost of the diseases for the reduction of PM_{10} concentrations in different scenarios.

METHODS

In second semester of 2017, 73 points were determined around Sergio Arboleda University, which were in an area (Fig. 1) of 252,000 m² (4.660995, -74.059804). The points were chosen from a composite random sample giving priority to corners, as they have the highest vehicular traffic. At each point for 3 hours (7-10h), PM_{10} concentrations were determined with the aerosol meter Dusttrak 8533. A total of 399,600 data were measured for the 37 days of sampling. Equation (1) was used to calculate in BenMAP the possible number of RDC that the university community could present (Ortiz, 2013).

$$C = (1 - e^{-A \cdot \beta \cdot \Delta}) * I * P \quad (1)$$

Where C is RDC, A is relation between PM_{10} and $PM_{2.5}$ (0.5), B is adjustment coefficient (0.00147), Δ is PM_{10} concentration change, I is the incidence (0.13) and P is population (9,576 people).

The economic value of each respiratory disease case was updated for 2017 and correspond to averages of the total costs that include medical appointments, laboratory tests, images, medicine, materials, supplements and hospitalization in Colombia (Bernal et al, 2017). Four scenarios of PM_{10} reduction were modeled: (1) 10% reduction of PM_{10} concentration, (2) 10 $\mu\text{g}/\text{m}^3$ reduction of all concentrations observed; (3) accordance with Colombian daily regulations (75 $\mu\text{g}/\text{m}^3$) and (4) accordance with the World Health Organization (WHO) guidelines (50 $\mu\text{g}/\text{m}^3$).

FINDINGS AND ARGUMENT

The highest concentrations of PM_{10} were recorded in the polygon formed between 76th Street, 11th Street, 75th Street and Caracas Avenue (Fig. 2). Else, lowest concentrations were reported between Caracas Avenue, 75th Street, 15th Street and 72th Street. According to the results, mobile sources produce the majority of the emissions (Jiménez et al., 2017) from surroundings areas of the university.

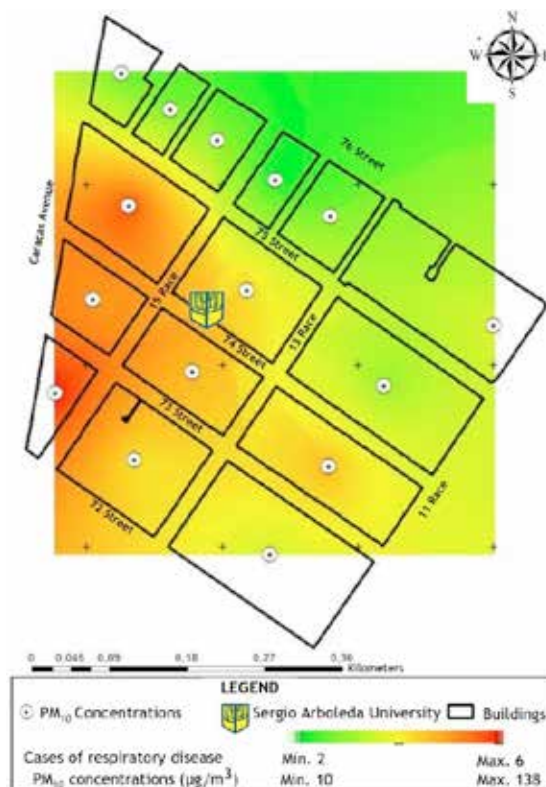


Figure 2. PM_{10} concentrations registered for 2017-II and Respiratory Disease Cases estimate through BenMAP, from surroundings areas of Sergio Arboleda University

PM₁₀ concentrations are directly proportional to RDC estimate through BenMAP, registering as there is no safe level of exposure (WHO, 2013). For the concentrations taken 51 RDC estimated with an approximate cost of \$14,487 USD, which is the economic value that enters the health system due to attending all the RDC.

Highest PM₁₀ concentrations can be observed in Caracas Avenue (Fig. 2), as it is a critical road in terms of mobility (Behrentz, 2017). However, 11th Street registered variations of PM₁₀ concentrations (Fig. 2), possibly due to trees, screening and meteorological variables (Arciniégas, 2012). The fourth scenario is the most promising, which complies with WHO guidelines, since is the one that reduces the most PM₁₀ concentrations, the scenario presents less RDC and has the greatest economic savings compared to the original scenario (Table 1).

Table 1. Respiratory Disease Cases (RDC) and its respective cost of modeled scenarios estimate through BenMAP, from surroundings areas of Sergio Arboleda University

SCENARIO	10% reduction of PM ₁₀ concentration observed	10 µg/m ³ reduction of all concentrations observed	Accordance with Colombian daily regulations	Accordance with WHO guidelines
Avoidable RDC	5	8	9	18
RDC total	46	43	42	33
RDC total cost (\$USD)	13,073	12,293	12,016	9,445

CONCLUSIONS

BenMAP software allows estimating that at time of analysis, 51 RDC would be presented with a total cost of \$ 14,487 USD, according to PM₁₀ concentrations recorded during study. Decreased of PM₁₀ lowers RDC and directly cost to pay for them, which happens because a safe level of exposure has not yet been determined.

Highest PM₁₀ concentrations were reported where there is more vehicular traffic, as it is on Caracas Avenue, which is a critical road in terms of mobility. Although 11th Street has a significant flow of vehicles, PM₁₀ concentrations were possibly varied by trees, screening and meteorological variables.

For management of PM₁₀ pollution from surroundings areas of Sergio Arboleda University, the most promising scenario of the modeling was that which complies with the WHO guidelines, since it was the one that reduced most PM₁₀ reduced, presenting 33 RDC and a saving of \$ 5,042 USD this compared to original scenario.

Analyze the atmospheric pollution concentrations is useful to now better the air quality presented in a place, the possible sources of pollution and their impact, how it presented in this work. But also, is important to use this information to stimulate the awareness of air quality in people, the reduction of pollution and to plan strategies of prevention and protection of the effects of pollution.

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ANALYSIS OF AIR POLLUTION DURING A TRUCKERS STRIKE IN BRAZIL, 2018

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Abstract: For a few days during May 2018, a Truckers Strike (TS) stopped several activities in Brazil. Due to the low circulation of vehicles during the TS, the event was an opportunity to evaluate the air quality. This study aims to investigate the behavior of air pollution before, during and after the TS, analyzing air pollutants datasets (O_3 , NO, NO_2 , NO_x and PM_{10}) of the city of Campinas, SP. It was used Principal Component Analysis (PCA), and Theil-Sen statistical analysis method. PCA indicated that May 23rd and May 24th were more affected by air pollution, while May 28th, May 29th and May 30th had lower concentrations in PM_{10} , NO_x and O_3 , during the TS. Trend analysis of PM_{10} and O_3 concentrations revealed that both decreasing day-on-day, an average rate of $2.21 \mu g \cdot m^{-3}$ per day and $5.35 \mu g \cdot m^{-3}$ per day, respectively. NO_x concentrations showed no significant trend. Finally, the results indicate that vehicular emissions are responsible for a great share of air pollution and investments in public policies for sustainable transportation are necessary.

Keywords: Principal Component Analysis, Trend analysis, Weekly cycle, Air pollution.

INTRODUCTION

High levels of air pollution emissions from vehicle traffic impact air quality in urban areas. Brazilian truckers went on a strike between 21 and 30 of May of 2018, with the most critical period between May 23rd and May 30th, that affected the population's routine, mainly because of the lack of fuel in most cities (BBC, 2018; G1, 2018). In these days there was a reduction of the fleet of vehicles in the streets, influenced, mainly, to the scarcity of fuel in gas stations. Thus, it is believed that the strike has directly influenced the air quality. The truck drivers' strike can be seen as an opportunity to evaluate the behavior of air pollutants. Thus, this study aims to evaluate the quality of the air during the period of that strike, in the city of Campinas, São Paulo, Brazil.

METHODS

Local and data characterization

The air quality data of this study was collected in Campinas, which is in São Paulo State, in Brazil. This city has an estimated population, in 2018, of 1,194,094 inhabitants and an area of 794.571 Km^2 (IBGE, 2019). The air quality data analyzed was obtained online, at the QUALAR platform (QUALAR, 2019), which is a database of CETESB's (the Environmental Company of the State of São Paulo, Brazil) automatic station in Campinas, located in Taquaral Park (South latitude $22^\circ 52' 28''$ and West longitude $47^\circ 03' 3''$). The air pollution parameters analyzed, in $\mu g/m^3$, were nitrogen dioxide (NO_2), nitrogen monoxide (NO), nitrogen oxide (NO_x), ozone (O_3) and particulate matter with an aerodynamic diameter smaller than 10 μm (PM_{10})

concentrations. The meteorological data were temperature (temp) [$^\circ C$] and wind speed (WS) [m/s].

The truckers' strike was divided into three different periods in this study: Before the Truckers Strike (BTS), from 05/01/2018 to 05/22/2018; During the Truckers' Strike (DTS), from 05/23/2018 to 05/30/2018; and After the Truckers' Strike (ATS), from 06/01/2018 to 06/30/2018.

Statistical analysis

All analyses were performed utilizing the R software (R Core Team, 2018). In the first place, Principal Component Analysis (PCA) was performed with daily concentration pollutants and meteorological data, in order to identify days more polluted in DTS period. Varimax rotation was performed to reflect the better relationship between the PCs and the original variable (Dominick et al., 2012).

In the second place, the trend analysis for the daily average concentration of pollutants was performed using the TheilSen function of the Openair package (Carslaw and Ropkins, 2012; Carslaw, 2018) for BTS, DTS and ATS periods. The non-parametric method of Theil-Sen is used in nonnormal and heterocedastic data series, and even in presence of outliers (Ancelet et al., 2015; Font and Fuller, 2016; Cho et al., 2017; Mateus and Gioda, 2017). In this analysis, the data series were deseasonalized (Mateus and Gioda, 2017; Gama et al., 2018). Bootstrap sampling was used to get the 95% confidence intervals and p-values (Font and Fuller, 2016; Cho et al., 2017; Mateus and Gioda, 2017).

FINDINGS AND ARGUMENT

Figure 1 shows the biplot of PC (Principal Component) for first and second components obtained from PCA. PC1 and PC2 explained 96% of the total variance after varimax rotation. Notice that May 23rd and May 24th were separated from the other days (Fig. 1). This occurred because these days were the most affected by truckers strike when the population began to realize the effects of the first of strike and started looking for gas stations to fuel their cars (BBC, 2018; G1, 2018). In the others days, population avoided getting out by car, in order to save fuel, and consequently, in these days (especially May 28th, May 29th and May 30th), there was a low circulation of vehicles and reduction of air pollutants concentrations.

Table 1 shows trend estimate and 95% confidence interval for trend estimate for air pollutants (PM_{10} , O_3 , NO_x , NO and NO_2), during BTS, DTS and ATS periods based in Theil-Sen method. Notice that only PM_{10} and O_3 presented trends significant. PM_{10} concentration presented negative trend in DTS period, as O_3 concentration.

Table 1. Trend estimate (before brackets) and 95% Confidence Interval (between brackets)

	Period	Estimate [95% CI]
PM_{10}	BTS	-0.59 [-1.44, 0.56]
	DTS	-2.21 [-3.89, -1.61]**
	ATS	0.33 [-0.57, 1.31]
O_3	BTS	-1.66 [-3.13, -0.50]**
	DTS	-5.35 [-8.89, -3.17]***
	ATS	0.32 [-0.02, 0.88]+
NO_x	BTS	0.37 [-0.49, 1.22]
	DTS	-0.55 [-2.47, 1.98]
	ATS	0.32 [-0.82, 1.26]
NO	BTS	0.14 [-0.07, 0.51]
	DTS	-0.08 [-0.39, 0.43]
	ATS	0.14 [-0.42, 0.67]
NO_2	BTS	0.49 [-0.81, 1.18]
	DTS	-0.95 [-4.21, 2.80]
	ATS	0.36 [-0.52, 1.04]

$p < 0.001 = ***$; $p < 0.010 = **$; $p < 0.050 = *$; $p < 0.100 = +$.

Figures 2 and 3 details trend analysis based on the Theil-Sen method for the PM_{10} and O_3 daily averages data, respectively, during DTS period. The trend was for PM_{10} concentration to decrease, showing a reduction of $2.21 \mu\text{g}/\text{m}^3$ ($p < 0.010$) per day in this period (Figure 2). The PM_{10} concentration average reduced from $36.85 \mu\text{g}/\text{m}^3$ to $16.00 \mu\text{g}/\text{m}^3$. The ozone concentration presented a reduction of $5.35 \mu\text{g}/\text{m}^3$ ($p < 0.001$) per day in DTS period, and the

concentration average reduced from 74.0 to 40.2 (Fig. 3).

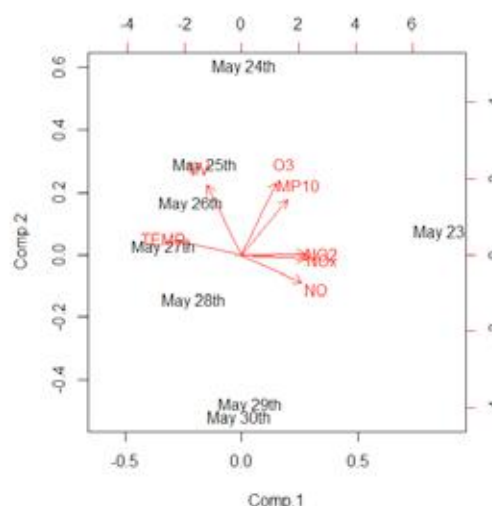


Figure 1. Biplot of days during DTS period

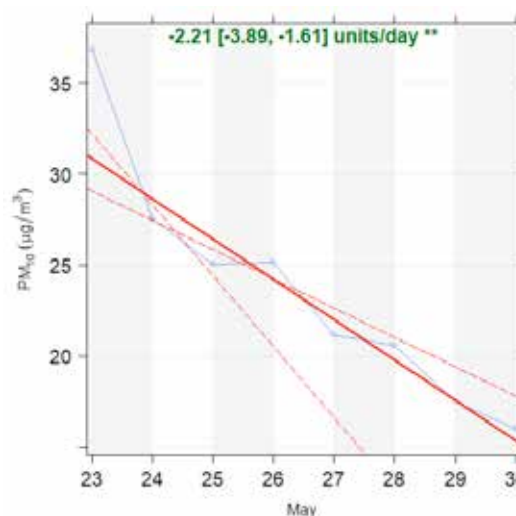


Figure 2. Trend analysis for PM_{10} concentrations in DTS period

The PM_{10} reduction (Fig. 2) may be explained to a reduction in the fleet of vehicles during this period. With the low circulation of vehicles in the streets, it was expected lower NO_x concentrations, but this behavior was not observed in the analyzed period (Table 1). In the other hand, occurred O_3 concentration reduction (Fig. 3). For ozone reduction, there are two possibilities, being a reduction in NO_x or in VOC (Volatile Organic Compounds) (Sillman, 1999). Reduction in NO_x will be effective if NO_x -sensitive chemistry predominates, and, reductions in VOC will be effective in reducing ozone if VOC-sensitive chemistry predominates (Sillman, 1999). So, we

believed that the atmosphere of Campinas had a reduction in VOC concentrations (ie, VOC-sensitive chemistry), and consequent, reduction in ozone concentration during DTS period. Unfortunately, the relation O_3 - NO_x -VOC are so complex, and lack of VOC concentration did not allow us to conclude this.

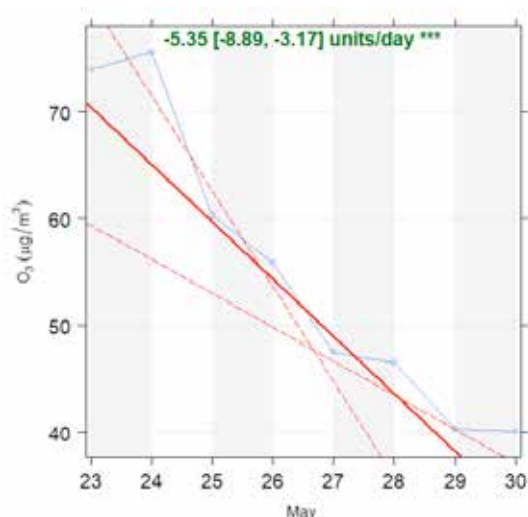


Figure 3. Trend analysis for O_3 concentrations in DTS period

CONCLUSIONS

The truckers strike was an opportunity to evaluate the air pollution caused by vehicles emissions. The DTS period, the results obtained in PCA indicated that May 23rd and May 24th were more affected because the population was searching for fuel in the gas station, increasing the traffic and the emissions. In the other hand, May 28th, May 29th and May 30th showed lower concentrations in PM_{10} , NO_x and O_3 , due to the reduction of the fleet of vehicles in the streets. The Theil-Sen analysis indicated on PM_{10} and O_3 concentrations decreasing day-on-day during DTS period. Finally, the results indicated that vehicular emissions are responsible for a great share of air pollution. Thus, investments in public policies for transportation are important to improve air quality.

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SOPRAR/SALVADOR AIR QUALITY FORECAST SYSTEM OF SALVADOR METROPOLITAN REGION

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Abstract:

Introduction: In Latin America - one of the most urbanized regions in the developing world - at least 100 million people are exposed to air pollution above recommended WHO concentrations. Key risk groups particularly vulnerable to this problem are children, elderly people and persons with poor health or low socio-economic status. SOPRAR-Salvador Project is an intersectoral mobilization aimed at addressing this issue in the Bahian capital, coordinated by the Gonçalo Moniz Institute of the Oswaldo Cruz Foundation (IGM-FIOCRUZ - Dr. Nelzair Vianna) and by the Secretariat of Sustainable City and Innovation of the City Hall of Salvador (SECIS - André Fraga), supported by Deutsche Investitions - und Entwicklungsgesellschaft (DEG) and ARIA Technologies.

Objective: SOPRAR-SSA will (1) adapt and introduce innovative air quality modeling system to assess and mitigate the impact of air pollution on health, (2) propose a warning system for health care management, civil defense and environmental planning in Salvador Metropolitan Area (RMS), (3) transfer related technical knowledge, know-how & capacity and (4) develop City-level action plans and protocols in order to protect the population from expected pollution events impacts.

Methods: Based on data provided by partners, public databases and well-established methodologies, ARIA will compile inventory of atmospheric emissions from point sources, vehicular and area sources in RMS. The emission inventory will be integrated in the Model Chain based on WRF-CHIMERE models. The system will produce an air quality database for environmental epidemiological assessment, to determine air quality and health risk indicators relevant to health surveillance and civil defense. The indicators will be integrated in the model chain for operational forecast purposes as the Early Warning System.

A Salvador City Level Action Plan will be developed with local partners, based on a Local Committee Board, to define actions to be taken when pollution levels are expected to reach certain thresholds. The Early Warning System will be considered into the Action Plan, incorporating protocols and recommendations, improving risk communication to hospitals, schools, other city government departments and asthmatic citizen ahead of high air pollution episodes, reducing health impact. In the future, the Early Warning System can be used to trigger specific actions, such as traffic restriction to force emission reduction and avoid an air pollution episode.

Conclusion: The project in Salvador is directly benefitting urban health planners, civil defense and environment managers, as it makes available an air quality modeling and an early warning system integrated to communicate the health impact associated with air pollution. The project builds on existing data and develops institutional capacity, transfers know-how on how to use existing streams of data and local institutions to enhance environmental management for the benefit of Salvador's citizen. This leads to decrease GHG emissions and to reduce the burden of air pollution on health - productivity, morbidity and mortality.

Keywords: Air Pollution, Modeling, Warning System, Public Health, Sustainable Cities

INTRODUCTION

In Brazil, municipalities are responsible for the promotion, coordination and execution of studies and research applied in the area of environmental health surveillance according to normative instruction nº 1 of 2005, published by the Secretariat of Health Surveillance-SVS (Brazil, 2005). However, the environmental agencies of many states and municipalities do not have infrastructure and staff, adequate to develop specific actions against contamination situations.

In Salvador, the association of the prevalence of respiratory allergies and air pollution has not been systematically described in local epidemiological investigations, although a study that addresses the asthma outcome has revealed a prevalence of 27.1% (Solé et al., 2001) in the city. Franco et al. (2007) demonstrated that large financial resources are allocated to control this disease in Salvador, so research, monitoring and prediction of environmental risk factors could be useful for the adoption of preventive measures and action plans,

contributing also for the optimization of these resources in the Unified Health System (SUS). Environmental management coordinated by the competent bodies in major metropolitan areas needs monitoring and planning tools to ensure an effective decision-making process. Air quality monitoring networks, when well dimensioned, act as an instrument to diagnose the present conditions, to evaluate the impact of accidental emissions and to consolidate a continuous database capable of representing the context of the exposure to the pollutants in diverse meteorological conditions. Between 2010 and 2016, an air quality monitoring network composed by 9 stations in the city of Salvador was operational. Currently, the metropolitan region of Salvador has no active air quality monitoring network.

However, monitoring is not as effective in defining guidelines for population mitigation and protection, especially when considering chronic exposure. The use of numerical models of meteorology and atmospheric chemistry is justified to anticipate the environmental concentrations of air pollutants and the conditions of the air quality in an area. The prior knowledge of these conditions allows managing population exposure to atmospheric pollutants, providing a long-term basis for the adoption of strategies for controlling air quality and sustainable economic development. In the short term, the forecast allows local health and environmental secretariats to articulate specific actions for alerts, preparation of health care device teams and civil defence, protecting the population.

The SOPRAR/Salvador Project (Operational air Quality Forecast System for the Metropolitan Region of Salvador), supported by DEG and ARIA Technologies aims to introduce innovative air quality modeling systems applied to health surveillance, contributing to prevent and mitigate the impact of air pollution on health in Salvador, Brazil. An intersectoral mobilization was organized including the Gonçalo Moniz Institute of the Oswaldo Cruz Foundation (IGM-FIOCRUZ), CETREL S. A. (Environmental Consultancy Private Company) and the Sustainable City and Innovation Office - City of Salvador (SECIS) to implement the project.

Primary beneficiaries of the project are local authorities, mainly departments of health, civil defense and the Environment and Sustainability Department. in charge of issuing air pollution warnings. The general public of RMS also benefits from this project, as early-warning air pollutions systems can protect human health and improve public health at reasonable cost. Further target groups are hospitals, education facilities, insurance companies and urban as well as transport planners that can profit from the provided information and data. Actors of the health sector, for instance, need information that allow them to understand the impact of air pollution peaks on the health of their patients. Urban planner, in contrast, will be

enabled to find the best solution with regards to traffic concepts, emissions permitting and industrial zoning.

METHODS

In close cooperation with local authorities, companies and research institutions, ARIA Technologies (AT) will (1) adapt and introduce innovative smart air quality modelling system to assess and mitigate the impact of air pollution on health, (2) integrate modern air quality modelling techniques for the first time in health care management, civil defense and environmental planning of a Brazilian metropolitan area, (3) transfer related technical knowledge, know-how & capacity and (4) demonstrate the multiple benefits for human health and the environment from such an approach. AT will use air quality modelling chain as commonly used in Europe/USA and adapt it to RMS - WRF/CHIMERE (Vautard, 2001).

The project is organized by 5 Work Packages (WP), and it is expected to deliver the operational system on mid-2020. Figure 1 illustrates the Work Plan proposed from June 2018.

The WP A1 quantified and sectorized the total emissions, by type of atmospheric pollutant and source typology, of the Metropolitan Region of Salvador, providing a current picture of these joint emissions and predict the additive of pollutants on the aerial basin to be controlled. In addition, the inventory will be used as input data in the WRF-CHIMERE model chain and will serve as a basis for the configuration of the SOPRAR system, which will allow the assessment of the contribution of the main emission sources to the formation of pollutants in the region and to differentiate the origin of the themselves.

The SOPRAR configuration (WP A2) is under development. FIOCRUZ will host the system and the meteorological simulations provided by CEMADEC (*Center for Monitoring and Alert of Civil Defense*) will be used as input to CHIMERE model. Three nested domains will be applied with 27, 9 and 3km resolution respectively.

In partnership with FIOCRUZ, a health impact assessment will evaluate the impact of air pollution on public health based on consolidates environmental epidemiology methodologies (WP A3). This assessment will also define indicators to be applied to the Systems Output, in order to facilitate the information dissemination. The WP A4 aims to integrate the indicators in the system and to interact with the operators from CEMADEC to design the warning system routine.

The Forecast system will be available on a Web Service (Figure 2), and the CEMADEC operators can check the predicted conditions and trigger specific protocols for risk communication. Those protocols will be defined in partnership with local institutions on WP B.

WP	Description	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A1	Emission inventory																								
A2	Air Quality Forecast System																								
A3	Health Impacts																								
A4	Warning System / Civil Defense																								
B	Air quality Events Action Plan																								
C	Awareness, Training, Events																								

Figure 1. SOPRAR/Salvador WorkPlan.



Figure 2 - Air Quality Forecast WEB Service example.

and citizens. Dr. Paulo Saldiva, one of the most relevant researchers in the international scientific community on the environmental health field contributed remotely (videoconf) with an inspiring Keynote Session. The Workshop gave a context about Air Quality in Salvador and its impacts on human health. Local institutions, such SECIS, CODESAL, FIOCRUZ, CETREL, UFBA, contributed with great summaries of the evidence and governmental instruments applied for air quality management in Salvador. The event description and the presentations are available online (<http://soprar.eco.br/>).

PROJECTS RESULTS (ON GOING)

This first term of the project was based mainly in the promotion of the project, search for engagement of local actors to provide input data that are key to consolidate the database representative of the current condition of the atmospheric pollutants emitted by the identified sources. At the early start of the project, we faced difficulties to get an involvement of local institutions such FIOCRUZ and SECIS due their lack of agenda. Finally, we had great interactions with Secretary André Fraga and Dra. Nelzair Vianna, and it was possible to schedule the Kick-off Workshop Event (delivered with a 2-month delay). The project was included on the workplan of the Memorial of Understanding signed between SECIS and FIOCRUZ, reinforcing their interest on the project.

We also proposed to the local partners institutions to sign a Cooperation Agreement called "Protocolo". This document states the contributions and counterparts of each partner on the SOPRAR Project., ARIA, SECIS (City of Salvador), FIOCRUZ and CETREL. Nevertheless, the document is still being analyzed by their legal department as we hand out this report.

We had a successful Workshop Event (Figure 3) to present the Project and to Build Awareness related to Air Pollution Impacts with about 100 participants including city managers, researchers, private sector



Figure 3. Opening Table of SOPRAR/Salvador Workshop.

In parallel to the event organization, ARIA team was involved to collect input data to build the Emission Inventory and the Air Quality Monitoring Database. The main difficulty was related to mobilizing institutions to contribute to the project with input data, due the lack of human resources and the non-inclusion of the project on the specific institution's workload. This difficulty induced a delay to the Emission Inventory tasks (Work package A1).

The Emission Inventory must be built based on local data regarding fuel consumption, traffic, road network, industries processes and land use. In this first inventory, the main industrial sources in the region and mobile emissions were considered,

including coherent assumptions for the lack of data cases. For the industrial sources, the emission data made available by CETREL for the year of 2017 were used, which each year receives updated information of the industries, for the enterprises installed in the Industrial Complex of Camaçari and Porto de Aratu. Due to the unavailability of physical and chemical parameters of the emitting sources necessary for the mathematical modeling, the inventory elaborated due to a doctoral thesis in the year 2003 of Dc. Diogenes (Lyra, 2008) was used as base. For the other industrial poles, due to the unavailability of more specific information, they were not considered.

The inventory of mobile sources, due to the delay in the availability of information by the city of Salvador, was built based on the HTAP 2 inventory (EDGAR, 2010), whose base year is 2010 (Figure 4). HTAP is an international scientific cooperation effort to improve understanding of intercontinental pollution transportation throughout the Northern Hemisphere.

Based on the inventory built, it was identified that the sources that contribute most to the emission of atmospheric pollutants in Metropolitan Region of Salvador are the industrial ones.

The air pollutants emission inventory was delivered, and the training session was organized. During half three days (not full days due the participants agenda commitments), it was possible to gather a heterogeneous audience (about nine to ten city managers who are part of several sectors such as: university, transport, civil defense and public health) to discuss the Emission Inventory Methodology and to present the results. The training gave rise to quite enriching discussions where the various sectors reported the difficulties, they find internally to disseminate the importance of preserving city air quality.



Figure 4 - Particulate Matter (MP) Emission in RMS - mobile sources - ton/year (base 2010).

The air quality forecast system is currently under tests in ARIA's infrastructure and it will be transferred to FIOCRUZ infrastructure on August. In the coming months those tests will generate the databases for the system's evaluation and integration with the health risk assessment that will be conducted in partnership with FIOCRUZ. Inter-

American Development Bank (IADB) will also give some resources to a complementary consultancy to support FIOCRUZ's contributions.

CONCLUSIONS

Monitoring and environmental risk factor forecasting systems are strategic points for the adoption of preventive measures, alerts and environmental health management. Currently, the municipal management of Salvador is committed to the problem and inaugurated the Center for Monitoring and Alert of Civil Defense (CEMADEC), promoting environmental risk monitoring in different areas of the city. Extreme rain events have a high impact on health and are monitored by measuring network, radars, satellite imagery and weather modeling. With the implementation of SOPRAR/Salvador, Civil Defense will start to launch some protocols, in partnership with other organizations (such as the Department of Health and Environment) to protect the population, including risk communication.

Salvador is part of the 100 Resilient Cities Initiative from the Rockefeller Center, and in 2019 it was published the Resilient Strategy (available at <http://100resilientcities.org/wp-content/uploads/2019/03/Resilience-Strategy-Salvador-Portuguese.pdf>) whereas include the SOPRAR Project as one of the actions listed for the axis of health management and social assistance, care for the population.

The project is based on existing data and builds institutional capacity, transfers know-how on how to use existing data streams and local institutions to improve environmental management for the benefit of Salvador citizens. The project brings together relevant institutions from the city of Salvador (FIOCRUZ, SECIS) and establishes a new cooperation mechanism to integrate the management of sectors such as health, industry and transportation, which influence each other. This leads to the reduction of GHG emissions and the costs of reduced productivity induced by pollution, as well as other spending on human health.

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Assessment of air quality in school environment

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Abstract: Exposure to particulate matter in the atmosphere is one of the main factors that negatively contribute to respiratory health, especially in urban areas and big cities. Studies about air quality indicate a negative and severe impact on health, which causes increase in morbidity and mortality. It is also noticed the increase of health problems at certain times of year. Thus, the aim of this work was to investigate the relationship between weather conditions and air quality of some public schools in Porto Alegre. Indoor and outdoor particulate matter concentrations were measured and analyzed throughout the four seasons. Mobile devices were used to measure particulate matter concentrations in nine micro-environments near schools and in the routes used by students. Temperature, humidity and wind were also measured. The particulate matter concentrations in the micro-environments were similar and mostly higher than the tolerated level recommended by the World Health Organization (WHO). It was observed that only in the autumn season the particulate matter concentrations remained close to the exposure levels recommended by WHO for 24 hours, and in some seasons, there was a relation between PM_{2.5} and temperature together with a weak relationship with humidity, which was not so significant.

Keywords: PM_{2.5} Measurements in Motion; Scholar Air Quality; PM_{2.5} Indoor and Outdoor; Air Pollution.

INTRODUCTION

World economic and industrial development, population growth and urbanization, as well as the increase in the number of motorized transport vehicles, causes an increase in the deterioration of the environment, increasing the levels of pollutants to which the population is exposed. This poses a threat to human health, current and future, especially in respiratory diseases in children, becoming a serious public health problem. This study evaluates the air pollution around 5 schools of Porto Alegre with the objective of measuring the differences between the external pollution and the air quality inside of the school.

METHODS

The measurements of air pollution were carried out in movement and in real time, using the most likely route to be daily traversed by the children to reach their school. Public schools were selected for this study, since their students often travel on foot. Each of the routes were traveled walking at two different times of the day: in the morning, corresponding to the school entry, and in the afternoon, corresponding to the time of the second round of the schools. These measures were repeated in each of the seasons (winter, spring,

summer and autumn). They were named Routes 1, 2 and 3. Each of the routes were traveled walking at two different times of the day: in the morning, corresponding to the school entry, and the afternoon, corresponding to the time of the second round of the schools. The samples collected on the routes and in front of the school were characterized as outdoor samples. Samples were also collected inside the classrooms, and these were called indoor samples.

The particulate matter and climatic conditions measurements were performed by accurate and sensitive equipment. The concentrations of particulate matter have been carried out on the DUST TRACK TM II Aerosol Monitor model 8532, with particulate matter filter of 2.5 micrometers.

The data was collected in a fraction of the 24 hours of day, and represent the concentrations of particulate matter which schoolchildren are exposed during walking to school. In this time there is the highest concentration of particulate matter in the atmosphere. The figure 1 demonstrates the routine of the measurement of particulate matter in the micro-environments: 3 minutes at morning and another 3 minutes afternoon for the single measurements, and 30 minutes, twice in a day, for each route.

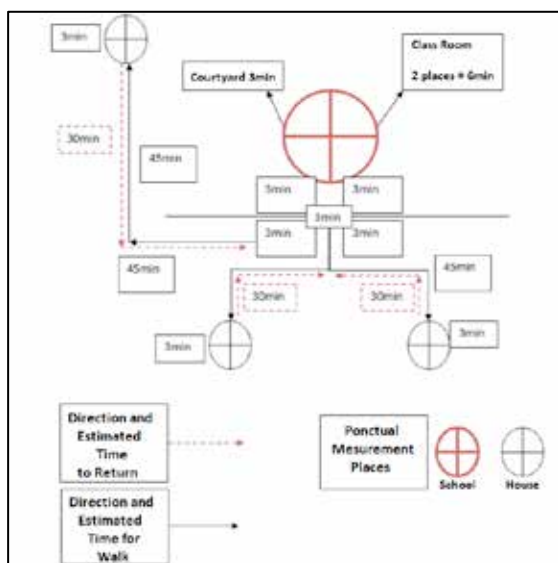


Figure 1 - Schematic of measurement

FINDINGS AND ARGUMENT

The table 1 shows the ration between indoor and outdoor (I/O) values for the particulate matter in all seasons for the 5 schools evaluated, named S1, S2, S3, S4 and S5.

	Winter	Spring	Summer	Autumn
S1	0,722	0,982	0,944	0,528
S2	1,188	0,992	0,978	0,811
S3	0,998	0,944	0,969	0,394
S4	1,066	0,960	0,980	0,367
S5	0,974	0,950	0,989	0,848

Table 1 - Ratio between indoor and outdoor

Autumn shows a better result from the other seasons the pollution inside of the buildings, except the in S1 and S5, are half or less then the outside. In the winter the pollution inside of the buildings S2 and S4 show almost equal or high then the outside. These occurrences could be explained by the geography of the regions, with wind variations. In the summer and spring, the ratio is close to 1, maybe explained by the high temperatures that obey the windows to be opened for a better air circulation.

CONCLUSIONS

The pollution from traffic increases the risks for respiratory diseases and symptoms, however, the methods for evaluating pollutant indicators should be validated, with the elaboration of more studies with adequate methodological design, to obtain a scientific basis solid.

This study shows that the architectonic buildings, could not be a good barrier for the external pollution, in some cases it is efficient but in other not. The buildings of the schools have no air conditioner devices, that in the summer, or hot days, the architectonic barrier has close to zero effect.

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Field experiment based quantification of air pollution exposure to in-pram babies and comparison with adult exposure

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Abstract: Babies, usually referred to young children with age less than 1 year, are more susceptible to adverse impacts of a similar level of air pollution exposure compared with adults (Buonanno et al., 2013; Galea et al., 2014; Kenagy et al., 2016; Kumar et al., 2017; Sharma and Kumar, 2018). The systematic assessment of their exposure is lacking. A multifaceted mitigation approach including soft (community empowering) and hard (technology driven) measures are needed to limit their exposure. Focusing on pollutants such as particulate matter (PM_{2.5}, PM₁₀), ultrafine particles (UFPs), and black carbon (BC), the aim of this work is to critically assess the comparative exposure levels of in-pram babies and to develop a strategic exposure mitigation framework combining technology, public policy and community engagement strategies. We classified various pram types based on criteria such as height, width and the seating capacity (single versus twin) and assessed the breathing heights of sitting babies in various pram types available in the market. Then, we designed field experiment plan for a range of scenarios designed to incorporate the effect of variations in exposure microenvironment (e.g., type of pram (single pram and double pram) and use of pram covers. Real-time field experiments were performed in single (facing parent and facing roadside) and double prams facing roadside. Primary data is analysed and a wide range of passive exposure control mitigation strategies (such as passive control at the receptor via enhanced filtration around the breathing zone and protection of prams) are critically evaluated (see table 1 for details of single field runs). We covered a total of 47 mornings and 46 evening runs covering a distance of 195km approximately. The preliminary analysis of primary data from field experiments suggested that babies transported in prams and breathing at relatively lower heights (within the zone of vehicle tailpipe's location) compared with adults are exposed to comparatively higher concentrations of different fractions of particulate matter (PM_{2.5}, and PM₁₀). Similarly, for double prams, the in-pram baby at the bottom seat of the pram is exposed to higher BC and PNC concentrations compared with baby sitting on the top seat. Overall, we concluded that in-pram babies are exposed to greater concentrations compared to adults since their breathing zone lies in the location of the vehicle tailpipe. Further in-depth analysis of the results is currently in progress.

Keywords: Baby Pram, Black Carbon, Exposure Assessment, Passive Control, Ultrafine Particles Exposure.

INTRODUCTION

Air pollution is found to be the largest cause of pollution-associated disease and is accountable for almost 6.4 million deaths per year with as much as 4.2 million caused by ambient air pollution and 2.8 million by household air pollution (Landrigan et al., 2017, 2018; Smith et al., 2014). These were the findings of the Lancet commission following the analysis of data from the Global Burden of Disease Study (Forouzanfar et al., 2016). To such a serious threat of air pollution exposure, particularly vulnerable are young children as they are very sensitive to environmental pollution during the windows of vulnerability during early development stages (see references of studies in table 2). Many studies have reported the adverse health impacts of

air pollution exposure to babies. Particularly, there are numerous studies pertaining to the distinctive health effects of air pollution to young children health on varying topics, such as, air pollution and neurodevelopment (Alemany et al., 2018; Perera, 2017), air pollution and respiratory effects (Bowatte et al., 2015; Bråbäck and Forsberg, 2009; Iskandar et al., 2011; Kanchongkittiphon et al., 2015; Khreis et al., 2017; McConnell et al., 2002; Perera, 2017), air pollution and cognitive development (Forns et al., 2015; Freire et al., 2010; Suglia et al., 2007; Sunyer Deu et al., 2017; Sunyer et al., 2015), air pollution and magnetic resonance imaging (Pujol et al., 2016). There are only a handful of studies from the past on in-pram babies' exposure which provides meaningful insight on elevated exposures of in-pram

babies by quantifying and comparing exposures at two different breathing heights, in-pram baby breathing height and adult breathing height. For example, Kumar et al. (2017) quantified the variability in concentration (size-resolved particle mass i.e., $PM_{2.5}$ in the range of 0.25-32 μm ; and particle number concentration i.e., PNC in the range of 0.2-1 μm) exposure for in-pram babies versus adults. They performed mobile measurement (64 runs over a distance of 87 km) in Guildford town centre area during morning and afternoon times. Their study revealed that in-pram babies are exposed to higher $PM_{2.5}$ ($PM_{2.5} = 47\%$, $PM_{10} = 31\%$) and PNC (31%) concentrations during the afternoon pick-up hours of children from school compared with morning drop-off hours. While they have discussed in detail the variability in the morning versus afternoon concentration exposure of in-pram babies, however, the study doesn't quantify the differential exposure of in-pram babies compared to adults. Similarly, Kenagy et al. (2016) performed stationary measurements along roadside environments in city of Edinburgh (UK) to assess the differences in NO_2 concentration exposure of in-pram babies compared to adults for their respective breathing height (i.e., in-pram breathing height = 0.8m and adult breathing height = 1.25m) above the ground level. They showed that measured concentrations at lower heights (0.8) were generally higher (5-15 %) relative to measured concentrations at moderately greater heights (2m) at a distance of 1.2 m from the kerbside of a busy traffic road. In a similar study, Galea et al. (2014) performed mobile measurements in Edinburgh city centre for pre-defined routes for $PM_{2.5}$ exposure at two different heights (i.e., in-pram breathing height = 0.74m and adult breathing height = 1.36m). However, their findings of this study were in contrast to other similar studies. They found that $PM_{2.5}$ exposure concentrations at in-pram baby breathing height were not higher than concentrations at adult breathing height, and, in fact, the reverse was found true, i.e., $PM_{2.5}$ exposure concentrations were found to be higher at adult breathing height by up to 17-51% than children in buggies (Galea et al., 2014). Garcia-Algar et al. (2015) performed simultaneous measurements of UFPs in Barcelona at two different heights, 0.55 m for an infant in a stroller and 1.70 m for an adult. They found that in-pram exposure to UFPs and $PM_{2.5}$ in the roadside environment was up to 10% higher than that for an adult while the corresponding values for NO_2 exposure were 5-15% higher for babies (Garcia-Algar et al., 2015). These findings were in line to those reported by Buzzard et al. (2009) emphasising that children breathing around tailpipe height are likely to be exposed to elevated concentrations of UFPs than those breathing at adults heights during walking or standing. None of the existing literature discussed above include quantitative findings of laboratory and field

experiments on efficacy of in-pram air pollution control technologies (such as, pram cover) which can be fitted inside prams. Also, there aren't any studies published so far which compare exposures in single pram facing roadside versus facing parent and similarly, comparison of in-pram exposure is missing for different baby breathing heights in double pram. Hence, there is a clear gap in understanding of in-pram exposure air pollution mitigation technologies and comparison of exposure in different types of prams at different baby-sitting heights such as, top seat versus bottom seat of double pram. Therefore, the present study aims to create a hitherto missing knowledge base for a low-energy, miniature, clean air system for removing gaseous pollutants and particles of varying size.

METHODS

Table 1 gives detail of field experiments for the data collection on selected route including details of field experiments with different scenarios for the data collection on the selected route. The targeted field measurements are divided into 8 different scenarios. The experiments were performed over 89 single runs (45 morning and 46 evening) covering a total distance of 187 km. First six scenarios include measurements in single prams with and without pram cover and industrial partner clean air prototype device (62 single runs) and for last two scenarios, measurements are performed in double prams (27 single runs).

Table 1. Details of the field run completed for selected Scenarios

Scenario	Description	Runs Completed
SP _{FP-WC}	Single Pram (facing parent-without cover)	10
SP _{FP-C}	Single Pram (facing parent-with cover)	10
SP _{FR-WC}	Single Pram (facing roadside without cover)	12
SP _{FR-C}	Single Pram (facing roadside with cover)	10
DP _{FR-WC}	Double Pram (facing roadside-without cover)	14

These scenarios differentiated on the basis of following criteria - (i) type of pram (single versus double) and (ii) use of pram cover. The field campaign is conducted for 40 days from during 6 August 2018 to 31 August 2018 and 7 November 2018 till 4 December 2018. Two runs are performed each day with 1 run in the morning (08:00h; local time) and 1 run in the afternoon (15:00h). The field campaigns are performed only during working days due to the school holidays on weekends. Pram covers are selected based on the filtration efficiencies of the pram covers to mitigate personal exposures of in-pram babies to pollutants (PNC,

PM_{2.5}, PM₁₀, and BC). The measurements were performed for PNCs, PM₁, PM_{2.5}, PM₁₀, and BC.



Figure 1. The route map showing field measurements for in-pram baby exposure.

The measurements were performed for 2 different heights i.e., typical in-pram breathing height (i.e., 0.7m) and breathing height of adult pushing the pram (i.e., 1.7m). The measurement was done utilizing the following instruments: (i) GRIMM aerosol spectrometer (EDM 107, GRIMM Technologies Inc., USA) for measuring particles in the 0.25-32 μm diameter range with sampling frequency of 6 seconds; (ii) P-Trak (Model 8525, TSI Inc., USA) UFP counter for measuring particles in the size range 0.02 to 0.1 μm with sampling frequency of 6 seconds; (iii) Q-Trak for CO measurements with sampling frequency of 10 seconds; and (iv) Microaeth (Model MA 200 and Model AE51) for BC measurements at sampling frequency of 10 seconds. The instruments were fitted into the prams at baby breathing height. For mimicking the exposure of in-pram babies and adults, we use 2 sets of similar instruments which are fitted into pram and backpack of the adult pushing the pram. The first set of instruments inside pram mimics the exposure at in-pram baby breathing height of 0.7m above the ground while the second set of instruments in backpack mimics exposure at breathing height. First set of instruments which are fitted into the pram includes GRIMM (EDM 107, GRIMM Technologies Inc.), P-Trak 8525 (TSI Inc.), Q-Trak and Microaeth (Model MA 200, Aethlabs, USA). The second set of instruments which is fitted into backpack includes GRIMM (11-C, GRIMM Technologies Inc.), P-Trak 8525 (TSI Inc.), Q-Trak (7575, TSI Inc.) and MicroAeth (Model AE51, AethLabs, USA). GRIMM data was obtained for every 6 seconds, however, these data points were averaged to 1 min subsequently to match the averaging period of other instruments utilised simultaneously. The location of the field worker was acquired per second (i.e. 1 Hz) with a Global Positioning System (GPS) Garmin Oregon 550 (Garmin Ltd., USA).

FINDINGS AND ARGUMENT

Here, we discuss some indicative results only while further analysis is still in progress. The morning time fine particle exposure concentration at in-pram breathing height (single pram facing roadside; $11 \pm 5 \mu\text{g m}^{-3}$) is 27% higher compared to adult height exposure concentration ($8 \pm 4 \mu\text{g m}^{-3}$) while this difference is increased to 44% during afternoon time (in-pram height, $16 \pm 7 \mu\text{g m}^{-3}$; adult height $9 \pm 3 \mu\text{g m}^{-3}$) (see Fig. 2). However, for coarse particle concentration, while, these differences are observed in opposite direction with morning time exposure higher by up to 33% at adult height ($9 \pm 12 \mu\text{g m}^{-3}$) compared to in-pram height ($6 \pm 18 \mu\text{g m}^{-3}$). The trend for coarse particle exposure during afternoon time was in a similar direction as that shown for fine particle exposure with 22% higher coarse particle concentration at in-pram height ($9 \pm 20 \mu\text{g m}^{-3}$) in contrast to exposure concentrations those at adult height ($7 \pm 17 \mu\text{g m}^{-3}$). It should be noted that for figure 2, the in-pram height in this section is referring to in-pram height for single pram facing roadside.

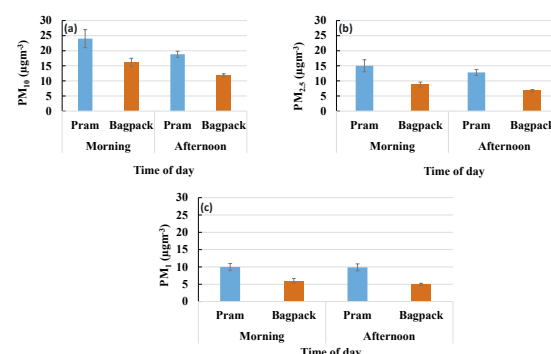


Figure 2. Morning and afternoon time concentration for pram versus backpack for different fractions of particulate matter such as: (a) PM₁; (b) PM_{2.5}; and (c) PM₁₀; Please note that y-axis denotes PM_x overall average concentrations for all runs combined.

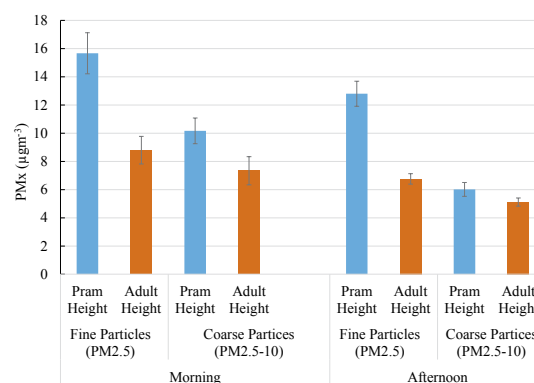


Figure 3. Fine and coarse particle exposure for baby vs. adults height during morning and afternoon time.

Please note that y-axis denotes PM_x overall average concentrations for all runs combined.

CONCLUSIONS

The analysis of primary data from field experiments suggested that babies transported in prams and breathing at relatively lower heights (within the zone of vehicle tailpipe's location) compared with adults are exposed to comparatively higher concentrations of PM_x (μgm⁻³), BC (μgm⁻³) and PNC (cm⁻³). Similarly, for double prams, the in-pram baby at the bottom seat of the pram is exposed to higher PM_x (μgm⁻³), BC (μgm⁻³) and PNC (cm⁻³) concentrations compared with baby, sitting on top seat. Overall, we concluded that in-pram babies are exposed to greater concentrations compared to adults since their breathing zone lies in the location of the vehicle tailpipe.

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SHORT-TERM IMPACTS OF AIR POLLUTANTS AND TEMPERATURE ON HOSPITALIZATIONS FOR MENTAL AND BEHAVIORAL DISORDERS

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Abstract: The effects of climate change and air quality on human diseases have been studied around the world. However, few analysis of the association of these environmental circumstances with disorders mental and behavioral changes have been made, especially in developing countries as Brazil. In this direction, a time series study was carried out to explore the associations between the air pollutants (SO₂, NO₂, NO₃ and PM₁₀) concentrations and mean temperature (T_m) and relative humidity (RH) over hospital admissions for mental and behavioral disorders for the cities of Curitiba and Araucaria. These cities are located in the southern region of Brazil and both municipalities are highly urbanized, with about 97% of their population residing in urban areas. The climate characteristics are similar; however, the urban morphology and the contributions of emissions sources to air quality conditions in the cities are different (Ardiles et al., 2017). The hospital admission for mental diseases (Chapter V, codes F00 to F99) were compiled from the online platform DATASUS (Department of Informatics of the Unified Health System) of the Unified Health System (SUS), and the meteorological and atmospheric pollutants data were obtained from the Environmental Institute of Paraná (IAP). All variables were analyzed daily for a time series from 2010 to 2014. It was used a Generalized Additive Model for Localization, Scale and Shape (GAMLSS) of negative binomial to Curitiba and negative binomial with inflation adjustment of zeros to Araucaria. The parameters analyzed in the probability distribution were modeled as non-parametric probability density functions smoothed through cubic splines. The health data were stratified by sex for both cities. For the city of Curitiba, the pollutants NO₂ and PM₁₀ presented a risk for both men and women, while in Araucaria SO₂ was the most expressive pollutant independent of sex. The temperature presented a risk for all groups.

Keywords: Temperature, emission sources, air quality, mental disorders.

INTRODUCTION

The problems related to air quality and health have been highlighted especially in the last two-three decades, mainly in the context of the marked climate change. The growing scientific interest in atmospheric aerosol particles is due to its great importance for the environment and health (Fuzzi et al., 2015). Atmospheric aerosols affect air quality and, in turn, human and ecosystem well-being (Héroux et al., 2015). Developing countries need studies relating diseases and air quality, for the promotion of sustainable and conscious development, as well as the collective health initiative and emission control.

METHODS

The average daily time series from 2010 to 2014 of the concentrations of SO₂, NO₂, O₃ and PM₁₀, temperature (T_m) and relative humidity (RH) were analyzed over hospital admissions for mental and behavioral disorders (MBD), stratified by sex, due to physiological differences (Ghisletta et al., 2018). The daily number of hospitalizations for primary diagnostic of MBD (Chapter V, codes F00-F99) classified according to International Classification of Disease (ICD 10) were compiled from the online public Single System of Health (SUS) Department of Informatics (DATASUS), webpage

(www.datasus.saude.gov.br), and the meteorological variables and air pollutants concentrations were obtained from the public Environmental Institute of Paraná (IAP - www.iap.pr.gov.br). Were used data from three air quality automatic stations located in Curitiba, and two in Araucaria. The stations used have at least 80% of valid data.

We used a generalized additive model (GAM), with the negative binomial distribution to model the explanatory variables for the outcome of mental disorders. For Araucaria, was used the negative binomial distribution inflated with zeros, due to the high percentage of null values, as proposed by (Lawless, 2006). To better fit the model some variables were added, weekdays and holidays were added as a binary indicator (0 or 1), to soften the characteristics of the highest number of hospitalizations on certain days in the week (Ardiles et al., 2017). The seasonality was modeled by natural cubic splines with 4 degrees of freedom per year.

The relative risk (RR) were calculated with the 95% confidence interval (CI) for each group, and all the statistical analyzes were performed using the statistical software R 3.5.3.

FINDINGS AND ARGUMENT

Figures 1 and 2 show the time series daily concentrations of analyzed pollutants in Curitiba and Araucaria, respectively. Except to ozone, the concentration of pollutants are larger in Araucaria. Although the cities are close, they present significant differences in air quality, these differences are directly linked to the emission pattern. In the case of Araucaria it is mainly industrial, while Curitiba presents mostly vehicular emissions (COMEC, 2015; IAP, 2013), which consequently the concentrations of SO₂ and PM₁₀ are significant higher in Araucaria.

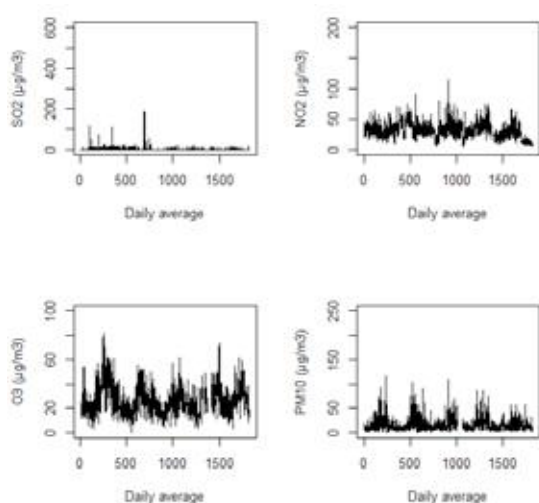


Figure 1 - Time series of daily average pollutant concentrations in Curitiba stations from 2010-2014.

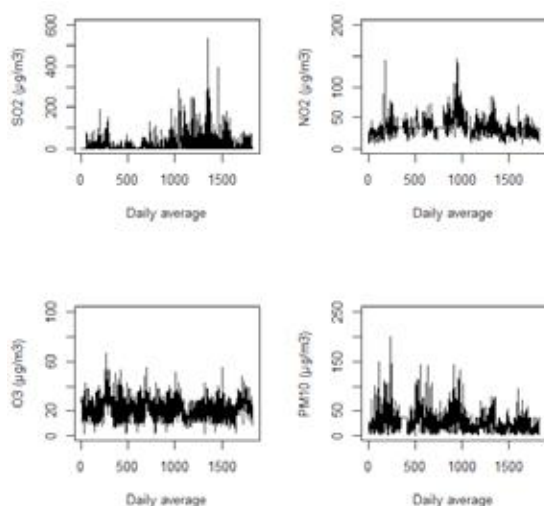


Figure 2 - Time series of daily average pollutant concentrations in Araucaria stations from 2010-2014.

The daily concentrations of pollutants in Araucaria exceed the limits established by CONAMA 491/2018 in many days in time series analyzed. The harmful effects of air pollution on brain activity present increasing evidence (Block et al., 2012). The nervous system responds first to environmental

variations, causing biological reactions that over time shape the emotional or behavioral character. Biophysical and meteorological factors cause changes in concentrations of neurotransmitters and eventually trigger mental or behavioral disorders (Yackerson et al., 2011).

Table 1. Relative risk of MDB to Curitiba.

Var	Men (RR - 95% CI)	Women (RR - 95% CI)
Tm	1.0133 (1.0009-1.0258)	1.0007 (1.0003-1.0142)
RH	0.9989 (0.9927-1.0052)	1.0020 (0.9953-1.0088)
SO ₂	0.9979 (0.9930-1.0028)	0.9993 (0.9935-1.0051)
NO ₂	1.0147 (1.010-1.0195)	1.0054 (1.0005-1.0103)
O ₃	0.9974 (0.9923-1.0026)	0.9990 (0.9937-1.0043)
PM ₁₀	1.0069 (1.0028-1.0111)	1.0024 (1.0021-1.0103)

Table 2. Relative risk of MDB to Araucaria.

Var	Men (RR - 95% CI)	Women (RR - 95% CI)
Tm	1.0818 (1.0099-1.1752)	1.0488 (1.0308-1.1359)
RH	0.9955 (0.9854-1.0088)	0.9982 (0.9897-1.0028)
SO ₂	1.0209 (1.0105-1.0569)	1.0019 (1.0005-1.0102)
NO ₂	0.9713 (0.9878-1.0065)	0.9945 (0.9740-1.0154)
O ₃	1.0291 (0.9801-1.0806)	0.9872 (0.9522-1.0236)
PM ₁₀	0.9846 (0.9595-1.0104)	0.9952 (0.9828-1.0077)

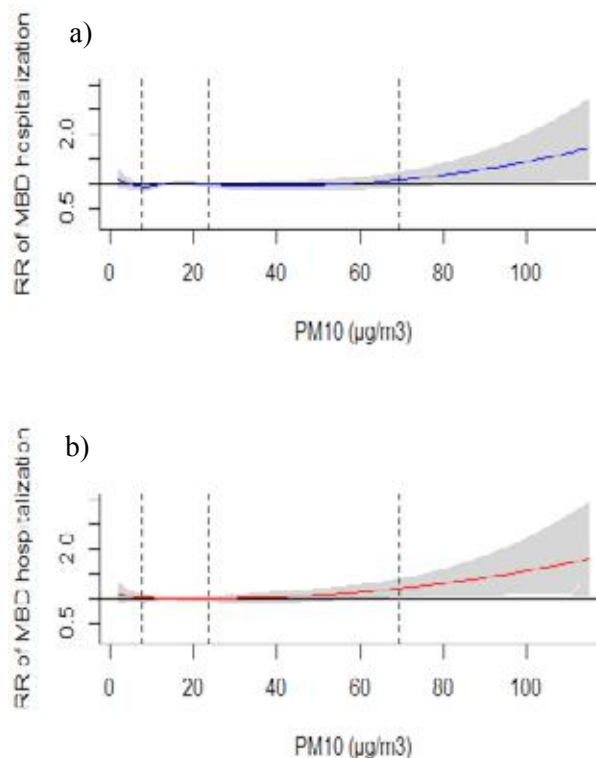


Figure 3 - Exposure-response curve of PM₁₀ and relative risk for mental and behavioral disorder (reference concentration of 13 µg/m³) for Curitiba. a) Men; b) Women. Vertical lines correspond to the 1st, 25th and 99th temperature percentiles.

In tables 1 and 2 are represented the relative risks of exposure to the pollutants analyzed in this study. For Curitiba NO_2 and PM_{10} represents risks for men and women, while in Araucaria SO_2 is the most significant pollutant associated with mental and behavioral disorders. As mentioned earlier, this difference is mainly related to the emission sources. Despite the relative high concentration of PM_{10} in Araucaria, when evaluated the effect of the pollutant together with the others, the risk is underestimated due to the influence of the other variables. However, when the model is composed only with the PM_{10} as an explanatory variable in conjunction with the control variables the RR obtained are of 1.0740 (95% CI: 1.0075-1.0269) for men and 1.0356 (95% CI: 1.0131-1.0169) for women. Temperature is also strongly associated with MDB, as observed in several studies (Cui et al., 2019; Peng et al., 2017). This is because extreme temperatures cause damage to nerve cells (Cramer & Jay, 2016; Lesk et al., 2016). In general, the men presented higher RR when compared with women. However, in this analysis the age was not considered, which was addressed in Silva et al. (2019).

Figure 3 shows the exposure-response curve for PM_{10} in Curitiba. It can be observed that the exposure to this pollutant is a risk factor in any concentration, due to the size of the particles, which allow it to reach the nervous system and its toxicity (Gao et al., 2017; Qiu et al., 2019).

CONCLUSIONS

It can be concluded that the air pollutants and temperature are risk factors to for mental disorders, and the type of the emission sources is an important aspect. In addition, this study reinforces the necessity of further deeper analysis of association between environment variables and mental disorders, as well as improvements in air quality.

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ANALYSIS OF PARTICULATE MATTER INSIDE A REST HOME IN SÃO PAULO, BRAZIL

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Abstract: Air pollution is a major environmental risk to human health, causing numerous adverse effects, for instance, respiratory, renal, cognitive, stroke and heart diseases. The elderly, among urban population, are distinctly susceptible to air pollution adversities and health effects, because of pre-existing health conditions, aging and cumulative toxic substances, such as smoking. Levels of outdoor air pollution in populous cities may not be adequately safe to the elder citizens and occasionally indoor air quality turns to be a risk as well. In particular, Brazil is the 5th most populous country in the world, with 30% of senior population. Globally, life expectancy at birth is projected to rise from 77 years in 2045-2050 and to 83 years in 2095-2100. Since elderly people spend 95% of their time in indoor environments, it is important to study levels of indoor and outdoor air pollution. This study aims to analyze (i) the mass of size-segregated particulate matter (PM) and black carbon (BC) in a rest home for elderly (Casa Ondina Lobo, Jardim dos estados, São Paulo - SP Brazil), (ii) evaluate the relationship between indoor and outdoor PM mass concentration, (iii) estimate respiratory deposition doses (RDD), and (iv) estimate MP ion composition. It was measured, simultaneously, indoor and outdoor PM in the 0.25-10 µm size range with five size ranges, using a Personal Cascade Impactor Sampler (PCIS; SKC Inc., Cat. No. 100-3000), during 24 hours data collection cycles. The PM mass of each sample was determined using a gravimetric method and PM₁₀ mass was calculated by summing all size ranges. Also, PM_{2.5} was analyzed by summing all sizes stages, except for PM_{10-2.5}. Concentrations of Black carbon (BC) were determined by optical reflectance with a smoke stain reflectometer (43D; Diffusion Systems Ltd). The MP ion composition was measured by ion chromatography during the first four stages. The means of PM₁₀ and PM_{2.5} were 39.1/31.5 µg/m³ and 23.8/19.1 µg/m³ for outdoor/indoor respectively, concluding on average, outdoor levels are 40% larger than indoor. PM_{2.5} and PM_{0.25} (particles with aerodynamic diameter of less than 0.25 µm) contributed 81 % and 34% of total PM₁₀, respectively. Nine samples of PM_{2.5} exceeded the standards set by the WHO, clearly indicating high exposure to fine particles by elderly. Furthermore, BC corresponds to 23.4% of PM_{2.5} mass, and the concentrations of BC were, on average, 6.7 and 5.2 µg/m³ for outdoor and indoor. The indoor/outdoor (I/O) ratios were calculated and we found values of 0.62 and 0.6 for PM₁₀ and PM_{2.5}, respectively, indicating external sources affecting indoor PM concentration. The RDD rates were applied for coarse and fine particles in outdoor measurements, 30% higher compared to indoor. The concentrations of ions were larger in outdoor samples, with sulfate and nitrate presenting the highest concentrations, 1.7 and 1.1 µg/m³, respectively. Our research suggests those elderly people living in São Paulo are exposed to high concentration of particles in indoor and outdoor environments, and when these concentrations exceed the WHO recommendation, adverse effects are presumed to affect elderly health. The I/O ratios and ion composition indicates that external sources, like road traffic, cigarette smoke, and dust, have a direct influence on internal PM. Our results propose the importance of controlling emissions of atmospheric pollutants, from both external and internal sources, in elderly residences and nursing homes to limit adverse health effects from particulate matter. Our conclusions suggest even in such wealth area, to control outdoor air pollution should be improved.

Keywords: Particle size, indoor/outdoor, rest home, elderly, respiratory deposition

1. Introduction

Air pollution is an important determinant of health. In 2016 air pollution was a cause 4.2 premature deaths worldwide (WHO, 2018). Many studies have been evidence the effects of air pollution on health. The airborne particulate matter (PM) are one of the most dangerous pollutants, causing lung cancer (NIELSE et al., 2016), heart diseases (DELFINO et al., 2005), respiratory diseases (POPE et al., 2011), neurodegeneration and cognitive dysfunction (LOANE et al., 2013), diabetes (HONDA, T et al., 2017) and anemia (HONDA, T et al., 2017b).

The effects to human health depends of differentes varies like age, pre-existing health conditions and others (PELED, R., 2011). The elderly population are more susceptible because of their depressed immune systems and pre-existing diseases (SUN & GU, 2008). The number of elderly worldwide will grow up from 21.5% in 2050 (United. N, 2015). Because of these aspects, the aim of this study is evaluate PM concentration and characterization in a rest home (São Paulo - SP), beside PM deposition dose in elderly.

2. Methods

2.1 Data collection and analysis

This study was made in a rest home localized in São Paulo - SP. We sampled the PM with a Personal Cascade Impactor Sampler (PCIS; SKC Inc., Cat. No. 100-3000), during 24 hours data collection cycles (indoor/outdoor) simultaneously, totalizing eleven measurements on may and june 2018. The indoor and outdoor collections was made at clinic and external area, respectively. The PCIS works with four filter stages and one post-filter: (A) referred 10-2.5 μm ; (B), 2.5-1.0 μm ; (C), 1.0-0.5 μm ; (D), 0.5-0.25 μm and (E), <0.25 μm (E) is a post-filter stage).

The PM concentrations were weighed by gravimetry using microbalance with scale of 1 μg (MX5; MettlerToledo, Columbus, OH, USA), black carbon concentration was measured by optical reflectance on post-filter stage with a smoke stain reflectometer (43D; Diffusion Systems Ltd) and ion chromatography was made to determine the concentrations of anions and cations on four first stages.

2.2 Estimation of PM deposition

We estimated the total *respiratory dose deposition* (RDD) in the respiratory system of elderly using equations given by (HINDS, 1999). We use elderly's respiratory parameters (male/female) given by (MUMOLI et al., 2013; PARREIRA et al., 2010).

3. Results and discussion

3.1 PM mass concentration

The average concentrations of fine particles ($\text{PM}_{2.5}$) were 25.6 $\mu\text{g}/\text{m}^3$. For fine particles there were not exceeded the CETESB's standards but the WHO guidelines was exceeded nine times, with eith outdoor and one indoor (Fig. 1). Fine particles were represented by sum of B, C, D and E stages and these particles represent 81% of all PM concentrations (Fig.1). The outdoor concentrations were 40% bigger than indoor.

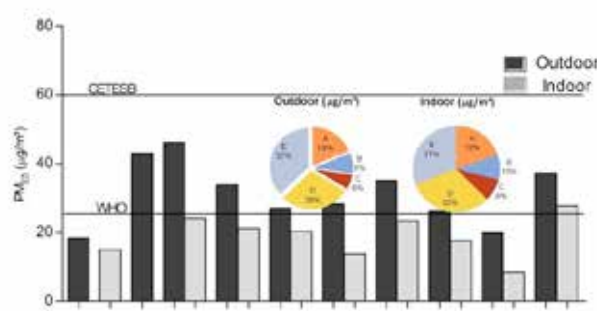


Fig.1 $\text{PM}_{2.5}$ mass concentrations (outdoor/indoor) and representation by PCIS stages.

The PM_{10} concentrations were measured by sum of all PCIS stages. Our mean PM_{10} was 31.8 $\mu\text{g}/\text{m}^3$ and the daily concentrations did not exceeded the CETESB's standards. The WHO guideline was exceeded two times in outdoor place (Fig.2). Like a fine particles, on PM_{10} outdoor concentrations were bigger than indoor (39% on average).

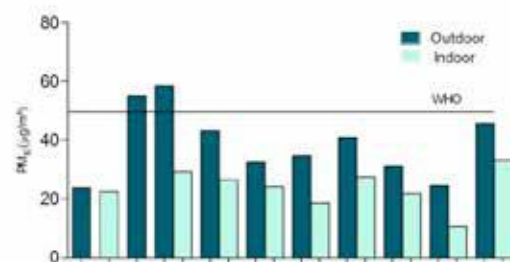


Fig. 2 PM_{10} mass concentrations (outdoor/indoor).

To understand the indoor/outdoor relationship between the mass concentration of PM_{10} and $\text{PM}_{2.5}$ we need to evaluate different characteristics. For example outdoor measurements are results for different sources in São Paulo like vehicular traffic, resuspension of dust, industry, pizzerias, bakeries, civil construction and steak houses (KUMAR et al., 2016). On indoor environment we have outdoor sources besides smoke from the burning of wood and cigarret (CHAO et al., 2012).

The outdoor place is frequent by cigarret smokers. Phillips et al (1998) reported smoker are exposed in a range of 46-94% higher PM_{10} concentration than non-smoker.

The I/O ratio is used to provide a relationship between PM mass concentration in indoor and outdoor environment. Our results show I/O <1 and indicate indoor particulate levels are penetrate from outdoors sources too.

3.2 Ion and BC concentrations

The concentrations of sulfate (SO_4^{2-}), nitrate (NO_3^-) and ammonium (NH_4^+) were major on D stage. SO_4^{2-} , NO_3^- and NH_4^+ are secondary inorganic aerosols originated by gas-particle conversion related to motor vehicle emissions (SEINFELD and Pandis, 2016). Nitrate is emitted by conversion of nitrogen oxides (NO_x), sulfate is produced from SO_2 oxidation and ammonium is related to ammonia and biomass burn (FINLAYSON-PITTS, 2000).

K^+ concentrations were higher on stages A and D, with 113.8 and 144.4 ng/m^3 , respectively, in outdoor (smokers area). K^+ is tracer representing a wood or biomass burning source (MUSTAFA et al., 2014). Ca^+ is higher on stage A with 973.4 and 756.8 ng/m^3 at outdoor and indoor respectively. Calcium is associated to resuspended dust and civil construction (WATSON, J 2004).

Concentrations of BC registered averages of 6.7 and 5.2 $\mu\text{g}/\text{m}^3$ for outdoor and indoor respectively. BC measurements represented 23.5% of $\text{PM}_{2.5}$ concentrations.

3.3 Respiratory deposition doses

The RDD was calculated using elderly respiratory parameters (tidal volume, respiratory frequency and minute ventilation). We estimate indoor and outdoor exposure for male and female, using mean particles diameter for each stage.

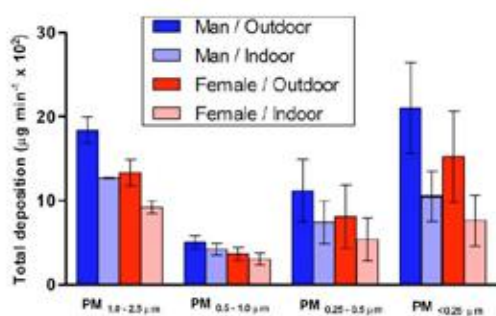


Fig. 3 Respiratory deposition doses (RDD) throughout the respiratory tract for elderly.

The highest concentrations were on stage E ($PM_{<2.5}$) representing 30% of all concentrations. For these reason, RDD was higher on this stage. These results is worrisome because smaller particles cause harmful effects on the human health (KELLY & FUSSELL, 2012).

Elderly mans have a higher respiratory parameters than elderly woman. Due to this, RDD was higher on man respiratory system than women.

Outdoor PM concentrations were higher than indoor, due to this, the RDD outdoor was on mean 32% higher than RDD indoor.

CONCLUSIONS

Our results identified elderly people, who live in nursing home, are expose to high PM concentrations. These people spend about $\geq 80 - 90\%$ of their time indoors. Our results indicated to PM characterization, indoor and outdoor sources, with indoor concentrations always lower than outdoors. Smoking cigarettes is another factor that might have contributed to increased outdoor PM concentrations. The RDD were higher for males than females and indicated highest PM deposition when elderly spend more time in outdoor. Our findings provide basis for mitigate adverse effects by air pollution on elderly health.

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Session 06
**Regulatory Modeling
and SIP Applications**

Impacts of Changing Heavy Trucks Fuel on Air Quality: A Case Study

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Abstract: The goal of this work is to estimate the abatement in air pollution emissions by changing the fuel of heavy trucks from diesel to liquefied natural gas (LNG) in road cargo transport, as well as its impact on air quality for the people living near Bandeirantes and Anhanguera roads. To estimate the transport activity in these roads, counting of vehicles at toll plazas are used. Emission factors for particulate matter (PM) and nitrogen oxides (NO_x) are used to estimate emission rates. The numerical model AERMOD performed simulations of pollutants transport and dispersion. The model was able to process prescribed meteorological conditions that, for this work, were obtained from a Weather Research and Forecasting (WRF) meteorological model simulation for 10 days during winter (6 to 15 August 2013). Results show that the area affected by the vehicular emission is highly influenced by atmospheric conditions. The emission plume may extend to a relatively large area and affect the population living near the roads. Calm winds conditions enhance pollutants concentration. The definition of the emission factor is key and there is still a large variability in values found. Liquefied natural gas has proven to be a cleaner fuel than diesel, however it demands investments in distribution infrastructure and regulatory changes.

Keywords: Air quality, liquefied natural gas, vehicular emission, AERMOD model.

INTRODUCTION

One of the greatest environmental issues of our time is air pollution and approximately 97% of the cities in low and mid income countries do not achieve the air quality guidelines of the World Health Organization

(<https://www.who.int/airpollution/data/cities/en/>). The transportation sector is a major contributor to air pollution and greenhouse gases in the state of Sao Paulo (CETESB 2013). In Brazil most of the commercial transport is done on roads (<https://www.cnt.org.br/analises-transporte>) by heavy duty vehicles (HDV).

In Sao Paulo state, the Environmental Company (CETESB) monitors air quality and estimates vehicular emissions. In 2017, for instance, CETESB estimated that heavy trucks emitted 18792 tons of carbon monoxide (CO), 89273 tons of nitrogen oxides (NO_x), 2693 tons of particulate matter (PM), 3596 tons of sulfur dioxide (SO₂), 3681 tons of volatile organic compounds (VOC) and 16250 tons of carbon dioxide equivalent (CDE), being responsible for 6% for CO, 58% for NO_x, 64% for PM, 77% for SO₂, 5% for COV and 39% for CDE of all vehicular emission (CETESB 2017).

The impact of air pollution on population health is substantial and it is estimated that 13000 people die every year because of air pollution in Sao Paulo (Gouveia et al. 2006; Veras et al. 2017; Saldiva et al. 2015; Rodrigues et al. 2015; Miranda et al. 2012;

https://www.saudeesustentabilidade.org.br/wp-content/uploads/2017/12/Cetesb_Saude_FINAL_V2_WEB.pdf).

Air quality in Sao Paulo has improved because of a national policy implemented since 1986 that limits new vehicles emission factors (EF) (Carvalho et al.

2015; Miranda et al. 2017; Ribeiro et al. 2016). However, local air quality standards (AQ_S) are exceeded during unfavorable meteorological conditions, particularly for ozone (O₃) during austral spring/summer, for which nitrogen oxides (NO_x) are precursors, and for particulate matter (PM) during winter. Therefore, more effective measures are needed to improve air quality (CETESB 2013).

In Sao Paulo, HDV only use diesel as fuel. Lately, it has a percentage of biodiesel (22%), but it still is a highly polluting fuel. Therefore, an alternative that has been evaluated is the usage of liquefied natural gas (LNG). Mouette et al. (2019) have investigated the costs and benefits of implementing blue corridors in Sao Paulo. Blue corridors are routes that aim to enable the use of LNG. They concluded that LNG costs up to 40% less than diesel, while reducing CO₂ equivalent emissions by up to 5.2%, PM by 88%, NO_x by 75% and eliminating hydrocarbon emissions. However, regulatory issues regarding the distribution of LNG in Brazil are an important barrier to implement blue corridors.

The present work intends to further explore the impacts of changing from diesel to LNG as HDV fuel on air quality and the population exposure to the pollutants emitted, in order to better evaluate the possible advantages of investing in a new fuel type for road transportation.

METHODS

This work only considers HDV in two main roads from Sao Paulo to Campinas, Anhanguera (ANR) and Bandeirantes (BNR), based in the design proposed by Mouette et al. (2019). To estimate the emission

abatement in using LNG instead of diesel, the current annual emission is estimated for the two considered roads as the multiplication of the EF for each pollutant, the distance traveled and the number of vehicles. The EF considered for NO_x is based on the CETESB data, considering different factors for different vehicle age (4.81 g km⁻¹). The EF for PM_{2.5} was the one calculated by Sanchez-Ccollyo et al. (2009) for HDV in road tunnels (0.558 g km⁻¹). The number of vehicles was obtained by toll plaza counting for 2016. Distance traveled by each HDV was estimated using the distance between consecutive toll plazas. The total abatement was estimated considering the study of Mouette et al. (2019): 88% abatement in PM and 75% abatement in NO_x. These factors were applied to the calculated total emission.

Then, to assess the impact of road pollution on the air quality of the population living near the roads, simulations with AERMOD model were performed (<https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models#aermod>).

AERMOD is a gaussian plume based model frequently used in licensing processes. The roads were considered as line sources that were defined to never be more than 200 m distant from the actual road. Daily emission rate was calculated using toll plaza counting of HDV vehicles and the EF mentioned before. For ANR, 19 sources were defined, and 9 sources were defined for BNR.

Meteorological conditions were obtained by an atmospheric model (WRF) for the period from 6 to 15 August 2013, representing austral winter conditions, that are not favorable for dispersion (Ribeiro et al. 2018). Therefore, the resulting concentration may be considered representative of the worst conditions. The results were then visually analyzed for Jundiaí city using Google Earth in order to observe the population impacted.

FINDINGS AND ARGUMENT

Total yearly emission for diesel and LNG are presented in Table 1. Changing the fuel only for the HDVs traveling between Sao Paulo and Campinas via ANR and BNR results in an abatement of 11% of PM (here considering PM₁₀, since CETESB does not estimate PM_{2.5} vehicular emissions) and 2% of NO_x of the total annual emission of the state (CETESB 2016).

Table 1. Total annual pollution emission by HDV between Sao Paulo and Campinas traveling in Anhanguera and Bandeirantes roads.

Emission (ton)	NO _x	PM _{2.5}
Diesel	3457	422
LNG	864	51

Local impact is even more substantial. Fig. 1 shows the maximum daily average concentration of PM_{2.5} simulated by AERMOD in current conditions (using

diesel as fuel), considering only HDV vehicles traveling ANR and BNR, over Google Earth images. BNR crosses Jundiaí city, passing near populated areas. Predominant conditions during the simulated period show NW winds that propagated higher concentration plumes to SE, fortunately away from populated areas. Highest concentrations are, as expected, near the roads, but there is a substantial contribution to pollution in populated areas. The period simulated included some calm winds conditions that greatly increased pollutants concentration.

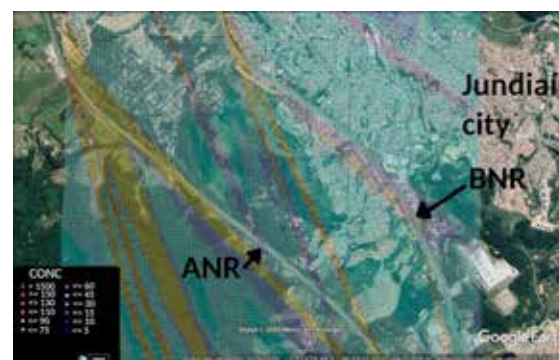


Figure 1. PM_{2.5} concentration in µg m⁻³ over Jundiaí area with current Diesel fuel.

When the simulation considers the usage of LNG as fuel (smaller EF), a considerable decrease in PM_{2.5} concentration is observed (Fig. 2). Most areas present a concentration lower than the WHO standard. Keeping in mind that this result only considers the contribution of HDV in ANR and BNR roads, it is important for the local administration to also promote measures to decrease PM_{2.5} pollution emission. The results show that, in addition to the contribution to the decrease on the state's total emission, changing diesel to LNG has a significant impact in local air quality conditions and consequently in public health for the population of Jundiaí city that live near the roads.

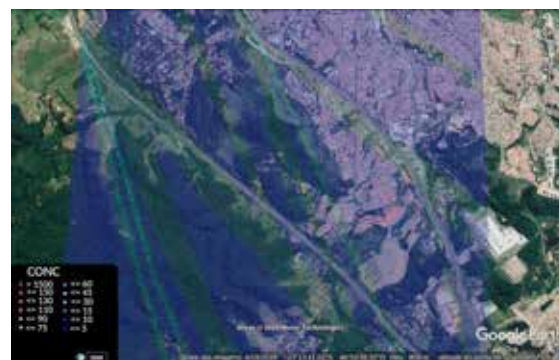


Figure 2. PM_{2.5} Concentration in µg m⁻³ over Jundiaí area with LNG.

The simulation considering NO_x also showed that ANR and BNR cause a substantial contribution to local emission (Fig. 3). Considering that the state AQS for nitrogen dioxide is 200 $\mu\text{g m}^{-3}$ in 1 hour, HDV emission in these roads definitely contribute to exceed that limit.

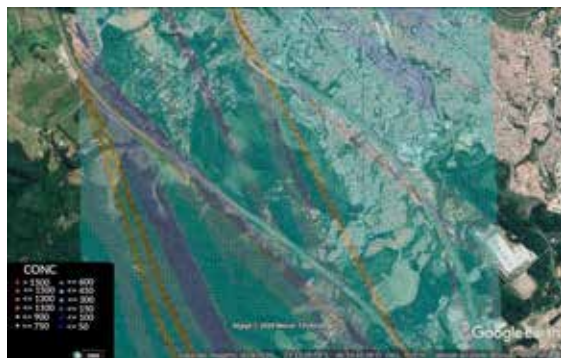


Figure 3. NO_x concentration in $\mu\text{g m}^{-3}$ over Jundiaí area with current Diesel fuel.

NO_x EF decrease from diesel to LNG is smaller than for PM_{2.5} and, therefore, concentration changes are not as intense. However, that are substantial improvement in air quality (Fig. 4). Some areas reduce ANR and BNR contribution in approximately half. Now, HDV traffic on ANR and BNR does not cause concentrations above the AQS over most of the area.

The contribution to decrease the total state emission of NO_x may not be impressive, but its impact in local air quality is substantial. It is important to stress that the simulations performed here represent unfavorable conditions for pollutants dispersion. The change, however, may considerably decrease AQS exceedances, greatly improving local air quality and, therefore, public health.



Figure 4. NO_x concentration in $\mu\text{g m}^{-3}$ over Jundiaí area with LNG.

CONCLUSIONS

This work is a first attempt to estimate local impacts of changing the fuel of highly polluting vehicles. There are challenges in determining the information used to address vehicular pollution as well as the uncertainties involved. Meteorological data is scarce and not easily available, but numerical models, when properly validated, are a helpful tool.

Meteorological conditions have a great influence on pollutant concentrations and the period simulated here was not favorable for dispersion, including periods of calm winds and subsidence that limited the mixed layer height. Concentrations were high for areas near the roads. When considering the health impact on the population affected by vehicular pollution, changing from diesel to LNG is an interesting option. Emission and concentrations may be substantially decreased.

Since LNG is already available in Brazil and is not yet used as fuel, it may be considered as a transition technology from highly polluting fuels to a more sustainable future. Differently than simulated here, a viable scenario is to convert only a part of the HDV fleet. Also, LNG needs to be included in Brazilian regulations and investments in infrastructure are needed to make LNG a viable choice of fuel.

Acknowledgments

The authors thank the Sao Paulo Research Foundation (FAPESP) for grant 2017/20148-3.

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EMISSION ESTIMATION AND DISPERSION MATHEMATICAL MODELING OF PARTICULATE MATTER FROM CONCRETE BATCHING FOR IMPACT ASSESSMENT ON AIR QUALITY

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Abstract:

The mathematical modeling of atmospheric pollutants dispersion has become an important computational tool to supply deficiencies present in the evaluation of air quality. However, there are still obstacles for certain situations, as the difficulty of measuring fugitive emissions, those that come from diffuse sources.

Thus, the present study aims to model the atmospheric dispersion of total suspended particles (TSP) and PM₁₀ of a concrete industry, whose atmospheric emissions are characterized as fugitives. For this, it was necessary an estimated material particulate emission rate of this industry, based on a methodology proposed by the United States Environmental Protection Agency (USEPA), which relates the industrial production capacity with atmospheric emissions, from an own emission factor for concrete batching, defined by the agency.

The Lagrangian model Micro Swift Spray (MSS) was chosen, which reproduces microscale scenarios, being more propitious for regions of rugged topography, which is the case of the region under study. When performing the modeling it was necessary to collect input data so that the program could generate the results for the analysis. Were used information of land use and topography, for creating a digital relief. Was also obtained meteorological variables, such as precipitation, humidity and temperature, obtained by the nearest meteorological station of the industry, administered by the National Institute of Meteorology.

The model generated dispersion plumes that were analyzed in two-dimensional scenarios. In order to better evaluate the potential pollution of the enterprise, two conditions were used, one without the presence of the fugitive emission control equipment and another considering the already installed ones, which is the current situation of the concrete batching.

The results showed that the control techniques are efficient in reducing the fugitive emissions of particulates from the concrete batching. The industry could interfere in the air quality in the region in the absence of control equipment. The local topography significantly interfered with the dispersion of the plume.

Keywords: Pollutant dispersion modeling, Fugitive emissions, Concrete Batching, Particulate matter, Micro Swift Spray (MSS).

INTRODUCTION

The emission of pollutants into the atmosphere has become a serious problem for the well-being of the population and for the environment, due to the accelerated industrial growth and the consequent increase of the emissions in the last years. In this context, over the last few years, the commitment to improving the quality of the environment, allied with the increasing demands of environmental agencies, has forced industries to mitigate their impacts on air quality in a variety of ways.

Techniques and specifically designed equipment to attenuate emissions throughout the production process, such as enclosure, confinement, local dilution ventilation, localexperative ventilation, cyclones, mango filters, water sprinkling, among others that can be effective measures in the control of atmospheric emissions (Lisboa and Schimer, 2007).

The implementation of emission control techniques in an industry must meet the emission standards of the local legislation in force. Besides that, if found that the sources significantly interfere in the air quality in the vicinity, the emission standards should also be taken into account. Therefore, the application of mathematical modeling of dispersion of atmospheric pollutants becomes useful, being an important tool to simulate the transport of air pollutants, both for air quality assessment in large urban centers, and also to identify regions that are not suitable for the installation of new enterprises, especially in the industrial sector (Batista et. al, 2018). Modeling makes use of softwares that are fed with different information, such as emission and weather data. It is an effective instrument for environmental monitoring and for assessing the air quality in locations close to emissions.

In the present study, the computational modeling was applied in a concrete batching, which over the last years has implemented atmospheric emission control techniques with the objective to reducing the emissions. Thus, through the plumes of concentration maps generated, was realized a comparative study of the scenarios before and after the implementation of the control measures. By treating of fugitive emissions, emission rates were estimated.

According to USEPA, Total Suspended Particles (TSP) and the Inhalable Particulate Material (PM_{10}), consisting, mainly, of cement and gaseous dust, but including some emissions of sand and gravel, are the major pollutants of concern for a particular concrete batching. Most of the sources are fugitive emissions, which include raw material transfer, truck loading, concrete mixer truck traffic and other trucks, and wind erosion from the raw material storage cells. The amount of fugitive emissions generated depends, among some factors, on the moisture content of the surface of these materials. In the case of fugitive emissions, there is a significant difficulty in measuring the pollutants.

METHODS

Initially, an analysis of the studied industry it was made, where information was gathered regarding the location of the facilities, the existing air quality monitoring data, the existing control systems, among other references. We also prioritized the search for data on meteorological conditions and methodologies for estimating fugitive emissions, mainly in concrete batching.

For the computational modeling, the two scenarios concerning the control systems were simulated through the ARIA Impact software of the company ARIA Technologies using the Micro Swift Spray - MSS model. This system uses the Micro Swift model, which generates the local scale wind field and the Micro Spray, a Lagrangian dispersion model. The MSS is suitable for calculating the wind field and pollutants at complex terrain sites.

Both for the calculations that were estimated as for the simulation performed considered that there was temporal modulation of the emissions. This tool is used to define a time dependent multiplicative factor that will be applied to the reference emission rate value of the source. This option allows you to consider the operation of the industry. In the current study was considered that the emissions from the operation and transportation activities occurred only during the industry work period from 6:00 a.m. to 6:00 p.m., from Monday to Friday, while the emissions from the storage had a frequency of 24 hours, every day of the week, since it is independent of operation.

In addition, two receptors close to the industry were determined, which allowed a punctual evaluation of the results obtained.

The software ARIA Technologies include topography preprocessors, land use, wind field and pollutant dispersion. For the relief was created a digital elevation model (MDE) from a file containing shape file of level contours of the city. The topography preprocessor of the interface generated a topography file with resolution of 30 meters. The land use data were obtained from a raster image with 30 meters of classified resolution and a classification file containing geophysical parameters such as albedo, surface roughness, Bowen ratio, soil heat (flux parameter) and leaf area.

Other important data refer to the source. Some of the sources were considered punctual, while others, source area or. For the estimation of the emission rates of the concrete batching, the following bibliographies were used as a basis: United States Environmental Protection Agency - USEPA (2014) e Sousa (2016). Firstly, emission factors were calculated for each point where there was emission, in both scenarios (without and with control systems), and later, from these factors, emission rates were calculated. The sources were divided into three categories for each scenario:

- **Without control technique**

1. **Operation:** Transfer of sand, gravel, gneiss powder; unloading of cement; loading of the cargo to the funnel; truck loading.
2. **Storage:** Stack sand, gravel, gneiss powder and cement.
3. **Traffic:** Transportation of concrete by concrete mixers and raw materials by trucks.

- **With control technique**

1. **Operation:** Loading the truck.
2. **Storage:** Stack sand, gravel, gneiss powder and cement silos filter.
3. **Traffic:** Transportation of concrete by concrete mixers and raw materials by trucks.

It is possible to notice that some of the activities of the operation phase weren't considered as sources in the second scenario. This is because according to the USEPA, with the adoption of control techniques, such as enclosure, the emissions in these sources became practically insignificant, being difficult to estimate the emission factors.

For the emission speed, since it is a matter of fugitive dust, the lowest value that the ARIA Technologies interface accepts, in this case, is 0.01 m/s. For the emission temperature the mean of the simulation period was 21.5 °C.

The software was also fed with weather information from the year of 2018 provided by the National Institute of Meteorology (INMETRO). The data were collected by the nearest meteorological station, being hourly values of wind direction, wind speed, temperature, precipitation, humidity, radiation and atmospheric pressure. The date chosen for simulation was the coldest week of 2018 (05/27/2018 to 06/02/2018), for being a period of greater atmospheric stability, which makes dispersion of the pollutants difficult.

The species modeled were the PTS and PM₁₀, the first being the main emission in the concrete batching. The parameters used to differentiate the species emitted were the density, dry deposition velocity (m/s), wet deposition coefficient (1/s), and particle diameter (μm). The informations about them shown in Table 1.

Tabela 1. Informações das substâncias.

Polluting	PM10	PTS
Diameter (μm)	10	30
Density (kg/m ³)	3000	3000
Washout (s-1)	4.00E-04	0.0012
Deposition rate (m/s)	1.30E-02	0.022

Reference: ARIA Technologie, 2014.

FINDINGS AND ARGUMENT

2D dispersion plumes were generated, which showed the worst situations (highest concentrations) for the simulated period and spreadsheets containing the maximum concentrations (peaks) in dates, hours and specific coordinates, including those of the predefined receivers.

Figures 1 and 2 present, respectively, the PTS dispersion maps before and after the installation of the control techniques. While Figures 3 and 4 are related to PM₁₀, for the two different scenarios. In Table 2 are inserted the values of the highest concentration, by receiver, with and without control, besides the differences of these averages.

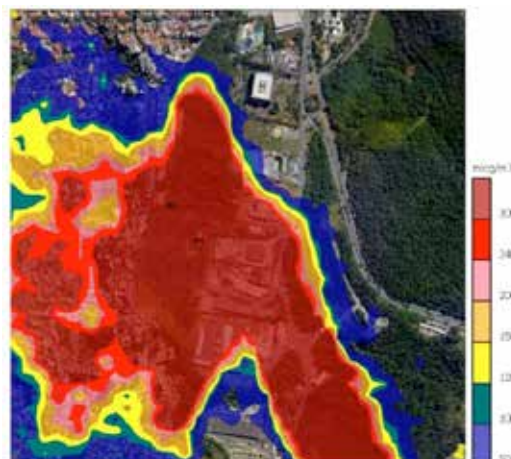


Figure 1. PTS - Scenario without emission control.

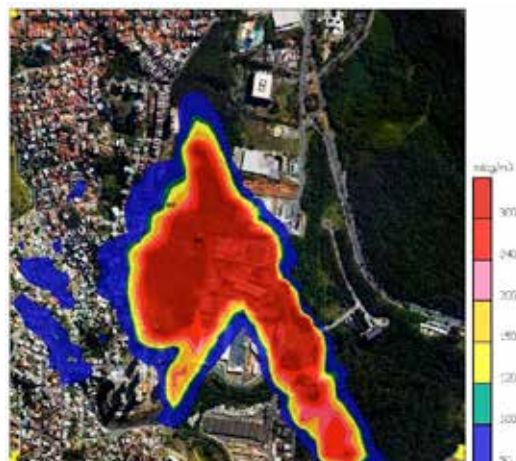


Figure 2. PTS - Scenario with emission control.

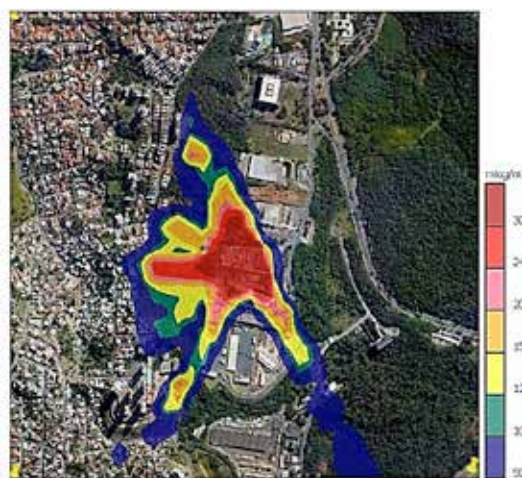


Figure 3. PM10 - Scenario without emission control.

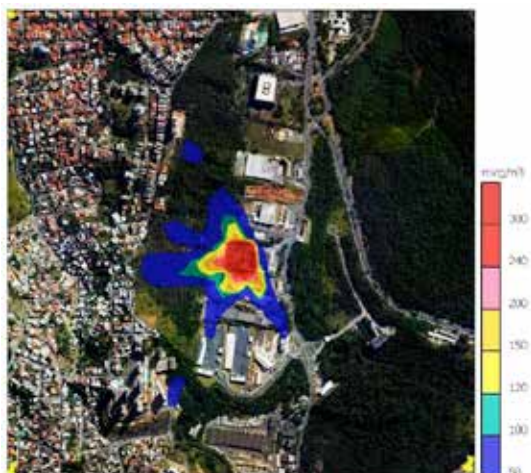


Figure 4. PM10 - Scenario with emission control.

Tabela 2. Higher concentrations in the receptors and difference between the scenarios.

Spot		R1	R2
Coord. X (km)		606.691	606.596
Coord. Y (km)		7801.23	7801.35
Without control	PTS (µg/m³)	1380,85	242,88
	PM10 (µg/m³)	55,25	17,26
With control	PTS (µg/m³)	212,77	35,57
	PM10 (µg/m³)	18,17	5,31
Difference	PTS (µg/m³)	1168,08	207,31
	PM10 (µg/m³)	37,08	11,95
	PTS (%)	84,60	85,35
	PM10 (%)	67,11	69,23

Reference: Personal collection

According to the resolution, the Primary Air Quality Standards are the concentrations of pollutants that, out of date, could affect the health of the population. Therefore, the statistical calculation used to generate the maps and the spreadsheets, calculated the worst concentration in several points of the defined domain and in the period of simulation chosen. After the calculations, from of inter-ratios, the model generated the concentration maps, in µg/m³. From this it became possible to make a comparison with the air quality standards established in CONAMA Resolution No.

491/2018, shown in Table 3, since the processing time defined for the calculations was 24 hours. The color scale of the maps refers to the ranges of the pollutant concentration plume and was defined taking into account the resolution limits.

Tabela 3. Air quality standards.

Standard	PM10 (µg/m³)	PTS (µg/m³)
Primary ¹	120	-
Secondary ¹	100	-
Finale ¹	-	240

¹ 24-hour reference period.

Reference: Resolution CONAMA, nº 491/2018.

Comparing the feathers of the non-inhalable particulates (PTS) and the inhalable ones (PM10), a significant reduction of the concentration in the surroundings of the enterprise was observed, since the reach of the feathers with control system was smaller. The PTS plume in the scenario without control equipment reached the residential neighborhood, as can be seen in Figure 1. In this situation, the limit of 240 µg/m³, shown in Table 3, would be exceeded even in the residential neighborhood. In contrast, for the scenario that considers mitigating measures for fugitive atmospheric emissions, shown in Figure 2, the PTS plume had a much smaller range. The residential district didn't receive concentrations higher than 240 µg/m³. Regarding the mean values of the maximum concentrations in the two receptors, there was a reduction of 83.00% and 76.30%, respectively, as recorded in Table 2.

The same occurred for the inhalable particulate material (PM10). At the recipients, the reduction of the mean maximum concentrations for the simulated period was 65.21% and 65.18%, respectively. In the uncontrolled scenario, whose plume is shown in Figure 4, concentrations above the established standard (120 µg/m³) are basically restricted only to the physical limits of the enterprise.

The topography of the local is bumpy. To the west, before the residential neighborhood, there is a mountain range that interferes in the shape of the plume. In Figures 1, 2 and 3 it is possible to note that, even if the tendency of the feathering direction to be east-west, following the predominant direction of the wind, is possible to perceive a busbar caused by the mountain range, that ends up functioning like an obstacle, causing that the rays of the plumes increase in the direction north-south.

Finally, it is possible to confirm the fact that fugitive emissions from concrete batching are, predominantly, from non-inhalable particulate

materials (PTS). At receiver 1, for example, in the emission control scenario, the mean for PM10 is 7.55% of the mean for PTS.

CONCLUSIONS

The results showed that the control techniques such as spraying, confinement and sweeping of the passageways of the trucks, are efficient in reducing the fugitive emissions of particulates from the concrete batching. It can be assumed that in a situation without emissions control and on cold days, where the atmospheric stability is greater and the boundary layer is low, the establishment could interfere significantly in the quality of the air in the surroundings, including in the residential neighborhood.

The achievement of the mathematical modeling of the dispersion of particulate pollutants, with the use of the Micro Swift Spray software, which was evaluated the contribution of each emission source of the establishment, to the scenario of without and with control, allowed to conclude that the mountains located just west of the sources served as a bush of the feathers, reducing its range in the east-west direction and doing the opposite in the north-south direction.

It is important to note that the "curtain" effect of the existing forest between the emission sources and the residential neighborhood east of the sources, wasn't considered in the present study. Therefore, this subject is suggested as continuity or for an improvement in future work.

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SIMULATION OF VEHICULAR EMISSIONS AND ITS DISPERSION AT PRESIDENTE ANTÔNIO CARLOS AVENUE, IN BELO HORIZONTE, BRAZIL

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Abstract: The vehicular emission of pollutants is a fundamental factor in studies of air quality in several metropolises in Brazil. The city of Belo Horizonte, capital of the state of Minas Gerais, is the sixth most populous city in the country and has the third largest fleet of vehicles. Presidente Antônio Carlos Avenue connects the populous districts located in the north to the economic center of this capital. Often, this avenue presents a large flow of vehicles that travel through its twelve lanes, four of which are exclusively used for public transport. This paper presents a case study in which vehicular emissions were estimated along stretches of this avenue and the values used to evaluate the dispersion process of these emissions around the avenue. The results of concentration of Particulate Material obtained at the end of the study were compared with information of monitoring carried out in the area surrounding the avenue. For the estimation of vehicular emissions, the TREFIC model, from the ARIANET company, was applied, based on information obtained from the transit management body in the municipality. This model also includes spatial information (length, width and height of the track) and presents hourly emission estimates. These estimates were inserted into the AERMOD dispersion model (AMS / EPA Regulatory Model Terrain Pre-processor), recommended by SUDEMA and USEPA (U.S. Environmental Protection Agency) to assess the behavior of the distribution of concentrations around the avenue. The obtained concentrations were compared with monitoring data and used to present levels of air quality based on standards established by CONAMA March 1990.

Keywords: Pollution, Air Quality, TREFIC, AERMOD, Particulate Matter.

INTRODUCTION

The increase in the number of vehicles in cities has been considered an important complicating factor in the issue of air pollution in urban centers and the concentration of particulate matter is a major governmental concern. This is because this pollutant is a mixture of solid and liquid particles in suspension and of various forms, size and composition that cause environmental damages and human health (MOTA, 2014).

As the city of Belo Horizonte is the sixth most populous city in the country (IBGE, 2014) and has the third largest vehicle fleet in Brazil (DENATRAN, 2015), the city has become an important site for the study of the air quality. Therefore, this research estimated the vehicular emission of particulate matter 10 micrometers or less in diameter (PM₁₀) from one of the main access roads of the city and with a large flow of vehicles, Presidente Antônio Carlos Avenue (APAC).

This estimate was made using the TREFIC software developed by ARIANET. This model considers type of vehicle, fuel consumption, average distance traveled and type of road (ARIANET, 2012). Two

methodologies of particulate emission rates for road fleet were used for later insertion in the AERMOD model: the method developed by the Austrian Institute IIASA, in the framework of the "RAINS Europe" project and the method proposed by Lohmeyer and his co-workers. In this way, this work will seek which of these methodologies is the most appropriate for the case of Belo Horizonte avenue.

Subsequently, the AERMOD software produced by Lakes Environmental was used, a program that simulates the atmospheric dispersion of pollutants from the emission rate. In this model, the concentration distribution is assumed to be Gaussian in both the vertical and horizontal for steady-state plume and takes into account the topography of the area of influence, the characteristics of the emission sources and the local meteorological conditions.

The concentrations obtained by this computational model were compared with the results obtained by MOURA (2016) and compared to the standard of Inhalable Particles (PM₁₀) present in Brazilian legislation CONAMA March 1990.

METHODS

Due to the great extension of Presidente Antônio Carlos Avenue (approximately 8 km), it was decided to divide it into four parts based on slope. For each of these stretches, a flow of vehicles provided by Transport and Transit Company of Belo Horizonte city (BHtrans) was considered, with the final and beginning limits of each stretch as well as the dates of the flows provided are contained in table 1.

Table 1. Definitions of stretches

STRETCHES'S NAME	STRETCHES'S BEGINNING	STRETCHES'S END	FLOW DATE
FLUXOSR	Santa Rosa Avenue	Anel Rodoviário	31/08/2015
FLUXOAR	Anel Rodoviário	Américo Vespúcio Avenue	01/09/2015
FLUXOAV	Américo Vespúcio Avenue	Viaduct Senegal	13/06/2014
FLUXOVS	Viaduct Senegal	Downtown	18/09/2015

Reference: Own author

The BHtrans provided for each of these stretches eight flow-hour data for each direction of the avenue. These times refer to local peak times (6am-10am and 4pm-8pm).

In addition to these flow data, it was considered in the software TREFIC that the stretches have a good surface condition, that the average speed of the vehicles is the maximum allowed in the avenue (60 km/h) and average inclination of the avenue as the one obtained by the generated profile in Google Earth (FLUXOSR = 15°, FLUXOVS = 15°, FLUXOAV = -15° and FLUXOAR = 15°). The fleet data used (types of vehicles, model, fuel, etc) refer to the Brazilian characteristic fleet and were supplied by the company ARIA DO BRASIL.

The TREFIC model generated eight hourly emission rates for two MP10 methodologies: IIASA and the method proposed by Lohmeyer and his co-workers. The average rate of each of these methodologies was inserted in the model AERMOD, being considered each of the stretches as source line volume.

To simulate the meteorological data of the study region, the AERMOD preprocessor AERMET was used. Three years (2013, 2014 and 2015) of data from the Pampulha station (code 86800) obtained by INMET were considered. The values of albedo, bowen ratio and surface roughness were respectively 0.18, 1 and 1, values based on the characteristics of land use and occupation, according to EPA (2013).

For the simulation of the AERMOD topographic preprocessor, the AERMAP, the topographic sheet SF-23-X-A obtained by the EMBRAPA electronic address was considered.

A discrete source was considered for the AERMOD in the same position used by MOURA (2016) in the samplings at APAC, Federal University of Minas

Gerais (UFMG). In addition, we considered a mesh with 500 meters of side.

After, the concentration results obtained by the dispersion model were compared with the emission standard of the Brazilian legislation *CONAMA March 1990* for Inhalable Particles (PM10) and the results of sampling of particulate material made by MOURA (2016).

OFINDINGS AND ARGUMENT

The average daily emission rates for each stretch obtained by TREFIC model for the two MP10 methodologies, IIASA method (PM IIASA) and the method proposed by Lohmeyer and his co-workers (PM LOH) are shown in table 2.

Table 2. Taxas de emissão obtidas pelo Trefic

STRETCHES	PM IIASA (g/s)	PM LOH (g/s)
FLUXOSR	0,25	2,40
FLUXOVS	0,27	1,80
FLUXOAV	0,24	1,02
FLUXOAR	0,55	5,29

Reference: TREFIC model

It is observed that the emission values for the Lohmeyer methodology are higher than for the IIASA methodology. This is because, in addition to the emission considerations due to combustion, abrasion of mechanical parts and road pavement, the Lohmeyer methodology considers the re-suspension of dust deposited in the road surface (ARIANET, 2002; NANNI, RADICE, 2004). These values were used in the AERMOD dispersion model. After statistical analysis of the meteorological data used, it was observed that almost 90% of the winds have a velocity lower than 3.60 m.s^{-1} , being classified by the Beaufort Scale as calm to smooth (MARINHA DO BRASIL, 2016). The predominant direction of the winds, according to figure 1, is from east to west.

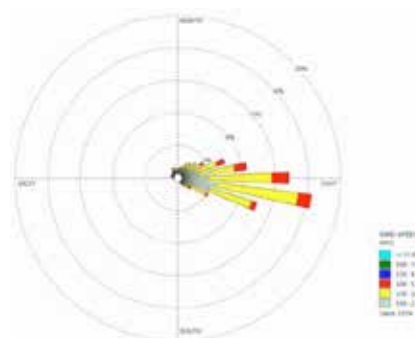


Figure 1. Wind Speed direction (blowing from)

After the simulation by the AERMOD software on the avenue, a maximum concentration of $572 \mu\text{g.m}^{-3}$ was obtained for the Lohmeyer methodology and $60.03 \mu\text{g.m}^{-3}$ for the IIASA methodology, both

for a 24-hour period. At the discrete point (UFMG ordinance), a value of $66.66 \mu\text{g.m}^{-3}$ was obtained for the Lohmeyer methodology and $6.82 \mu\text{g.m}^{-3}$ for the IASA methodology. In samples taken by MOURA (2016) at the same point, between June 2014 and March 2015, an average concentration of particulate matter equivalent to $48.09 \mu\text{g.m}^{-3}$ was obtained.

Figure 2 shows all the PM10 concentration results obtained by the sampling performed by MOURA (2016) and the results obtained by the AERMOD for the discrete point. It is observed that the concentration results for the IASA methodology are much lower than the sampling data.

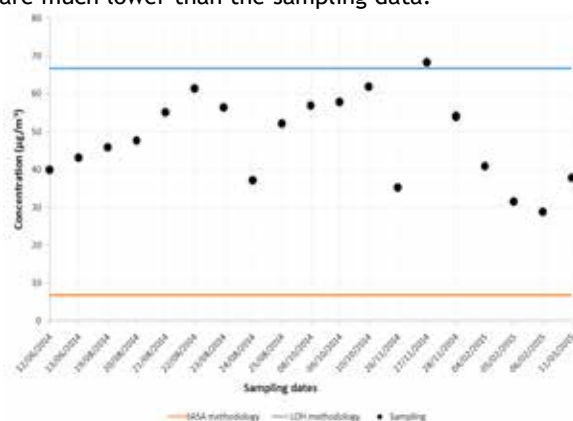


Figure 2. PM10 Concentrations

Although the main emitting source of MP in the APAC is of vehicular origin, other polluting sources such as civil construction, industries, anthropogenic emissions, among others, can not be disregarded. In this way, a concentration of particulate matter from the road fleet was expected to be lower than the total concentrations of particulate matter in the atmosphere. However, although the average concentration obtained by the Lohmeyer methodology is higher than the average obtained in the samplings, this would be the methodology that best represents the reality of vehicular particulate emission. This is because this methodology considers the re-suspension of surface dust and is more representative of the results of sampling.

The Brazilian legislation CONAMA March 1990 establishes that the maximum limit of inhalable particle concentration (PM10) is $150 \mu\text{g.m}^{-3}$ for a period of 24 hours. According to the concentration results for this same period for the Lohmeyer methodology, the maximum concentration was superior to the legislation. However, as already observed, the results for this methodology were overestimated. Already, the maximum result for the IASA methodology represent about 40% of the maximum allowed by the legislation.

CONCLUSIONS

The estimated emissions rates for the PM10 from the TREFIC software have proved to be very different from each other. The concentration obtained by the Lohmeyer methodology is almost ten times higher than the IASA methodology. The results for the Lohmeyer methodology although superior to the actual concentration results obtained by sampling, are more representative considering the re-suspension of dust deposited in the road surface.

This work, however, is an initial study of the evaluation of vehicle emission software as a way of assessing atmospheric pollution. This is because it was considered an average emission rate for the whole day, a fact that does not represent the reality of vehicular emission, since the flow varies constantly throughout the day. In addition, the characteristics of the fleet in APAC were considered in the software TREFIC as being the same Brazilian characteristic, not representing the reality of the avenue.

ACKNOWLEDGMENT

This research project is supported by the following Brazilian institutions: Nuclear Technology Development Center (CDTN/CNEN), Research Support Foundation of the State of Minas Gerais (FAPEMIG), GELAI/PBH and BHtrans.

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Multi-isotopic fingerprint (MIF) approach to improve tracing and discrimination of atmospheric pollutant sources in megacities

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Abstract: Urban atmospheric pollution is a global environmental problem with prominent effects on public health and climate. Considering the risks of high particulate matter (PM) concentration and the consequential metal species exposure to humans, the identification and discrimination of air pollutant sources is of great importance to monitoring programs and to policy decisions. Apart from traditional source apportionment tools, the combination of multiple isotope systems promises unparalleled insights into sources and pathways of metals in the atmosphere. Here, we perform a critical comparison of Pb, Zn and Cu MIF in PM and main pollutant sources from São Paulo, London and Barcelona in order to check if similar patterns of air pollution reflect common isotope signatures of urban anthropogenic sources and how can MIF improve source discrimination resolution. In São Paulo 450 samples of PM and urban sources (fuels, tires, cement, road dust, non-exhaust and road furniture) were analysed along 14 years (1999 to 2013), whereas in London, 86 samples, and in Barcelona 20 samples were analysed. All data and methodology details were published in previous work. We critically compared the isotope signatures of Pb, Cu and Zn in the main urban sources and PM from São Paulo, London and Barcelona using $^{206}\text{Pb}/^{207}\text{Pb}$ vs $\delta^{66}\text{Zn}_{\text{JMC}}$ and $\delta^{66}\text{Zn}_{\text{JMC}}$ vs $\delta^{65}\text{Cu}_{\text{NIST}}$ bivariate plots. In these diagrams, Zn isotopes discriminate between non-exhaust and exhaust traffic and industrial emissions with isotopically heavier, slightly light and lighter signatures, respectively. Industrial emissions from São Paulo and road dust from São Paulo and London were successfully separated using Pb isotopes. Additionally, vehicular traffic, road dust and cement sources were distinguished by Cu isotopes. These multi-isotopic diagrams demonstrated as a powerful tool to discriminate between many sources in complex systems as polluted atmospheres in urban areas. The Pb and Zn isotopic signatures of non-exhaust emissions from São Paulo and London have showed similar values, indicating that this isotopic fingerprint is reproducible in these different cities and has potential to be used as reference in future studies. Road dust from London differ from São Paulo city due to the less radiogenic isotopic signatures associated to re-mobilized Pb from leaded gasoline, which remains an important source to road dust from London. The heavier isotope compositions of Zn and Cu of aerosol from São Paulo and London had similar signatures to vehicular traffic (exhaust + non-exhaust), road dust, road furniture and cement, whereas isotopically lighter Zn found in aerosols from São Paulo was associated to industrial emissions. It is mandatory for future investigations to improve MIF characterization of the main air pollutant urban sources to obtain a global picture of air pollution in the bigger cities of the planet.

Keywords: Multi-isotopic fingerprint, Pb Cu Zn isotopes, aerosol, urban pollution, pollutant sources.

INTRODUCTION

Air pollution is the major environmental threat to the public health in the world. More than 80% of people who live in urban areas, with air quality monitoring, are exposed to pollution levels that exceed the World Health Organization (WHO) limits. Source apportionment of atmospheric pollutant sources of particulate matter (PM) is imperative to the air quality control and make-decision actions. Usually, elemental analysis in conjunction with multivariate statistics have been applied to this end. However, these traditional tools show some drawbacks for source identification and discrimination of trace metals in atmosphere.

In the last decade, investigations of emerging metal stable isotope systems (e.g, Cu and Zn) and radiogenic isotopes (e.g, Pb) have been tested as tracers of pollutant sources in the atmosphere. Of special interest are the elements Pb, Cu and Zn, since they are important constituents of several man-made materials technological devices whose cycles are drastically altered by anthropogenic activities.

In this study, we compare the results critically with previously determined the Pb, Cu and Zn isotopic compositions for Sao Paulo, London and Barcelona, in order to identify spatial and city specific differences and to test critically the wider potential for Cu, Zn and Pb isotopic signatures for pollutant tracing in urban atmospheres.

METHODS

The measurements of Pb, Zn and Cu isotopic compositions in PM and pollutant sources were obtained in previous studies carried out in São Paulo, London and Barcelona cities. In São Paulo, Pb isotopic ratios were measured in 450 PM and pollutant sources samples along 14 years (1999 to 2013), whereas Zn and Cu were measured in 101 and 32 samples during 2013, respectively (Aily, 2001; Gioia et al. 2005, 2010, 2017; Souto-Oliveira et al. 2018). In London, Pb isotopic ratios were determined in 74 samples approximately during two campaigns in 1994 and 2010, whereas Zn and Cu isotopic compositions were measured in 38 samples between 2010 and 2015 (Monna et al. 1997; Ochoa et al. 2016; Dong et al. 2017). In Barcelona, Zn and Cu isotopes were determined in 43 samples (Ochoa et al. 2016; Dong et al. 2017).

All sample digestion and purification steps were conducted in clean room conditions followed by measurements in high-resolution mass spectrometers (MS) equipped with magnetic sector and multiple collector (MC), containing two possible ionizations systems, thermal ionization (TIMS) or Inductivity coupled plasm (MC-ICP-MS). Those procedures are detailed in each work.

FINDINGS AND ARGUMENT

The PM from São Paulo and London showed distinct Pb isotopic signatures, as showed in $^{208}\text{Pb}/^{206}\text{Pb}$ vs $^{206}\text{Pb}/^{207}\text{Pb}$ plot (Fig. 1A). The $^{206}\text{Pb}/^{207}\text{Pb}$ ratios measured in PM from São Paulo (1.16 and 1.31) are more radiogenic and variable than in London (1.114 to 1.136).

Lead isotopic signatures of Non-exhaust and road furniture, such as road paint, manhole cover and surface tarnac, from London (red dashed circle) present slightly similar with those vehiular traffic from São Paulo (green dashed circle) (Fig. 1B). The lead found in road dust from São Paulo has the major contribution of vehicular traffic (fuel and tire), whereas road dust and PM from London (closed red circle) contains Pb provided of non-exhaust, re-mobilized Pb from leaded gasoline, used before phase out in 1996, and road furniture (Fig. 1B) (Dong et al., 2017; Souto-Oliveira et al., 2018). More radiogenic lead ($^{206}\text{Pb}/^{207}\text{Pb} > 1.20$) observed in PM from São Paulo are related to emissions from an industrial area (Cubatão), located 48 Km southeast from sampling point (Fig.1C) (Gioia et al., 2016; Souto-Oliveira et al., 2018).

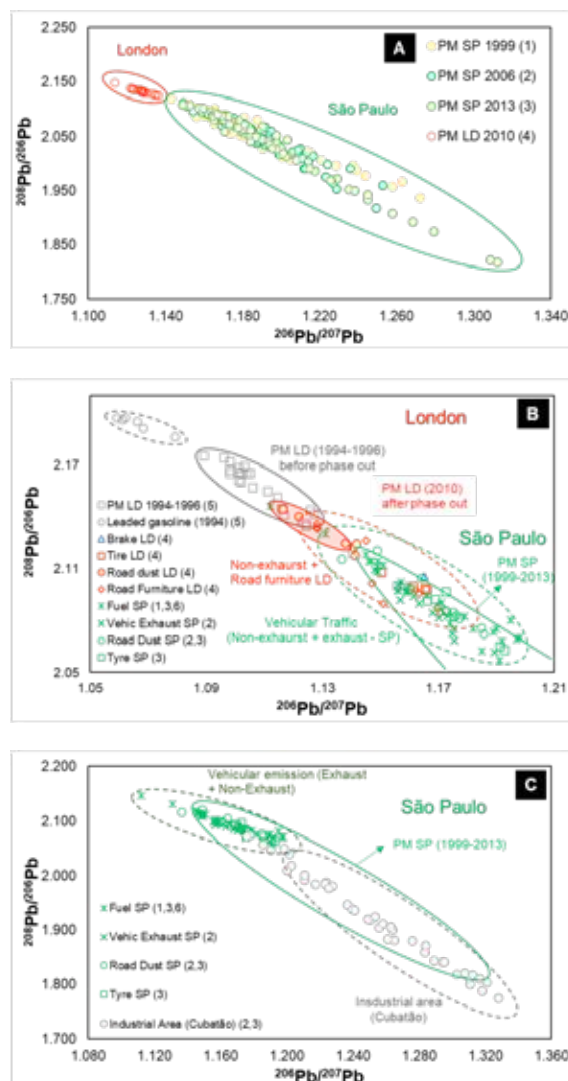


Figure 1. Three-isotope plot ($^{208}\text{Pb}/^{206}\text{Pb}$ vs $^{206}\text{Pb}/^{207}\text{Pb}$) of PM and pollutant sources from São Paulo (SP) and London (LD) megacities. A) Comparison of isotopic signatures of PM from two cities. B) Pb signatures of PM and vehicular sources of London and São Paulo. C) Vehicular and industrial sources from São Paulo (1-Aily,2001, 2-Gioia et al.,2017, 3-Souto-Oliveira et al.,2018, 4-Dong et al., 2017, 5-Monna et al., 1997, 6-Gioia et al.2005).

The Zn isotopic signature of PM from São Paulo ($\delta^{66}\text{Zn}_{\text{JMC}} = -1.36$ to $+0.18\%$) is more variable but similar with those found in PM from London ($\delta^{66}\text{Zn}_{\text{JMC}} = -0.29$ to $+0.79\%$), Fig. 2A, and Barcelona ($\delta^{66}\text{Zn}_{\text{JMC}} = -0.21$ to $+0.17\%$), Fig. 2B.

Zinc isotopes showed a good resolution to differentiate between non-exhaust and exhaust vehicular emissions in São Paulo (Fig 2A), which probably can be extrapolated to London (dashed red lines). While non-exhaust has shown heavier Zn

isotopic signature ($\delta^{66}\text{Zn}_{\text{JMC}} > +0.00\text{‰}$), observed in tires and brakes, exhaust emissions presented remarkably lighter ones ($\delta^{66}\text{Zn}_{\text{JMC}} = -0.18$ to -0.58‰ , Fig. 2A). In São Paulo, PM collected in road tunnel, representative of vehicular traffic budget, have $\delta^{66}\text{Zn}_{\text{JMC}}$ values between -0.06 and -0.23‰ , demonstrating a mixture of non-exhaust and exhaust contributions, (Fig. 2A) (Souto-Oliveira et al., 2018).

Road dust from São Paulo and London showed similar Zn signatures (Fig. 2A), characterized by isotopically heavy Zn ($\delta^{66}\text{Zn}_{\text{JMC}} = -0.03$ to $+0.34\text{‰}$), which contains dominant Zn of non-exhaust emission ($\delta^{66}\text{Zn}_{\text{JMC}} = 0.00$ to 0.22‰) (Souto-Oliveira et al., 2019).

Isotopically lighter Zn found in PM from São Paulo ($\delta^{66}\text{Zn}_{\text{JMC}} < -0.60\text{‰}$) was related to industrial emissions from metallurgical plants, assigned with characteristic lighter Zn signatures (Fig. 2B) (Mattielli et al., 2009; Yin et al., 2015; Souto-Oliveira et al., 2018).

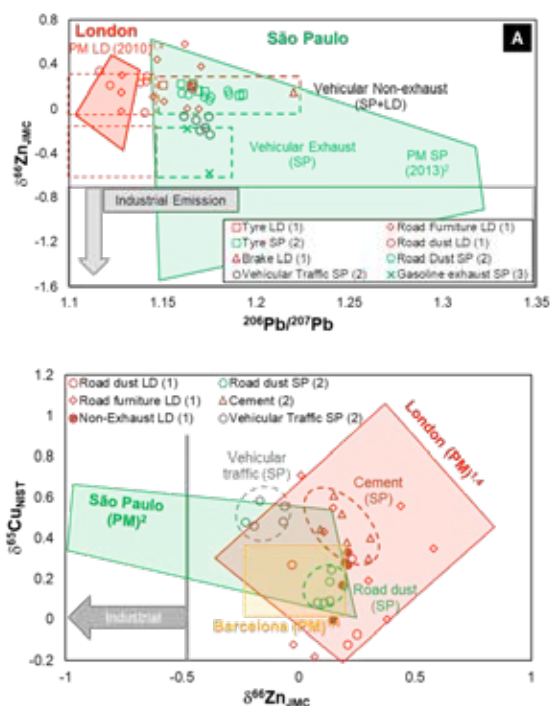


Figure 2. Comparison of Pb, Zn and Cu isotopic signatures of PM and pollutant sources from São Paulo (SP), London (LD) and Barcelona. A) $^{206}\text{Pb}/^{207}\text{Pb}$ vs $\delta^{66}\text{Zn}_{\text{JMC}}$ plot, B) $\delta^{66}\text{Zn}_{\text{JMC}}$ vs $\delta^{65}\text{Cu}_{\text{NIST}}$ (1- Dong et al., 2017, 2-Souto-Oliveira et al., 2018, 3-Gioia et al. 2008, 4- Ochoa et al., 2016).

PM samples from São Paulo, London and Barcelona have shown similar Cu isotopic signatures ($\delta^{65}\text{Cu}_{\text{NIST}} = -0.01$ to $+0.55\text{‰}$) (Fig. 2B). These signatures are associated to road dust ($\delta^{65}\text{Cu}_{\text{NIST}} = -0.28$ to

$+0.30\text{‰}$), road furniture ($\delta^{65}\text{Cu}_{\text{NIST}} = -0.12$ to $+0.55\text{‰}$), vehicular traffic ($\delta^{65}\text{Cu}_{\text{NIST}} = +0.46$ to $+0.59\text{‰}$), non-exhaust ($\delta^{65}\text{Cu}_{\text{NIST}} = +0.27$ to $+0.62\text{‰}$) and cement ($\delta^{65}\text{Cu}_{\text{NIST}} = +0.10$ to $+0.61\text{‰}$) contributions. In São Paulo an important improvement was related to differentiation of cement from vehicular traffic and road dust signatures using Cu isotopes (Souto-Oliveira et al., 2019).

CONCLUSIONS

The main pollutant sources of São Paulo, such as vehicular exhaust and non-exhaust, road dust, industrial emissions and construction (cement), were discriminated by combination of Pb, Zn and Cu isotopes. The Pb and Zn isotopic signatures of non-exhaust emissions from São Paulo and London have showed similar values, indicating that this isotopic fingerprint is reproducible in these different cities. São Paulo presented lighter Zn signatures associated with industrial emissions. Therefore, Pb, Zn and Cu isotopes demonstrated a great improve to discriminate and trace sources in those megacities. Although, enhancement of MIF characterization in PM from other megacities and pollutant sources, and combination with elemental data and other isotopic systems is mandatory to improve source discrimination and modelling using MIF approach.

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AIRBORNE PM_{2.5} POLLUTION IN THE GREATER BOGOTA AREA AND ITS SOURCES

(TREBUCHET MS, 14 FONT SIZE, BOLD, ALL CAPS, CENTERED)

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Abstract: Bogota is the 3rd most polluted capital in Latin America. Air quality has been monitored for 20 years, and the dynamics of pollution and its sources is reasonably well understood in the city. However, air pollution in the west part of the Greater Bogota area, with more than 1 million inhabitants, has not been studied with the same interest and, therefore, little is known about the factors that affect it. This work investigated the source contribution to the organic fraction of PM_{2.5} in two sites with a strong industrial activity, using the CMB receptor modeling and back-trajectory analysis. Sample collection was carried out for two-months at each site between September and November 2014. Chemical analysis included elemental and organic carbon, water-soluble organic carbon, inorganic ions and organic tracers. Average PM_{2.5} mass concentrations were 23 and 26 $\mu\text{g m}^{-3}$ at these sites. Organic matter was the major component of the PM_{2.5} mass (63%-68%), while secondary inorganic ions (ammonium, sulfate and nitrate) constitute about 10% of it. The CMB model results suggested the following 5 types sources of PM_{2.5} organic fraction: wood smoke, diesel vehicles, gasoline vehicles, natural gas combustion and industrial coal combustion. Differences between both sites are attributable to local sources, although transport of pollutants by easterly winds suggest that there is a regional effect on PM_{2.5} composition and source contribution.

Keywords: Source contribution, organic tracers, chemical mass balance, Greater Bogota.

INTRODUCTION

Bogotá is Colombia's capital and largest city, with ca. 8 million inhabitants. It is located on a plateau in the middle of the oriental branch of the Colombian Andes, at 2,600 m.a.s.l. Air pollution has been monitored for more than 15 years, showing that particulate matter is the most concerning air pollutant, frequently exceeding the Colombian ambient air quality standards, which is much higher than the WHO air quality guidelines. Several studies have determined PM₁₀ source contributions using receptor models and estimated emission inventories. The city government, through its environmental agency, Secretaría Distrital de Ambiente - SDA, is currently implementing a ten-year pollution abatement plan that started in 2010, based on some of these studies. However, the plan does not include other counties of the *Sabana de Bogotá*, but only its main urban center, the Distrito Capital. The rest of the region involves 3 counties (*Sabana Centro*, *Sabana Occidente* and *Soacha*) with 21 municipalities and a population of ca. 1,455,000 inhabitants, and is under the jurisdiction of a different environmental agency, *Corporación Autónoma Regional de Cundinamarca* - CAR. These counties have their industrial areas and are currently facing a challenging growth process of their economy and their population. Some of their towns have suffered serious air pollution impacts for

many years and others are recently starting to experience them. Particulate matter has been clearly identified as the most concerning pollutant of the area under the jurisdiction of CAR, frequently exceeding the Colombian ambient air quality standards. The contribution of different sources to particulate matter air pollution is rather well known in Bogotá, but it is uncertain in the rest of the *Sabana*. Therefore, in addition to improving emission inventories, the characterization of airborne particulate matter and the application of receptor models are necessary and valuable to determine the source contribution and, then, design an appropriate and prioritized air pollution abatement plan.

The first goal of this work is to determine the chemical composition of PM_{2.5} in two sites, one in Mosquera, in the *Sabana Occidente* county, and the other in the *Soacha* county. Both are influenced by industrial activities and the transit of a high volume of trucks, buses and vehicles, but only Soacha is influenced by mining of construction materials. We focus on PM_{2.5} because of its higher association with health effects than PM₁₀. The second goal is to determine the source contribution to the organic fraction of PM_{2.5}, based on organic tracers' concentrations and the application of the chemical mass balance (CMB) model.

METHODS

Sampling sites description

The Mosquera sampling site (4° 42'9.75" N, 74° 13'54.94" W) was located at a 7-m high monitoring platform regularly used for manual particulate matter monitoring, in the middle of the *Villa Olímpica* public sport fields. Mosquera has ca. 83,000 inhabitants and has an important industrial corridor where the food & beverage, metal work and plastics sectors are significant contributors.

The Soacha sampling site (4° 35'4.59" N, 74° 13'11.62" W) was located on the roof of the 5-story Mario Gaitán Yanguas Public Hospital building. The hospital is on a narrow but congested street, with a medium volume of vehicles and small buses, at 620 meters from Autopista Sur, the main corridor connecting Bogotá with southern and western Colombia and one of the most congested highways in the country, particularly because of a massive volume of heavy-duty trucks. Soacha has a large industrial corridor. Construction materials mining is also a significant activity in this city, which keeps growing at an alarming rate under insufficient planning provisions.

Sampling methods

Simultaneous sampling of 24-h integrated PM_{2.5} filters was performed between 9/12/2014 and 11/11/2014 using paired samplers at both sites. In Soacha, three 16.7 lpm speciation samplers (Rupprecht & Patashnick, USA), one loaded with a PTFE filter (Zefluor membrane, 2 µm, 47 mm, Pall Corporation, USA) and two loaded with quartz filters (QMA, 47 mm, Whatman, USA), were used. In Mosquera, one 16.7 lpm speciation sampler was loaded with a PTFE filter and one high volume sampler equipped with a brushless motor (TE-1000, 200 lpm, Tisch Environmental, USA) was loaded with a 100-mm quartz filter, cut from a larger sheet (QM-A, 203.2 x 254 mm, Whatman, USA). PTFE filters were used to determine PM_{2.5} mass, ions and trace metals, and quartz filters to determine ECOC and organic tracer speciation. Before and after sampling, filters were stored and transported in Petri dishes, with internal aluminum foil holders and an external Teflon tape seal, refrigerated at -20°C until chemical analyses.

In order to ensure an appropriate mass loading for chemical speciation, filters compositing was performed. Composites from stage 1 corresponded to 3 groups of consecutive days of the same week: Monday-Tuesday, Wednesday to Friday and Saturday-Sunday, which were analyzed for WSOC and ions. Any differences in these components between weekdays and weekends could be detected in this way. Composites from stage 2 corresponded

to weekly groups, which were analyzed for metals and organics. As a result, 25 composites from stage 1 and 9 weekly composites of each filter material at each site were formed.

Mass concentration and chemical analysis

Teflon filters used for gravimetric analysis were conditioned in a room with controlled temperature (20±2°C) and relative humidity (35±5%) for 24-48 h before being weighed with a microbalance (MX5, ±0.001 mg, Mettler Toledo, USA). Each filter was weighed three times and re-weighed if a difference higher than 15 µg in consecutive weights was found.

Chemical composition was achieved through the analysis of water-soluble organic carbon (WSOC), ions, elemental and organic carbon (EC/OC), metals and organic tracers. The analytical methods used in this work follow those described by Villalobos et al., 2015, Wang et al., 2005, Schauer et al., 2003, Nolte et al., 2002.

Source apportionment

The chemical mass balance model software developed by the US EPA (EPA CMB v8.2) was used to estimate primary source contributions to organic carbon (Watson et al., 1984). The model was run with eight weekly composite samples. Due to the resources and the particulate matter mass required for the organics analysis, it was not feasible to analyze individual daily samples for organic tracers. Organic compounds selected as tracers were stable during the transport from the source to the receptor, they did not react or volatilize, and all main sources were included in the model in order to obtain good results (Schauer et al., 1996). Source profiles were selected according to the organic tracer analysis results and the sources present in each site. We selected natural gas combustion (Rogge et al., 1993), diesel vehicles (Lough et al., 2007), gasoline vehicles (Lough et al., 2007), wood smoke and industrial coal burning, mixed quality. CMB results were considered acceptable if R² ≥ 0.9.

FINDINGS AND ARGUMENT

PM_{2.5} concentrations during the sampling period were 31 ± 15 µg/m³ in Soacha and 26 ± 12 µg/m³ in Mosquera. Chemical analyses achieved a PM_{2.5} mass reconstruction of 104% ± 25% and 103% ± 26% in Soacha and Mosquera, respectively, using an Organic Carbon (OC) to Organic Material (OM) factor of 1.6 for both sites. OM constituted a large fraction of PM_{2.5}, with 68% ± 19% and 63 ± 19% in Soacha and Mosquera, respectively. Organic tracers used in the CMB model made up a small fraction of OM, but they are useful to identify and quantify the OM and PM_{2.5} sources. CMB model results show that the main contributor to OC in Soacha was wood combustion (4.03 ± 1.43 µg/m³) followed by diesel vehicles (2.59

$\pm 1.05 \mu\text{g}/\text{m}^3$), gasoline vehicles ($2.06 \pm 0.47 \mu\text{g}/\text{m}^3$), coal combustion ($0.43 \pm 0.28 \mu\text{g}/\text{m}^3$) and natural gas combustion ($0.10 \pm 0.05 \mu\text{g}/\text{m}^3$). In Mosquera, the main contributors were diesel vehicles ($3.59 \pm 1.02 \mu\text{g}/\text{m}^3$), followed by gasoline vehicles ($3.32 \pm 0.93 \mu\text{g}/\text{m}^3$), wood combustion ($1.64 \pm 0.27 \mu\text{g}/\text{m}^3$) and natural gas combustion ($0.14 \pm 0.10 \mu\text{g}/\text{m}^3$). Secondary organic aerosol (SOA) and unidentified sources, calculated as the difference between the measured OC and the sum of the contributions of the identified primary sources, make up 33% and 22% of organic carbon in Soacha and Mosquera, respectively.

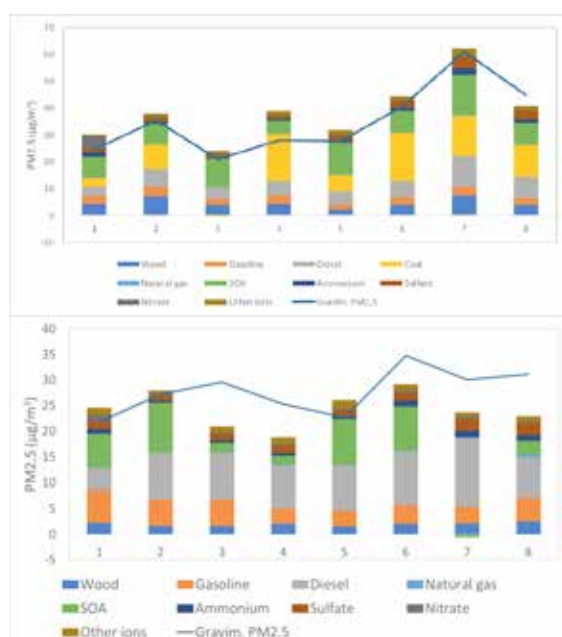


Figure 1. Source contribution to PM_{2.5} in Soacha (upper) and Mosquera (lower).

Source contributions to OC were converted into PM_{2.5} contributions using specific OC/PM_{2.5} factors for each source. The unidentified fraction was converted using an OC/PM_{2.5} factor of 0.5. The main contributor to PM_{2.5} in Soacha is coal combustion ($10.13 \pm 6.68 \mu\text{g}/\text{m}^3$), followed by SOA and unidentified sources ($9.16 \pm 3.10 \mu\text{g}/\text{m}^3$), diesel vehicles ($6.36 \pm 2.59 \mu\text{g}/\text{m}^3$), wood combustion ($4.72 \pm 1.73 \mu\text{g}/\text{m}^3$) and gasoline vehicles ($2.65 \pm 0.61 \mu\text{g}/\text{m}^3$). In Mosquera, the main contributor to PM_{2.5} is diesel vehicles ($8.81 \pm 2.50 \mu\text{g}/\text{m}^3$), followed by SOA and unidentified sources ($4.92 \pm 3.97 \mu\text{g}/\text{m}^3$), gasoline vehicles ($4.28 \pm 1.20 \mu\text{g}/\text{m}^3$) and wood combustion ($1.97 \pm 0.32 \mu\text{g}/\text{m}^3$). Reconstructed mass from this source apportionment was $38.84 \pm 11.51 \mu\text{g}/\text{m}^3$, 113% of measured PM_{2.5} mass, which means that the selected sources explain most of the observed mass. In Mosquera, there was an undetermined PM_{2.5} mass of $3.66 \pm 0.91 \mu\text{g}/\text{m}^3$ after reconstruction from CMB results.

CONCLUSIONS

This study apportioned OC and PM_{2.5} at two receptors of the Greater Bogota area, Soacha and Mosquera, using organic tracers and the CMB receptor model, during an 8-week period between September and November 2014. The model and the PM_{2.5} reconstruction derived from it were able to resolve the contributions of 6 main sources to OC and PM_{2.5}: diesel and gasoline vehicles; natural gas, wood and coal combustion; secondary organic aerosols. To the best of our knowledge, this kind of apportionment had not been previously achieved in Colombia. An important difference with previous studies in Bogota's Capital District is the high contribution of wood combustion in these receptors. This may be associated with the stronger use of wood for cooking and even for heating in both towns. More stringent controls are needed to reduce emissions from coal burning facilities in Soacha, and from diesel vehicles in both towns.

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Session 07
Remote Sensing
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AIR QUALITY MONITORING ON URBANS & INDUSTRIALS SITES USING COMBINATION OF INNOVATIVE LOW CONSUMPTION CERTIFIED ANALYZERS AND SMART MICROSENSORS

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Abstract: The integration of industrial sites in increasing urban environment and residential encroachment into previously non-resident areas represent a major challenge for municipalities. Combined with intolerance of nuisances (of any kind) by residents, it forces industrial and local environmental authorities' players to manage and control diffuse emissions of pollutants in a more stringent and efficient way.

Among these diffuse pollutions generated by urban activities or photochemical reactions (SO₂, NO₂, O₃, ...), hydrogen sulfide (H₂S) and ammonia (NH₃) have been identified as 2 important sources of nuisance as they are associated to odors. Beyond the olfactory discomfort, these gases have high adverse effects on health, the severity of which increases with the duration and level of exposure. They must be detected, monitored and controlled in advance.

This paper presents real-time and continuous monitoring and detection systems based on advanced state-of-the-art amperometric sensors of the industrial ambient and diffuse emissions. It consists of an autonomous network of Micro-Sensors associated with a software monitoring platform such as ClairCloud making the acquisition and data processing of each measurements point. This solution combined to the data provided by certified air quality monitoring stations available for the local authorities makes it possible to detect precisely a diffuse emission, thanks to the mesh of being able to go back to the source and to be able to control it by anticipation. The data may be also used to feed air quality modelling software for predictive and forecasting of air pollution.

An introduction and exclusive presentation of a highly sophisticated autonomous air quality stations with criteria pollutants certified and reference monitoring analyzers will be disclosed. This new concept of eco-conceived certified monitors with extremely low consumption of energy (making possible the solar panel powering) and, highly resistant to extreme conditions will be presented (making possible to operate with a surrounding ambient temperature up to 45°C) ...

The results will show the contribution of such a monitoring network based on high precision microsensors, combined to reference stations and hence building a so called "hybrid network" configuration to improve the mesh of the area of interest with an increase of accurate data and consequently, optimize the air pollution nuisance's management.

Keywords: micro sensors, reference analyzer, ambient air, autonomous station, Cairsens.

INTRODUCTION

Knowing that one of the main obstacles to measure the air quality in some merging or developing countries is the lack of availability of electricity grid, a major technological advance finally open the way to pollution monitoring in remote places where power supply is not available. According to the World Health Organization (WHO), more than 90% of air pollution-related deaths occur in low- and middle-income countries. Africa and some of the Western Pacific have a serious lack of air pollution data.

The reference (Type approved monitors: US EPA, EU QAL1 or others) station is essential for the reliability of all-weather measurements. The station powered by solar panels or batteries is an exclusive solution available from ENVEA for sites with little infrastructure without degrading the performance of measuring devices. Beside the fact that the monitors have been adapted to be powered by 24Vdc, those same reference analyzers can stand temperatures that can rise up to 50°C without need of air conditioning room.

The poor lack of data, as well as incomplete legislation in the countries concerned could finally

evolve, thanks to these highly innovative and autonomous air quality measurement stations.

Reference stations are essential for the reliability and precise measurements for ambient air and usually settled at a single location, some applications need to spread out sampling point at a very large scale (i.e. modeling or sources apportionment). This can be done by innovative and cost-effective micro-sensors Cairsens® (Cairpol products developed and manufactured by ENVEA) with high QA/QC standards.

The micro-sensors, while being not Type approved, in certain situations, can be a good alternative in order to have indications on ambient air pollution especially for industrial stations (H₂S, NH₃, TVOC, ...) but, in specific climatic situations the differences can be very large and therefore the measurement results must be subject to interpretations. These can be, now, corroborated using the autonomous reference stations.

METHODOLOGY

In the context of the rise of micro-sensors in Air and of their great variability of quality, plus the growing of projects based on it, the European Working Group

WG42 (of CEN TC264 - "Air Quality") work mainly on the validation of the Micro-Sensors. There will be 3 categories of sensors according to whether they respect: the indicative method, the objective estimation and the informative methods (table 1).

Table 1: Category of the micro-sensors according to them accuracy class (reference Air quality guidelines)

Pollutant	"Measurement" Method			
	Reference	Indicative	Modelization	Objective estimation
SO ₂ , NO ₂ /NO _x , CO	± 15%	± 25%	± 50%	± 75%
Benzene	± 25	± 30%	± 50%	± 100%
Pm ₁₀ /PM _{2.5}	± 25%	± 50%	± 50%	± 100%
O ₃	± 15%	± 30%	± 50%	± 100%

The Cairpol micro-sensors (Cairsens®) manufactured by ENVEA, are in the "indicative" class. These air quality monitoring devices are very sensitive and make reliable measurements (Berthelot^(a) et al. 2017) down to ppbv levels for several parameters and with a response time of 90 s. The Cairsens are embeddable on autonomous and real-time monitoring Cairnet® mini station for Ambient Air. To improve sensor performances, they are calibrated in ENVEA metrological laboratory using AQMS reference monitors. Figure 1 shows the good correlation between Cairsens® measurements and the reference AF22e UV Fluorescence TRS analyzer for H₂S monitoring on field for 5 days.

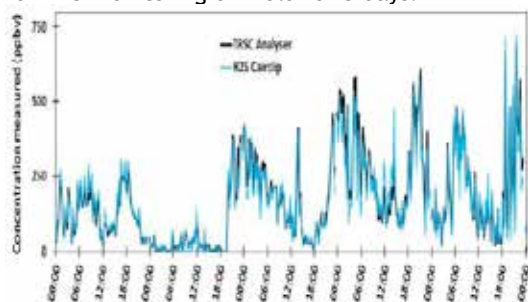


Figure 1: 5 days field monitoring of H₂S by Cairsens and validated by UV Fluorescence TRS analyzer

Unlike reference monitors, micro-sensors measurements are not standardized nor approved. Moreover, electrochemical sensor measurements may be influenced by different parameters, such as temperature, humidity and cross-sensitivity when they monitor ambient air on field (Spinelle^(b) et al., 2015). Despite their calibration in metrological laboratory, there is a need and a high valuable interest for the validation and periodic re-calibration of sensors measurements. Thus, ENVEA air quality stations including reference analyzers are unavoidable near industrial sites using several micro-sensors stations.

Envea fulfill a new and even more ambitious challenge to create a 100% autonomous AQMS reference station powered by solar panel and possibly wind turbine.

This station is equipped with specific US EPA approved analyzers such as the AF22e to monitor the SO₂, CO12e to monitor the CO, O342e to monitor the O₃, AS32M to monitor direct NO₂ and MP101M to monitor the PM₁₀ and/or PM_{2.5} particles and one weather multiparameter station is included to monitor the external temperature, pressure and humidity. The monitors have been especially eco-designed for low consumption operation and high temperature operation. Hence, the station is continuously powered by a set of photovoltaic panels (quantity according the energy needed) which feed four batteries during the night.

While maintaining outstanding metrological performance, the analyzers are now available with 24 V power supply. Their already very low energy consumption has been halved to reach a total of 300 W/h for the 5 gas and particulate analyzers, where other monitors on the market require over 1,300 W/h. Thanks to these unparalleled features, this unique 100% autonomous Reference AQMS station is able to withstand temperatures up to 50 °C without air conditioning and without connection to the power grid.

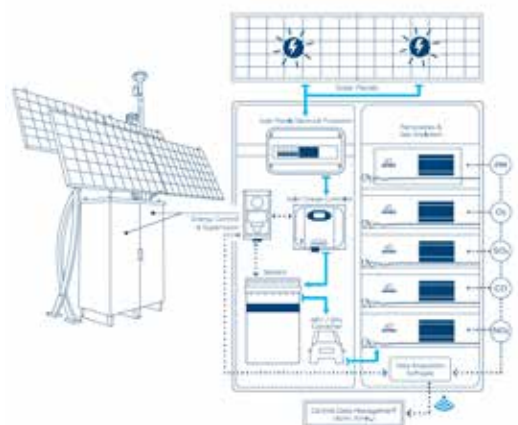


Figure 2: working principle scheme of the autonomous reference station (envea™ design)

Knowing that one of the main obstacles to measuring the air quality in some countries is the lack of the electricity grid, these major technological advances finally open the way to pollution monitoring in remote places as well as to developing countries. Also, this able the combination of mini-stations (based on micro-sensors) and of the 100% autonomous reference station to permit good and more local pollution measurement.

3. RESULTS AND DISCUSSION

The reference analyzers have been tested in a climatic chamber in order to measure the temperature influence on the measurement. An AC32e, which measure the NO, NO₂ and NO_x concentrations have been also tested. Inside the climatic chamber, the temperature can be controlled at $\pm 0.5^{\circ}\text{C}$. The tests were performed at 10, 20, 30 and 40°C . To generate two gas concentrations of NO₂, SO₂ and CO, gas cylinder and a gas dilutor MGC101 was used. To generate two gas concentrations of O₃, we used the internal O₃ generator of the gas dilutor MGC101. The concentrations of the different gases are presented in the table 2. Each analyzer have been tested with zero air to measure the temperature influence at zero point and with a span gas concentration which is roughly 80% of the full range.

Table2: Gas concentrations generated for the tests

analyser	Measure range	Gas measured	Gas concentration 1	Gas concentration 2
CO12e	50 ppm	CO	0 ppm	30 ppm
O342e	500 ppb	O ₃	0 ppb	400 ppb
AF22e	1 ppm	SO ₂	0 ppb	800 ppb
AS32M	1 ppm	NO ₂	0 ppb	800 ppb
AC32e	1 ppm	NO ₂	0 ppb	800 ppb

The test results are summarized in the table 3

Table 3: Influence of the temperature on the analyzers measurements

Analyser	Drift for 30°C		Drift for 1°C	
	At 0 ppb	At span point	At 0 ppb	At span point
CO12e	-180 ppb	700 ppb	-6 ppb	20 ppb
		2.33 % of the measured value		0.08 % of the measured value
O342e	0.44 ppb	-2.49	0.015 ppb	-0.083 ppb
		-0.62 % of the measured value		-0.02 % of the measured value
AF22e	-4.49 ppb	-29.85 ppb	0.15 ppb	-1 ppb
		-3.59 % of the measured value		-0.12 % of the measured value
AS32M	0.41 ppb	3.84 ppb	0.014 ppb	0.13 ppb
		0.48 % of the measured value		0.016 % of the measured value
AC32e	0.23 ppb	12.77 ppb	0.01 ppb	0.43 ppb
		1.55 % of the measured value		0.05 % of the measured value

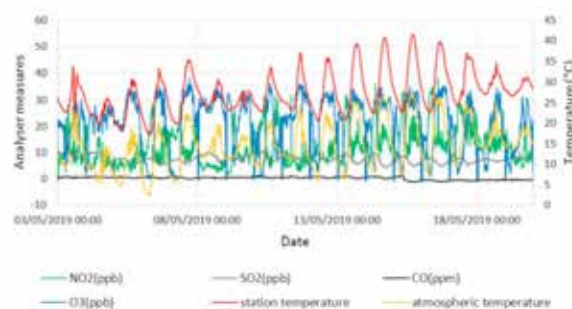


Figure 3: Measures of SO₂, CO, O₃ and NO₂ inside the station during the month of May 2019 in the suburb of Paris (France).

The temperature inside the station follow the atmospheric temperature with an offset of $+ 15^{\circ}\text{C}$. No dysfunction on the analyzers has been observed even when the temperature inside the station rises to 40°C .

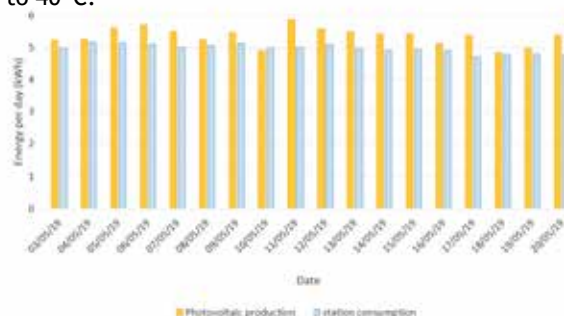


Figure 4: Station consumption and photovoltaic production during the month of May 2019 in the suburb of Paris (France).

The station consumption is less than 5000 Watt per day. The solar panels can supply this consumption during May 2019. The production may be higher but as the production is limited to the energy necessary, we cannot know the highest production.

CONCLUSIONS

Developing a combined solution of reference stations & sensors-based detectors stations for air quality mapping measurements with a scheduled correction to reduce sensor uncertainties will provide a strong cost effective monitoring network.

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Abstract: Atmospheric particulate matter (PM) is one of the main air pollutants, being characterized by the heterogeneity of its composition, which can include organic and inorganic components, originating from both natural and anthropogenic sources. The objective of this study was the assessment of the air quality in an urban environment, as well to carry out the source apportionment of the metallic elements Al, Ba, Cd, Pb, Cu, Cr, Fe, Mn, Hg, Ni and Zn in the PM_{2.5} and PM_{2.5-10}. The collection of PM_{2.5} and PM_{2.5-10} was performed monthly, from September 2015 to July 2017, using a dichotomous Stacked Filter Unit (SFU) sampler. The source apportionment of the metallic elements was carried out using the EPA PMF 5.0 receptor model. The Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model developed was used to obtain an overview of the air mass origins related to the episodes of higher concentrations of PM. The source apportionment made it possible to identify three Factors for PM_{2.5} and two Factors for PM_{2.5-10}. For PM_{2.5}, Factor 1 was highly loaded with Cu (81.0 %) and was characterized as Vehicular emissions; Factor 2 was highly loaded with Fe (97.6 %) and was characterized as Earth's crust and Factor 3 was highly loaded with Al (77.3 %), Mn (83.3 %) and Zn (91.4 %) and was characterized as Earth's crust/Industry. For PM_{2.5-10}, Factor 1 was highly loaded with Al (80.6 %), Fe (98.8 %), Mn (100.0 %) and Zn (89.4 %) and was characterized as Industry/Earth's crust emissions due to the mixture elements mostly originated from natural sources (Fe and Mn) and elements from anthropogenic sources (Zn and Al). Factor 2 was highly loaded with Cu (100.0 %) and was characterized as Vehicular emissions. The source apportionment demonstrated that vehicular and industrial emissions are the main anthropogenic sources contributing to the concentration of metallic elements in the PM. The integrated use of air mass trajectories with receptor models can provide useful information regarding the origin of atmospheric pollution.

Keywords: Air pollution, Particulate Matter (PM), Metallic elements, Source apportionment, HYSPLIT.

INTRODUCTION

The degradation of air quality in urban environments has become an issue of global concern, especially due to the problems related to human health and the environment. Atmospheric Particulate Matter (PM), which can be defined as comp

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The objective of this study was to evaluate the air quality of an urban area through the determination

of the concentrations of the metallic elements Al, Ba, Cd, Pb, Cu, Cr, Fe, Mn, Hg, Ni and Zn in the $PM_{2.5}$, $PM_{2.5-10}$ and the source apportionment of the metallic elements, which was carried out using the EPA PMF 5.0 receptor model.

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Samples were collected monthly from September 2015 to July 2017 using a low-volume dichotomous Stacked Filter Unit (SFU) sampler (Hopke et al., 1997). The collections were conducted for 24-hour periods, using 47 mm diameter polycarbonate membrane filters (Millipore®, Isopore Membrane Filter) with 2 μm and 10 μm pore size for $PM_{2.5}$ and $PM_{2.5-10}$, respectively. Before and after the sample collections, filters were conditioned in a desiccator for at least 72 hours (temperature of $25 \pm 5^\circ C$ and relative humidity of 30-40%) to achieve a constant weight for gravimetric analysis (Abiye et al., 2013). Ba and Zn were determined by flame atomic absorption spectrometry (SpectrAA 110, Varian), Al, Cd, Pb, Cu, Cr, Fe, Mn and Ni by graphite furnace atomic absorption spectrometry (ZEE nit 600, Analytik Jena AG) and Hg by fluorescence (Mercur, Analytik Jena AG).

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10 (µg m ⁻³) and metallic elements (ng m ⁻³)						
	Specie	N	Mean	Median	Min.	Max.
PM _{2.5}	PM	28	20.12	13.89	6.61	150.46
	Al	22	1477.18	250.06	8.39	21278.46
	Ba	22	273.54	21.41	0.31	5394.74
	Cd	22	5.09	0.04	0.03	81.31
	Pb	23	9.16	1.53	1.24	83.09
	Cu	22	48.81	11.63	0.17	375.05
	Cr	23	3.24	0.83	0.71	23.79
	Fe	22	139.54	52.07	1.18	1338.32
	Mn	22	9.07	3.92	0.23	40.20
	Hg	22	0.04	0.02	0.01	0.26
	Ni	21	6.78	1.91	0.78	81.02
	Zn	21	76.52	14.62	5.21	904.00
PM _{2.5-10}	PM	31	50.96	33.07	7.31	358.80
	Al	22	3589.26	401.94	42.60	30929.16
	Ba	21	30.26	21.41	9.87	107.43
	Cd	22	0.88	0.04	0.03	6.62
	Pb	23	7.71	1.86	0.73	34.70
	Cu	21	489.87	22.10	0.19	9322.30
	Cr	23	3.61	0.87	0.71	20.11
	Fe	21	419.62	46.85	1.12	2776.38
	Mn	22	24.99	12.41	0.06	150.51
	Hg	21	0.04	0.02	0.01	0.42
	Ni	22	19.44	2.08	1.01	171.01
	Zn	19	160.81	52.82	0.81	2059.76

The source contributions to $PM_{2.5}$ and $PM_{2.5-10}$ are shown in Figure 1.

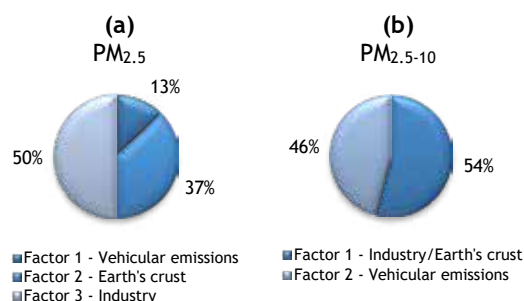


Figure 1. Source contributions to (a) $PM_{2.5}$ and (b) $PM_{2.5-10}$

With relation to $PM_{2.5}$, Factor 1 was highly loaded with Cu (81.0 %) and was characterized as Vehicular emissions. Factor 2 was highly loaded with Fe (97.6 %) and was characterized as Earth's crust. Factor 3

was highly loaded with Al (77.3 %), Mn (83.3 %) and Zn (91.4 %) and was characterized as Industry (Figure 1a). In $PM_{2.5-10}$, Factor 1 was highly loaded with Al (80.6 %), Fe (98.8 %), Mn (100.0 %) and Zn (89.4 %) and was characterized as Industry/Earth's crust emissions due to the mixture elements mostly originated from natural sources (Fe and Mn) and elements from anthropogenic sources (Zn and Al). Factor 2 was highly loaded with Cu (100.0 %) and was characterized as Vehicular emissions (Figure 1b).

The highest concentration of $PM_{2.5}$ and $PM_{2.5-10}$ in the atmosphere of the sampling site occurred in November 26, 2015, when the concentration of $PM_{2.5}$ was of $150.46 \mu g m^{-3}$ and the concentration of $PM_{2.5-10}$ was of $358.80 \mu g m^{-3}$. Figure 2 shows backward trajectory of the air masses related to this episode.

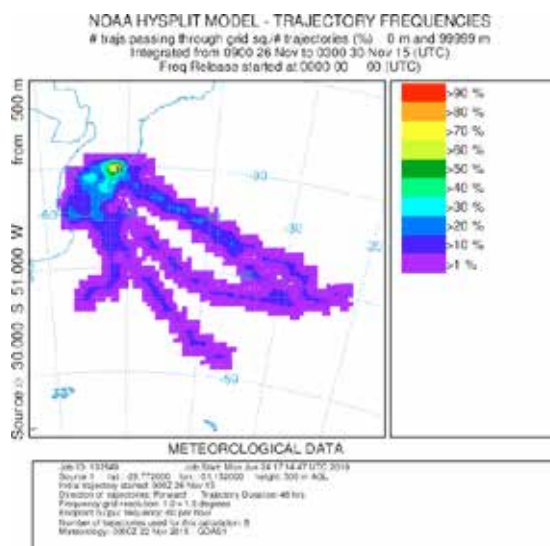


Figure 2. Trajectories of air masses related to the event of highest concentrations of $PM_{2.5}$
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Figure 2 illustrates an episode, where it is possible to verify that the origins of the air masses are not from earth, which would be suggestive of anthropogenic sources, but most of them come from the ocean and go to the sampling site, which suggests that most of the concentration of PM is from natural sources. In fact, even being from natural sources, the potential of causing problems to the human health and the environment can not be underestimated.

CONCLUSIONS

The source apportionment resulted in factors which represent the natural (Earth's crust) and anthropogenic (Vehicular emissions and Industry) contributions to the increase of the concentrations of metallic elements to the $PM_{2.5}$ and $PM_{2.5-10}$ in São Leopoldo, demonstrating that vehicular and

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The trajectories of the air masses calculated using the HYSPLIT model for the episodes of highest concentrations of $PM_{2.5}$ and $PM_{2.5-10}$ indicated the SE as the directions related with the origin of the PM, indicating that the emissions related to this event was not originated from anthropogenic sources, but from marine sources, which demonstrates the high influence of natural sources on the concentrations of PM.

The integrated use of different methodologies in environmental assessments allows a greater understanding of the behaviour of the main variables responsible for the degradation of the air quality.

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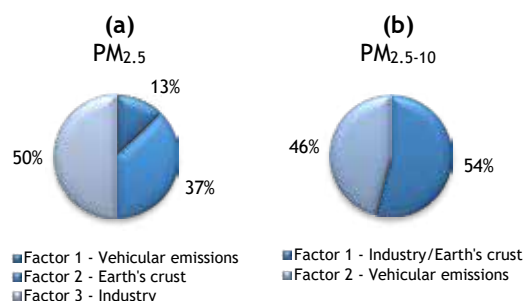


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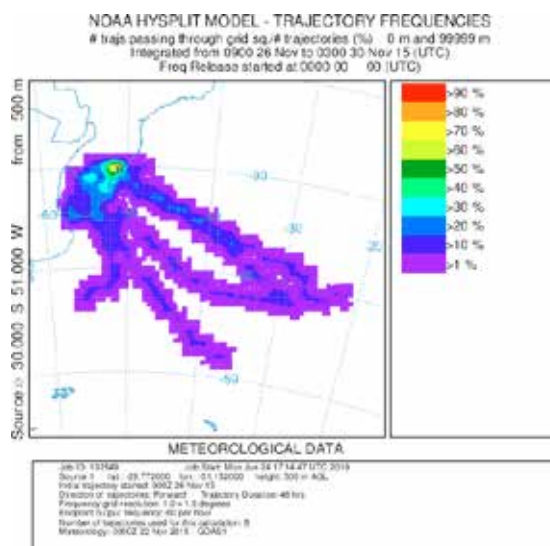


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MICROBIOLOGICAL ANALYSIS OF BULK AND WET DEPOSITION IN LAVRAS, MG

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Abstract: Bioaerosols, aerosols of organic nature, are transient particles in the terrestrial system, which can comprise up to 50% of atmospheric particles with a diameter greater than 0.2 μm . The main suspended bioaerosols are fungi, pollen, bacteria and viruses. These microorganisms present in the atmosphere can be transported, processed, and integrate physical, chemical and climatological processes. Understanding how these microorganisms act in the atmospheric processes is critical, since studies show that fungal spores, pollen and bacteria are suitable candidates for initiating ice nucleation, and bacteria can act as a cloud condensation nuclei (CCN) which may influence the hydrological cycle. Besides the relevance to the atmospheric sciences, the study of bioaerosols are pertinent to microbiology, since they can carry pathogenic microorganisms affecting agriculture, public health and microbial biogeography. Furthermore, they can indirectly affect human health through the deterioration of water quality. In Brazil, there are no established networks for routinely monitoring atmospheric deposition. Thus, there is a lack of studies on the processes and influence of bioaerosols in the atmosphere. The objective of this study was to verify and quantify colony forming units (CFUs) present in samples of bulk deposition (BD) and wet deposition by microbiological techniques and to adjust the methodology of sampling and cultivation of the microorganisms. After enumerated the colonies were classified from their colorations in C1, C2, C3, C4 and C5, with the following definitions: White, yellow, Orange, whitish and fungal. Given the importance of knowledge of the behavior and the factors that influence the permanence and interaction of bacteria in the atmosphere, the data presented infer the following conclusions: bacteria are influenced by seasonality, as seen in Figure 2, where C3 and C5 were prevailing in spring and knowing that C5 is fungus and observing the positive linear correlation of the same with the temperature of humid bulb, it is seen that this colony is present in moist environments. For colony C1 it can be inferred that its presence does not depend on specific environmental characteristics. The next step of this study is to identify the species of these colonies in order to ascertain in literature which participate in atmospheric processes.

Keywords: bioaerosols, bacteria, wet deposition, bioprecipitation, aeromicrobiology

INTRODUCTION

Atmospheric Deposition is a mechanism for removal of air pollutants and particulate matter. This process occurs mainly from the influence of gravity and phenomena such as precipitation, atmospheric turbulence, chemical properties and the surface's nature. Moreover, deposition is characterized by the several agents of influence [5]. Atmospheric removal could undergo by direct incorporation into the cloud droplets and rain droplets on their way to the Earth's surface, named wet deposition, in addition dry deposition refers to the sedimentation of the particles under gravitational action in the absence of precipitation, so the simultaneous contribution of these two processes results in total atmospheric deposition. Aerosols are solid or liquid particles suspended in the atmosphere [7]. Bioaerosols comprise aerosols derived from biological systems, which may correspond to bacteria, fungi, pollen, viruses, microalgae, etc. [2][6]. The main sources of bioaerosols are found in the biosphere mainly from the soil, leaf surfaces and water bodies, due to phenomena of particulate material ascent. Such aerosols sources are also

modified by seasonality, meteorological factors and altitude [2]. Recent studies have shown that airborne bacteria are likely to play an important role in cloud formation and precipitation. [3] *Pseudomonas* bacteria are excellent candidates for Ice Nucleotides showing more abundance during summer indicating a likely role in precipitation [4]. In addition, the discovery of metabolically active microorganisms in the clouds has raised questions about their possible influences on cloud chemistry [2]. In the literature there are several studies that seek to determine the true influence of microorganisms on the atmosphere, but there is a shortage of studies for Brazil.

In this sense, the detection, quantification and / or studies of bacterial diversity can help characterize environmental microbiological quality with other complementary variables. The present study evaluated the density of bacteria by means of quantification in the total and dry deposition in the municipality of Lavras-MG. This analysis will make it possible to know the microbiological characteristics of precipitation and to compare the density of bacteria with meteorological variables.

METHODS

Sampling Procedures and Site

The study was conducted in the southern region of Minas Gerais, specifically in the city of Lavras (21 ° 14' 42 "S 45 ° 00' 00" W). The sampling period ranged from September 2018 to March 2019.

Atmospheric Deposition Sampling

The total deposition samplings were made in 20L high density polyethylene containers previously conditioned with deionized water. The container, protected with nylon screen to prevent deposition of macroscopic material, is housed inside a PVC structure with anti-UV bath (Figure 1). This set is arranged on a wooden stand with a height of 1.50 m, which is installed in the vicinity of the Air Pollution Laboratory of the Department of Water Resources and Sanitation.

Figure 1 - Coletor bulk deposition



The samplings were carried out in the period of seven days, after which, each sample was transferred to the laboratory for analysis. In the absence of a precipitation event, a volume of 60 mL of deionized water was added with a pipette so as to "wash" the entire sampler area for the material analysis.

The wet deposition samples were collected during a rainfall event with the help of a previously autoclaved funnel and container following M. Akila et al (2018) sampling procedures.

Conditioning

When it was not possible to inoculate microbiological deposition after sampling, the contents were conditioned in polyethylene bottles, at 4°C until inoculation, not later than 24 hours.

Microbiological analysis

The culture medium preparation, and temperature, incubation period followed Standard Methods 9215 [1]. With the aid of a disposable sterile volumetric loop an aliquot of 0.001 ml of sample was inoculated into Petri dishes containing the solid R2A medium, the samples were performed in triplicates as well as control plates were made throughout the inoculation process of the samples. The inoculated plates were incubated for 7 days at 28 ° C. After incubation period, colonies were counted to determine Colony Forming Units (CFUs). After quantification of the colonies, the bacterial density was obtained from the following equation:

$$\text{CFU} = \frac{\text{colonies counted}}{\text{mL} \times \text{actual volume of sample in dish, mL}}$$

Meteorological Data

They were obtained from the virtual repository of the National Institute of Meteorology of Brazil (INMET). To study the following variables were used: Precipitation, Relative Humidity, Humid Bulb Temperature and Wind Speed.

Correlation and Cluster Analysis

For statistical analysis we applied Pearson correlation and a cluster analysis following Ward's hierarchy method with Euclidean distance as surrogate similarity variable.

FINDINGS AND ARGUMENT

The enumerated colonies were classified according to their coloration, observed in Table 1.

Table 1 - Classification of the colonies regarding coloration.

C1	C2	C3	C4	C5
White	Yellow	Orange	Milky	Fungal

Source: Of the authors, 2019.

The colonies showed variability throughout the sampling period, which can be observed in the following Image 2.

Image 2 - Seasonal variability of the colonies in atmospheric deposition

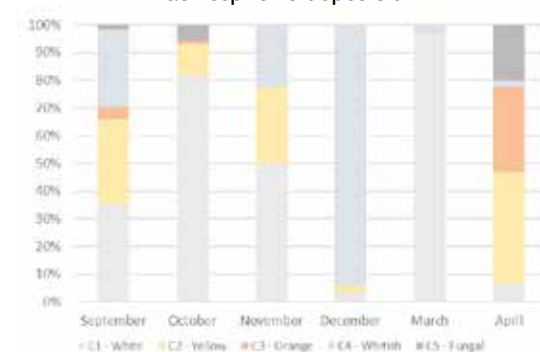
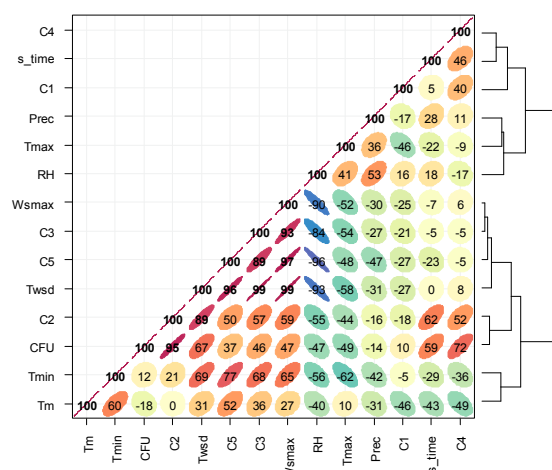


Figure 2 highlights the colonies seasonal variability of C2, C4 and C5. In the months of September, October and November corresponding to austral spring, temperatures are milder and pluviometric indexes increases, which contributed for such pattern. From December, early summer, where precipitation and temperature increase occur, we observe a lower frequency of C3. At the end of summer the colonies C2 and C3 reappeared in samples.

Seasonality is directly related to meteorological variables, this correlation can be observed in Figure 3.

Figure 3 - Cluster analysis and Pearson Correlation of meteorological variables and bioaerosols



* S_time: sampling period; Prec: Precipitation; Tmax Maximum Temperature; RH: Relative Humidity; Wsmax: Maximum wind speed; Twstd: standard deviation of Wet Bulb Temperature; Tm: average temperature; Tmin: Minimum temperature.

High similarities were observed between sampling time and CFU and C2, which were positively correlated to wet bulb temperature (67% and 89%) and inversely related to relative humidity (-47% and 55%). It was also observed that the C1 obtained only weak correlations with the analyzed meteorological variables. C4 presented negative linear correlation with average and minimum temperature (-49% and -36%). It is also important to note the positive correlation between sampling time and CFU and C2 colonies around 60%.

CONCLUSION

Given the importance of behavior knowledge and influence factors for the interaction of bacteria in the atmosphere, the data presented implies the following conclusions: bacteria are influenced by seasonality, where C3 and C5 were prevailing in Spring. Fungi colonies, as C5 were expected to show the positive linear correlation with wet temperature due to its presence in moist environments. For colony C1 one can imply that environmental variables did not show significant linear correlation with its colony density. The next step of this study is to identify the species of these colonies in order to find out in literature that they participate in atmospheric processes.

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INTERMEDIATE-SCALE HORIZONTAL ISOPRENE CONCENTRATIONS AND IMPLICATIONS FOR HETEROGENEITY OF EMISSIONS IN CENTRAL AMAZONIA

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Abstract: Intermediate-scale heterogeneity in VOC emissions over Amazonia has long been considered as a key possibility for closing the discrepancy observed at larger scales between measured and modeled VOC concentrations, but the possibility has been based on process modeling rather than in situ measurements. The measurements presented herein quantify horizontal VOC concentration gradients in the near-canopy atmosphere across different forest sub-types at the intermediate scale of several hundred meters. The implication is that previous top-down estimates, largely based on tower or aircraft measurements, may have bias when taken as representative of regional Amazonia. For comparison, bottom-up small-scale leaf-level approaches can be accurate locally but extrapolation to larger domains is challenging. The results herein demonstrate how complementary original data sets collected by UAV-enabled technologies provide a fifth platform that can fill a missing niche among leaf-level, tower, aircraft, and satellite scales. In that context, the results show that additional information at intermediate horizontal scales hitherto unavailable can be quantified, as needed for accurate understanding and predictions in evolving forests under climate stress. **Objective:** This study represents an advance in the quantitative and qualitative understanding of VOC under different forest subtypes in the Amazon. In the context of emission knowledge gaps and VOC processes on an intermediate scale. **Method:** simultaneous air samplings were performed in February and March 2017, with a flow of 200 sccm.min⁻¹ for 5 min, in cartridge tubes packed with Tenax TA and Carbograph 5TD (32 tubes were collected), with the help of a UAV equipped with the VOC sampler was launched and recovered from a platform (3.5 m × 3.5 m) atop the MUSA tower in the Ducke Reserve (Manaus-Brazil). The tower corresponded to location A of the study (3.0032° S, 59.9397° W). Ground level was 120 m asl at location A. Location B (2.997° S, 59.936° W) was 711 m distant from the tower. Ground level was 85 m asl or -35 m aghl at location B. Thermal desorption gas chromatography was used to analyze the samples. Detailed procedures can be found in Faiola et al. (2012). **Findings:** Heterogeneity in VOC emissions over Amazonia has long been considered as a key possibility for closing the discrepancy observed at larger scales between field-measured and modeled VOC concentrations, but the possibility has been based on process modeling rather than in situ measurements. The isoprene concentrations in the near-canopy atmosphere over the former were 80% greater than those over the latter. A gradient transport model informed by these data sets constrains emissions as 250% to 400% greater for the plateau forest as compared to the slope forest, which is significantly greater than available model simulations. The results presented herein highlight VOC concentration gradient in the near-canopy atmosphere across different forest sub-types at intermediate-scale of several hundred meters. The implication is that previous top-down tower- or aircraft-based emission estimates taken as representative of Amazonia may have biases at this scale. The measurements of this study tested the accuracy of leaf-level bottom-up approaches of VOC emissions and show that additional information at intermediate scale can be quantified, emissions, and other processes at the intermediate scale can improve predictions for present-day and possible future ecologies and other shifting Earth systems, as needed for accurate emission predictions.

Keywords: Amazon, isoprene emission, landscape heterogeneity, intermediate scales, Manaus.

INTRODUCTION

Volatile organic compounds (VOCs) emitted from forests have important roles in signaling among plants, animals, insects, and microbes, ecosystem functioning

and health, and atmospheric chemistry and climate (Laohawornkitkul, 2009). Tropical forests are the major global VOC source but are comparatively less studied and understood than their temperate and

boreal counterparts (Guenther, 2012). Tropical forest landscapes can have great heterogeneity and many forest sub-types at scales of 100's of meters (i.e., intermediate horizontal scales) (ter Steege, 2013). In central Amazonia, rolling hills underlying the tropical forest north of the Amazon River give rise to plateaus interspersed by water-logged valleys, all dissected by streams and rivers and joined by sloped regions, at scales of hundreds of meters. Myriad forest sub-types and biodiversity result across this intermediate scale for reasons of water, sunlight, and soil, among other factors and variations (Laurance, 2004; Myster, 2017). The landscape variability at intermediate scales is thought to be associated with variability in VOC emissions at the same scale (Kaser, 2015). For any VOC, some tropical forest sub-types can have high emissions of that VOC whereas other sub-types can exhibit low emissions or pockets of net deposition, even as the forest as a whole emits in net. Measurements of VOC variability over the forest sub-types are needed to investigate this possibility as well as to improve predictive capabilities for models of emissions and reactive chemistry over these landscapes. Herein, results are reported for investigating the heterogeneity of isoprene concentrations in the near-canopy atmosphere over contiguous plateau, slope, and valley forest sub-types in central Amazonia during the wet season of 2018. Isoprene is the non-methane VOC emitted in greatest quantities by land surfaces on Earth, as represented in the *Model of Emissions of Gases and Aerosols from Nature* (MEGAN) (Guenther, 2012). One estimate is that isoprene emissions alone represent 70% of total VOCs emitted by plants globally into the atmosphere (Sinderalova, 2014). Leading models such as MEGAN and others, however, are not presently able to predict emissions heterogeneity at the intermediate horizontal scales across forests, even as differences are thought to exist, in large part because of the absence of historical measurement platforms and data sets. For investigation of forest sub-types at intermediate scales without disturbance of the underlying landscape, chemical sampling and sensing by use of unmanned aerial vehicles (UAVs or “drones”) represents an emerging frontier in atmospheric chemistry (Villa, 2016). Data sets of isoprene concentration were collected at intermediate scales by use of the UAV.

METHODS

Tower. The UAV equipped with the VOC sampler was launched and recovered from a platform (3.5 m × 3.5 m) atop the MUSA tower in the Ducke Reserve. The tower corresponded to location A of the study (3.0032° S, 59.9397° W). Location B (2.997° S, 59.936° W) was 711 m distant from the tower (Figure 1).

Unmanned Aerial Vehicle. The UAV was a DJI Matrice 600 Professional Grade. It was a hexacopter design with onboard stabilization. The UAV had a nominal flight time of 30 min. The VOC sampler was mounted to the flight platform (McKinney, 2019).

Sampler. In brief, samples were collected by drawing air through cartridge tubes packed with Tenax TA and Carbograph 5TD (C2-AXXX-5149, Markes International) (Brown, 2014). A sample flow rate of 0.15 L min⁻¹ was used for collection. Additional samples were collected directly from the tower platform at location A using a handheld pump (GilAir PLUS, Gilian) to draw air through cartridge tubes, after the tubes were capped and stored in a refrigerator prior to chromatographic analysis.

Sampling Strategy. During a UAV flight, a sampling period for a single cartridge was 2.5 min. More specifically, as an example, two flights on one day between 09:00 and 10:00 corresponded to 5 min of sampling with one cartridge tube. In the same cartridge tube, samples were collected at the same period of the day (e.g., 09:00 to 10:00) for four days in a week to ensure sufficient material for chemical analysis, corresponding to 20 min or 3 L of sampling for this cartridge tube.

Analysis. Thermal desorption gas chromatography was used to analyze the samples (McKinney, 2019; Faiola, 2012).

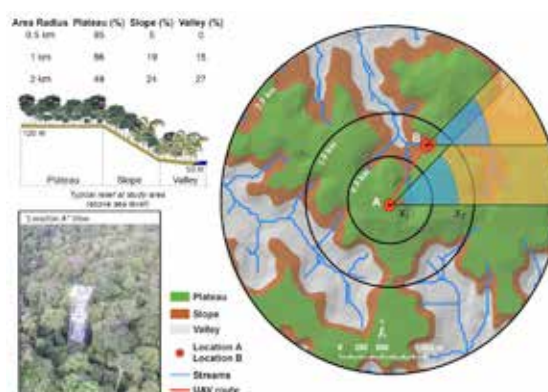


Figure 1. Local topography surrounding the tower (location A) at the Manaus Botanical Gardens (“MUSA”) of the Adolfo Ducke Forest Reserve in the central Amazon, Brazil. The UAV flight route from location A over the plateau forest to location B over the slope forest is shown by the red line.

FINDINGS AND ARGUMENT

Different forest sub-types. The Ducke Reserve (10 km × 10 km) is located on the northern outskirts of Manaus, Brazil, in central Amazonia. Valley and plateau regions in the tower vicinity are approximately 50 m and 120 m above sea level (asl), respectively, and they are joined by sloped regions. The UAV collected samples for two different locations above the Ducke Reserve across four weeks during the wet season from February 20 to March 15, 2018. Biodiversity in Ducke Reserve is well characterized by tree inventory surveys. The plant species and occurrence in the reserve has three major forest classifications, described as valley, slope, and plateau forest sub-types (Ribeiro, 1999; Schiatti, 2013; Ribeiro, 1994). Some important families include Arecaceae (commonly referred to as palm trees), Caryocaraceae, Clusiaceae,

Fabaceae (legumes), Lecythidaceae, Meliaceae, Mimosaceae (specialized legumes), Rapataceae, Solanaceae (nightshades), and Sapotaceae. The species that grow in abundance are distinct for each forest sub-type.

Concentrations in near-canopy atmosphere. Many compounds were identified in the collected samples, including isoprene, α -pinene, β -pinene, nine other monoterpenes, β -caryophyllene, and three other sesquiterpenes, together representing a progressive set of C_5 , C_{10} , and C_{15} compounds. The isoprene concentrations were consistently higher over the plateau forest compared to over the slope forest. The mean weekly differences for isoprene concentration over the slope compared to over the plateau forest ranged from 1.5 to 2.7 ppb. For the overall data set, the mean isoprene concentration was 2.4 ppb over the slope forest, which can be compared to 4.4 ppb over the plateau forest, representing an increase of +80% for the latter. The calculated probability (p value) for a two-way ANOVA analysis in location and time is < 0.001 for the null hypothesis that the two sets of isoprene concentrations were the same over locations A and B. An implication is that measurements from a single tower placed at either location A or location B would have significant bias if taken as representative of the regional area of Ducke Reserve. The ratio of the isoprene concentration to the α -pinene concentration is plotted in Figure 2.

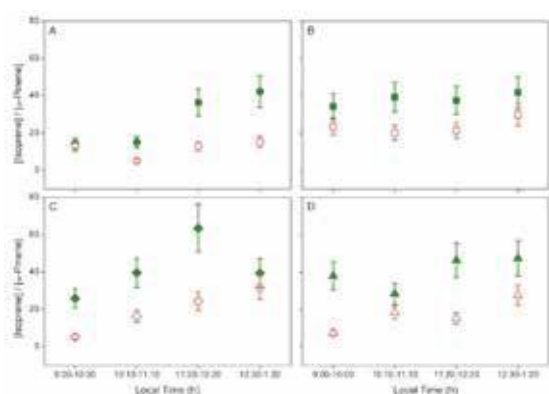


Figure 2. Isoprene-to- α -pinene concentration ratios measured during morning hours. (green) Over the plateau forest for 15 m above local canopy height at location A of Figure 1. (orange) Over the slope forest for 47 m above local canopy height at location B. Panels A, B, C, and D represent weeks 1, 2, 3, and 4, respectively.

α -Pinene is typically the monoterpene emitted in largest quantities by the forest. Unlike isoprene concentrations, the α -pinene concentrations and time variability were similar over the plateau and slope forests. The p value was 0.61 for the null hypothesis that the two sets of α -pinene concentrations were the same over location A and location B. An advantage of the concentration ratio, compared to the isoprene concentration alone, is mitigation of some possible confounding factors related to differences in transport and reactive loss to locations A and B compared to

differences in emissions from forest sub-types at locations A and B.

CONCLUSIONS

The measurements presented herein quantify horizontal VOC concentration gradients in the near-canopy atmosphere across different forest sub-types at the intermediate scale of several hundred meters. The results suggest that there are biases in both top-down estimates, based on satellite or aircraft measurements that are too coarse to compare with specific locations, and bottom-up approaches, based on leaf or tower measurements that are difficult to extrapolate to larger domains. The results demonstrate how observations collected by UAV-enabled technologies fill a missing niche among leaf-level, tower, aircraft, and satellite scales. Information at this previously unavailable scale is needed for accurate understanding and predictions in evolving forests under climate stress.

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boreal counterparts (Guenther, 2012). Tropical forest landscapes can have great heterogeneity and many forest sub-types at scales of 100's of meters (i.e., intermediate horizontal scales) (ter Steege, 2013). In central Amazonia, rolling hills underlying the tropical forest north of the Amazon River give rise to plateaus interspersed by water-logged valleys, all dissected by streams and rivers and joined by sloped regions, at scales of hundreds of meters. Myriad forest sub-types and biodiversity result across this intermediate scale for reasons of water, sunlight, and soil, among other factors and variations (Laurance, 2004; Myster, 2017). The landscape variability at intermediate scales is thought to be associated with variability in VOC emissions at the same scale (Kaser, 2015). For any VOC, some tropical forest sub-types can have high emissions of that VOC whereas other sub-types can exhibit low emissions or pockets of net deposition, even as the forest as a whole emits in net. Measurements of VOC variability over the forest sub-types are needed to investigate this possibility as well as to improve predictive capabilities for models of emissions and reactive chemistry over these landscapes. Herein, results are reported for investigating the heterogeneity of isoprene concentrations in the near-canopy atmosphere over contiguous plateau, slope, and valley forest sub-types in central Amazonia during the wet season of 2018. Isoprene is the non-methane VOC emitted in greatest quantities by land surfaces on Earth, as represented in the *Model of Emissions of Gases and Aerosols from Nature* (MEGAN) (Guenther, 2012). One estimate is that isoprene emissions alone represent 70% of total VOCs emitted by plants globally into the atmosphere (Sinderalova, 2014). Leading models such as MEGAN and others, however, are not presently able to predict emissions heterogeneity at the intermediate horizontal scales across forests, even as differences are thought to exist, in large part because of the absence of historical measurement platforms and data sets. For investigation of forest sub-types at intermediate scales without disturbance of the underlying landscape, chemical sampling and sensing by use of unmanned aerial vehicles (UAVs or “drones”) represents an emerging frontier in atmospheric chemistry (Villa, 2016). Data sets of isoprene concentration were collected at intermediate scales by use of the UAV.

METHODS

Tower. The UAV equipped with the VOC sampler was launched and recovered from a platform (3.5 m × 3.5 m) atop the MUSA tower in the Ducke Reserve. The tower corresponded to location A of the study (3.0032° S, 59.9397° W). Location B (2.997° S, 59.936° W) was 711 m distant from the tower (Figure 1).

Unmanned Aerial Vehicle. The UAV was a DJI Matrice 600 Professional Grade. It was a hexacopter design with onboard stabilization. The UAV had a nominal flight time of 30 min. The VOC sampler was mounted to the flight platform (McKinney, 2019).

Sampler. In brief, samples were collected by drawing air through cartridge tubes packed with Tenax TA and Carbograph 5TD (C2-AXXX-5149, Markes International) (Brown, 2014). A sample flow rate of 0.15 L min⁻¹ was used for collection. Additional samples were collected directly from the tower platform at location A using a handheld pump (GilAir PLUS, Gilian) to draw air through cartridge tubes, after the tubes were capped and stored in a refrigerator prior to chromatographic analysis.

Sampling Strategy. During a UAV flight, a sampling period for a single cartridge was 2.5 min. More specifically, as an example, two flights on one day between 09:00 and 10:00 corresponded to 5 min of sampling with one cartridge tube. In the same cartridge tube, samples were collected at the same period of the day (e.g., 09:00 to 10:00) for four days in a week to ensure sufficient material for chemical analysis, corresponding to 20 min or 3 L of sampling for this cartridge tube.

Analysis. Thermal desorption gas chromatography was used to analyze the samples (McKinney, 2019; Faiola, 2012).

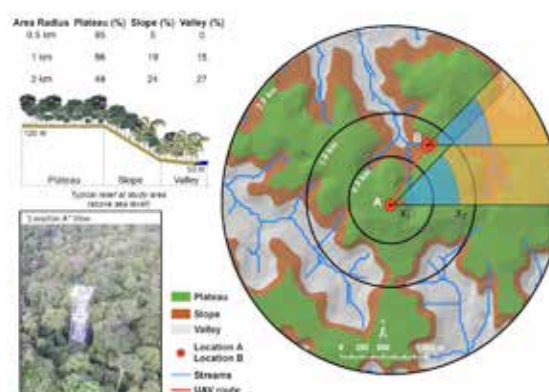


Figure 1. Local topography surrounding the tower (location A) at the Manaus Botanical Gardens (“MUSA”) of the Adolfo Ducke Forest Reserve in the central Amazon, Brazil. The UAV flight route from location A over the plateau forest to location B over the slope forest is shown by the red line.

FINDINGS AND ARGUMENT

Different forest sub-types. The Ducke Reserve (10 km × 10 km) is located on the northern outskirts of Manaus, Brazil, in central Amazonia. Valley and plateau regions in the tower vicinity are approximately 50 m and 120 m above sea level (asl), respectively, and they are joined by sloped regions. The UAV collected samples for two different locations above the Ducke Reserve across four weeks during the wet season from February 20 to March 15, 2018. Biodiversity in Ducke Reserve is well characterized by tree inventory surveys. The plant species and occurrence in the reserve has three major forest classifications, described as valley, slope, and plateau forest sub-types (Ribeiro, 1999; Schietti, 2013; Ribeiro, 1994). Some important families include Arecaceae (commonly referred to as palm trees), Caryocaraceae, Clusiaceae,

Fabaceae (legumes), Lecythidaceae, Meliaceae, Mimosaceae (specialized legumes), Rapataceae, Solanaceae (nightshades), and Sapotaceae. The species that grow in abundance are distinct for each forest sub-type.

Concentrations in near-canopy atmosphere. Many compounds were identified in the collected samples, including isoprene, α -pinene, β -pinene, nine other monoterpenes, β -caryophyllene, and three other sesquiterpenes, together representing a progressive set of C_5 , C_{10} , and C_{15} compounds. The isoprene concentrations were consistently higher over the plateau forest compared to over the slope forest. The mean weekly differences for isoprene concentration over the slope compared to over the plateau forest ranged from 1.5 to 2.7 ppb. For the overall data set, the mean isoprene concentration was 2.4 ppb over the slope forest, which can be compared to 4.4 ppb over the plateau forest, representing an increase of +80% for the latter. The calculated probability (p value) for a two-way ANOVA analysis in location and time is < 0.001 for the null hypothesis that the two sets of isoprene concentrations were the same over locations A and B. An implication is that measurements from a single tower placed at either location A or location B would have significant bias if taken as representative of the regional area of Ducke Reserve. The ratio of the isoprene concentration to the α -pinene concentration is plotted in Figure 2.

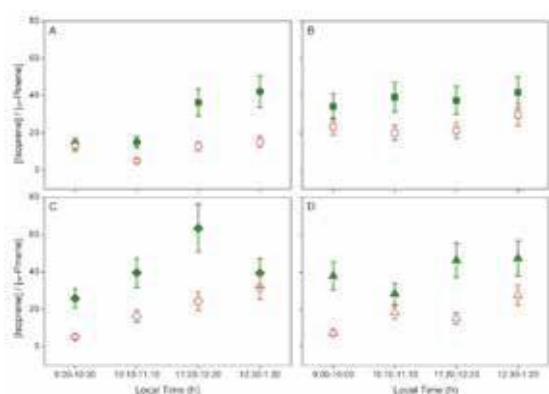


Figure 2. Isoprene-to- α -pinene concentration ratios measured during morning hours. (green) Over the plateau forest for 15 m above local canopy height at location A of Figure 1. (orange) Over the slope forest for 47 m above local canopy height at location B. Panels A, B, C, and D represent weeks 1, 2, 3, and 4, respectively.

α -Pinene is typically the monoterpene emitted in largest quantities by the forest. Unlike isoprene concentrations, the α -pinene concentrations and time variability were similar over the plateau and slope forests. The p value was 0.61 for the null hypothesis that the two sets of α -pinene concentrations were the same over location A and location B. An advantage of the concentration ratio, compared to the isoprene concentration alone, is mitigation of some possible confounding factors related to differences in transport and reactive loss to locations A and B compared to

differences in emissions from forest sub-types at locations A and B.

CONCLUSIONS

The measurements presented herein quantify horizontal VOC concentration gradients in the near-canopy atmosphere across different forest sub-types at the intermediate scale of several hundred meters. The results suggest that there are biases in both top-down estimates, based on satellite or aircraft measurements that are too coarse to compare with specific locations, and bottom-up approaches, based on leaf or tower measurements that are difficult to extrapolate to larger domains. The results demonstrate how observations collected by UAV-enabled technologies fill a missing niche among leaf-level, tower, aircraft, and satellite scales. Information at this previously unavailable scale is needed for accurate understanding and predictions in evolving forests under climate stress.

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MASS SIZE-SEGREGATED OF AMBIENT AEROSOL IN BOGOTA

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Abstract: Together with mass concentration and chemical composition, aerosol size distribution is key to determine its health effects and source contribution. This study presents the aerosol mass size distribution in Bogotá, Colombia. Particulate matter samples were collected using an eight-stage cascade impactor, which simulates the particulate deposition in different fractions along the human respiratory system. Average concentrations of PM_{10} and $PM_{2.5}$ and $PM_{1.1}$ were $61.13 (\pm 27.7)$ and $30.21 (\pm 15.02)$, respectively and the $PM_{2.5}/PM_{10}$ ratio was 0.5. The aerosol mass size distribution was bimodal, with the coarse mode at $4.4 - 5.4 \mu m$ and the accumulation mode at $0.8 - 1.1 \mu m$. Approximately 48% (± 5.1) of the PM mass could penetrate into the terminal bronchi and 27.2% (± 4.3) into the alveoli. Further work include characterizing the chemical composition of particles in several size fractions.

Keywords: Particulate matter, size distribution, mass concentration.

INTRODUCTION

The issue of urban air quality is receiving increasing attention as a growing share of the world's population is now living in urban centers and demanding a cleaner urban environment. The exposure to certain atmospheric compounds is responsible for potential harmful effects on human health and the environment. (Vasconcellos et al., 2011).

In urban areas the most common air pollutant is the particulate matter (PM). This pollutant is emitted by a wide range of sources including vehicular traffic, industry activities, biomass burning, volcano emissions, soil erosion, vegetation and sea, among others. According to aerodynamic diameter of PM can be classified by different categories of sizes, which describe penetrating ability to penetrate into the respiratory tract.

Environmental Authorities on the world had regulatory frameworks based on two size categories; PM_{10} : particles with diameters less than $10 \mu m$ (coarse mode) and $PM_{2.5}$, particles with diameters less than $2.5 \mu m$ (fine mode). However, these two sizes didn't describe the total effect of exposure to PM, because the effects depend on anatomy of respiratory tract, airflow patterns in the lungs and PM size. For instance, in nasal breathing, the cilia and the mucus act as a filter of particles exceed $10 \mu m$. Particles between 5 to $10 \mu m$ are most likely deposited in the tracheobronchial tree, while those between 5 to $2.1 \mu m$ are deposited in the bronchioles, the PM_{10} have behaviour like the gas molecules and will penetrate the alveoli, where gases exchange occurs. The ultrafine particles can have a larger potential for lung deposition and escape into the blood stream to translocate into the cell tissue, circulatory system and arrive at the brain, via olfactory nerve. (Kim, Kabir, & Kabir, 2015).

Overall, studying the sized distribution and size resolved chemical composition of ambient is useful to understand its sources, formation mechanisms, toxicity and complements well the information obtained from the bulk aerosol composition. In South America, there are few studies including mass size distribution and their chemical, especially in densely populated cities.

This study presents the mass size distribution of PM collected in a site of Bogotá, the capital of Colombia, with ca. 8 million inhabitants where small and medium industry, vehicle traffic and residential areas. Air pollution in the city is moderate (Ramirez, Sánchez de la Campa & de la Rosa, 2018), mostly emitted by local sources. (Vasconcellos et al., 2011). The results of this work will help to strengthen definite conclusions about the specific consequences of exposure to ultrafine particle (HEI, 2013) and is expected to support the definition of appropriate strategies to reduce PM emissions and their impacts.

METHODS

The sampling site was located in the West of Bogotá, at the Fire Station of the Fontibon District, ($4^{\circ}40'12.36''$ N, $74^{\circ}8'29.58''$ W, 2591 m.a.s.l.). Samplers were installed over the roof of the main building, approximately 9 m above the ground. This site is about 40 meters from an arterial road and 2.2 km from El Dorado international airport. The main industrial areas of the city are located within 4 km. The site was selected to represent the levels of air pollution in the urban area of Bogotá, a large residential area, affected by industrial and vehicular emissions.

Meteorological parameters were taken from El Dorado airport station, which is the nearest to sampling site. In general, the average annual temperature and precipitation in Bogotá are $14^{\circ}C$ and 840 mm/year, respectively. The months with the highest rainfall levels are April-May and

October-November. Winds from NE-E and SE-E prevail with average speeds of 1.5-3.5 m/s and average maximum values of 10 m/s (IDEAM, 2015).

Nineteen sets of size-segregated ambient aerosol samples were collected over two periods: March-June 2018 and October-November 2018, using a Tisch® ambient eight-stage cascade impactor (Serial 436, Model 20-800, TISCH Environmental, USA) at a flow rate of 28.3 L/min, during for 3 days.(72hr)The impactor separates particles into the following 9 inhalable fractions: <0.43, 0.43-0.65, 0.65-1.1, 1.1-2.1, 2.1-3.3, 3.3-4.7, 4.7-5.8, 5.8-9 and >9 μm .

Quartz filters of 81 mm- diameter (Whatman®, TE-20-QZ) were used as impaction substrates in the impactor. Filters were baked at 600°C for 8 h to remove carbonaceous impurities. Before and after field sampling, filters were weighed on a microbalance analytical (Sartorius Research, R200D) to determine the mass concentration after the filter had been conditioned at 22.8 ± 1.4°C and 40.6 ± 5.8% relative humidity for 24 hr. The exposed filters were stored individually in sealed containers wrapped with aluminum foil and kept in plastic bags, then immediately transported to the laboratory by keeping in an ice box.

For the chemical composition, elemental and organic carbon content was determined by thermal decomposition using charring correction (Sunset Labs®, USA). A fraction of quartz filter was extracted in 1,5 mL deionized water and analyzed by ion chromatography for ions (ammonium, sodium, potassium, magnesium, calcium, chloride, nitrate, sulfate and oxalate). (Van Pinxteren et al. 2009).

Particle concentrations were calculated by dividing the weight of the collected particulate matter by the volume of air sample adjusted to standard ambient temperature and pressure (25 °C, 1 atm). The concentration of $\text{PM}_{2.1}$ and PM_9 was obtained by adding the concentrations of stages with a cutoff diameter smaller than 1.1 μm and 5.8 μm , respectively.

FINDINGS AND ARGUMENT

The average concentration of PM_9 was $61.13 \pm 27.7 \mu\text{g}/\text{m}^3$ and $\text{PM}_{2.1}$ was $30.21 \pm 15.02 \mu\text{g}/\text{m}^3$, which are close to the Colombia's National Air Quality Regulations for 2017 (100 and $50 \mu\text{g}/\text{m}^3$ for 24 hours, respectively). However, the y are well above the WHO guidelines.

The Puente Aranda air quality station, located in the same study area, reported that $\text{PM}_{2.5}$ constituted 40% of the PM_{10} mass. In our study, the ratio between $\text{PM}_{2.1}/\text{PM}_9$ was consistent at 49.63%, for most of the sets. This ratio indicated that there is a high

contribution of combustion sources (industrial and traffic) around point of measurement. Besides, this relation means that the population is exposed to a high concentration of matter particulate and almost the half of these particles could penetrate the trachea, secondary bronchi or alveoli.

Particle size fractions were classified into three different size ranges according to their mechanism of formation: ultrafine particles (nuclei mode, $d_{ae} < 0.4 \mu\text{m}$), fine particles (accumulation mode, $0.4 \mu\text{m} < d_{ae} < 2.1 \mu\text{m}$) and coarse particles ($d_{ae} > 2.1 \mu\text{m}$). The average concentrations of ultrafine, fine, and coarse particles in the sample during were 31.6, 22.8, and $6.8 \mu\text{g m}^{-3}$, respectively.

The average distribution (see Figure 1) is bimodal and indicates that particle mass is fairly evenly divided between accumulation and coarse particle modes. The coarse mode has a mass median diameter (MMD) between diameters 4.4 and 5.4 μm and an accumulation mode are between diameters 0.8 and 1.1 μm . In all sets, the value of MMD does not coincide exactly with the peak of the distribution.

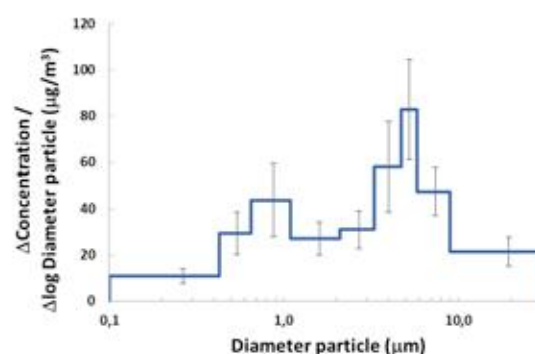


Figure 1. Average mass size distribution in Fontibon, Bogotá.

According to Figure 1, the largest fraction of particles in the coarse mode >2.1 μm (52% of total particle mass), 48% (± 5.1) of particles were smaller than 2.1 μm . These particles could penetrate into terminal bronchi and the 27.2% particle matter smaller than 1.1 μm and could deposited into the alveoli.

Preliminary results from chemical compounds in some sets of the collected sets show that organic carbon is one of the main constituents of PM in all sizes. Elemental carbon is more concentrated in fine particles. Sulfate ions and organic carbon are abundant in coarse mode.

CONCLUSIONS

This study measured the aerosol mass size distribution in Bogotá D.C. The distribution was

bimodal, with the coarse mode at 4.4 - 5.4 μm and the accumulation mode at 0.8 - 1.1 μm and its largest fraction of particles was in the coarse mode >2.1 μm (52% of total particle mass). The $\text{PM}_{2.5}/\text{PM}_{10}$ ratio were 49.63%, indicating a high contribution of combustion sources (industrial and traffic) around point of measurement.

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DETERMINATION OF POLYCYCLIC AROMATIC HYDROCARBONS (PAHs) IN ATMOSPHERIC PARTICLES IN THE METROPOLITAN REGION OF PORTO ALEGRE, RS

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Abstract: The emission of Polycyclic Aromatic Hydrocarbons (PAHs) associated with particulate matter (PM) to the atmosphere in metropolitan areas is emitted mostly by anthropogenic sources. Therefore, this work had as objective to evaluate the concentration of 16 PAHs in samples of atmospheric particles in the metropolitan region of Porto Alegre-RS. Samples of PM_{2.5} and PM₁₀ were collected by the dichotomous sampler with PTFE filters in the cities of Novo Hamburgo and Canoas and their concentrations determined by gas chromatography coupled to mass spectrometry, which aimed to identify the 16 PAHs classified as priority by the United States Environmental Protection Agency (US EPA). As results greater concentration of PM₁₀ and PM_{2.5} in Canoas in relation to Novo Hamburgo. It was identified 10 PAHs from the 16 PAHs classified as priorities by the US EPA, in which the majority are associated with PM_{2.5}. The presence of benzo(a)pyrene in PM₁₀ was not detected. However, it was detected in PM_{2.5} along with benzo(b)fluoranthene, benzo(k)fluoranthene and naphthalene in Novo Hamburgo. The highest concentrations of PAHs were of fluorene and phenanthrene in PM₁₀. In Canoas the predominant wind direction comes from the east and southeast direction where the BR116 and Canoas Air Base are located. In Novo Hamburgo the predominant wind direction is the east direction where the residential area is located with small industries.

Keywords: Atmospheric monitoring, polycyclic aromatic hydrocarbons, atmospheric pollution, particulate matter.

INTRODUCTION

The urbanization, the industrialization and the extraction of natural resources around the world have been responsible for the high content of atmospheric pollutants (MARTINS, et al., 2017). The accumulation of pollutants into the atmosphere causes climatic changes and damages the health of humans, bringing short, medium and long term consequences mainly to children and the elderly (ILLI, et al., 2016).

Among these pollutants, the particulate matter (PM_{2.5} and PM₁₀) can be defined as a mixture of heterogeneous particles composed of dust, solid particles, liquid particles, smoke and soot that change in space and time according to the source emitted (GALVÃO, et al., 2017). In the PM are numerous pollutants associated with it, among them the PAH, composed only of carbon and hydrogen with two or more aromatic rings condensed in its structure (BAIRD, CANN, 2011).

According to its source, PAHs can be emitted into the atmosphere by the process of resuspension, volatilization and incomplete combustion (DIAS, et al. 2016). PAHs of lower molecular mass, formed by four or fewer benzene rings oxidize in the atmosphere, forming even more toxic compounds, such as oxy-PAHs and nitro-PAHs. Over four benzene rings, PAHs are found adsorbed to PM (GALVÃO, et al., 2017).

The main sources of these pollutants (PAHs) into the atmosphere in metropolitan areas are caused by

the burning of fossil fuels through the incomplete combustion of motor vehicles in major roadways and by the processing industries (PHILIPPI JR, et al., 2004).

The objective of this work was to identify and evaluate the concentration of 16 PAHs classified as priority by the US Environmental Protection Agency (EPA) in samples of atmospheric particles in the metropolitan region of Porto Alegre, RS.

METHODS

PM collection was performed in the city of Canoas (29°55'19.79"S and 51°10'43.05"W) and Novo Hamburgo (29°40'12.40"S and 51°7'15.73"W), both characterized by the proximity to the routes of intense traffic of vehicles. The collection of PM_{2.5} and PM₁₀ was done by the dichotomous sampler that fractionates the sampling flow in 900 m³ min⁻¹ for PM_{2.5} and in 100 m³ min⁻¹ for PM₁₀. The filter used was Millipore PTFE 47 mm diameter and 0.5 µm porosity previously weighed. The sampling period was from January 2018 to September 2018 every 15 days for 48 hours.

The procedure for extracting the PAHs retained in the PM filters was carried out in a soxhlett apparatus where the samples were extracted in laboratory with approximately 250 mL of dichloromethane (CH₂Cl₂), for 24 hours at 45°C.

After extraction, the samples underwent the Clean Up process to remove already in the first fraction with 20 mL of hexane the aliphatic

hydrocarbons that interfere in the sensitivity of the gas chromatograph detector. The second and third fraction of 20 mL of hexane and dichloromethane (1:1) and (3:1) were collected and concentrated with nitrogen gas (N₂) and injected into GC/MS mass spectrometry gas chromatograph. The mode of detection of PAHs used was Electron Ionization (IE) through Selective Ion Monitoring (SIM) scanning (SCAN). Samples were quantified in duplicates.

FINDINGS AND ARGUMENT

The PM₁₀ and PM_{2.5} samples were collected from January 9 to September 13, 2018. Their concentrations were determined and compared to the CONAMA Resolution 491/2018 that defines the emission standards of atmospheric pollutants in Brazil, and also with the quality standard recommended by the World Health Organization (WHO). The figure 1 shows the concentrations of PM₁₀ obtained in the city of Canoas and Novo Hamburgo and compares them with the emission standards of CONAMA Resolution 491/2018 (120 µg m⁻³) and also with the WHO standard (50 µg m⁻³).

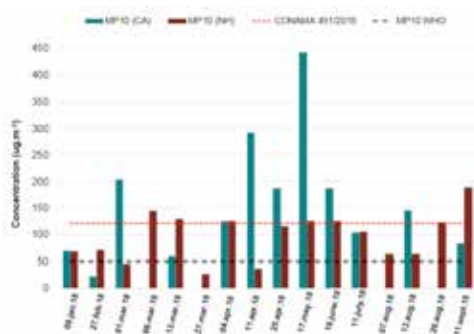


Figure 1. Concentrations of PM₁₀ obtained in the cities of Canoas and Novo Hamburgo

A total of 12 PM₁₀ samples were collected in Canoas and 16 samples in Novo Hamburgo.

As can be observed in Figure 1, the highest concentrations of PM₁₀ were obtained in the city of Canoas (CA), 441.53 µg m⁻³ concentration, where the sampling point is located a few meters from BR 116, about 50 m. Comparing the results obtained with the CONAMA Resolution 491/2018 and the quality standard recommended by the WHO, it is verified that seven samples of PM₁₀ in Canoas as well as in Novo Hamburgo obtained concentrations above the limit imposed by Resolution CONAMA 491/2018.

Regarding the WHO quality standard, 11 PM₁₀ samples had above-standard concentrations in Canoas and 13 samples in Novo Hamburgo also had concentrations above the recommended level.

The figure 2 shows the concentration results of PM_{2.5}.

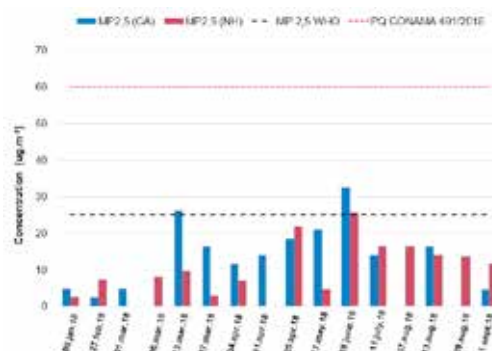


Figure 2. Concentrations of PM_{2.5} obtained in the cities of Canoas and Novo Hamburgo

Figure 2 shows the concentrations of PM_{2.5} obtained in the city of Canoas and Novo Hamburgo. In total, 13 samples of PM_{2.5} were collected in Canoas and 14 samples in Novo Hamburgo.

Analyzing the results of the PM_{2.5} concentrations expressed in figure 2, it is possible to observe that in relation to CONAMA Resolution 491/2018 in any sample there was a concentration above the quality standard (60 µg m⁻³), both at the sampling point in Canoas and in Novo Hamburgo. However, in relation to the standard determined by WHO (25 µg m⁻³), three samples had above-standard concentrations, two at the sampling point in Canoas and one in Novo Hamburgo.

From the total samples of PM₁₀ and PM_{2.5} collected, it was only possible to analyze the concentrations of PAHs present in PM from eight sets of filters (PM 10 µm and 2.5 µm) due to technical problems presented by GC/MS during the period of this study.

The Figure 3 shows the PAHs detected in the CG/MS and their respective concentrations found in PM₁₀ and PM_{2.5}.

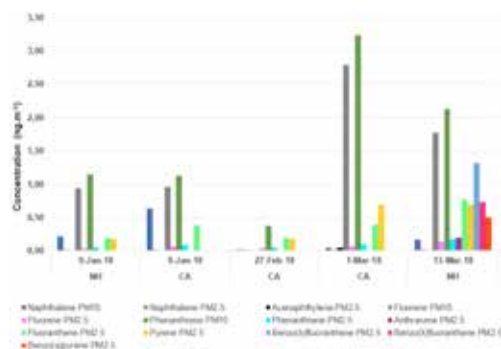


Figure 3. Concentration of the 10 PAHs determined according to the sampling date

Of the 16 PAHs classified as priority by US EPA, 10 were identified, Acenaphthylene (ACY) in MP_{2.5}, Anthracene (ANT) in MP_{2.5}, Benzo(a)pyrene (BaP) in MP_{2.5}, Benzo(b)fluoranthene (BbF) in MP_{2.5}, Benzo(k)fluoranthene (BkF) in MP_{2.5}, phenanthrene (PHE) in MP_{2.5} and MP₁₀, Fluoranthene (FLA) in MP_{2.5}, Fluorene (FLE) in MP_{2.5} and MP₁₀, Naphthalene (NAP) in MP_{2.5} and MP₁₀ and Pyrene (PYR) in MP_{2.5}. Not

identified acenaphthene (ACE), Benzo(a)anthracene (BaA), Benzo(ghi)perylene (BghiP), Chrysene (CHR), Dibenzo(a,h)anthracene (DahA), Indene(1,2,3-cd)pyrene (IcdP).

From Figure 3 it is possible to verify that the majority of the identified PAHs were associated with $MP_{2.5}$. As predicted by the literature, the aerodynamic diameter of the $PM_{2.5}$ favors its adsorption (MEINCKE, 2018). In addition to being easily associated with $PM_{2.5}$, studies also indicate that in the $PM_{2.5}$ the most toxic PAHs are found, which was also found in this study when detecting PAHs benzo(a)pyrene, benzo(b)fluoranthene, benzo(k)fluoranthene and naphthalene, classified as belonging to groups 1, 2B, 2B and 2B respectively by International Agency for Research on Cancer (IARC) at the sampling point of Novo Hamburgo (TEIXEIRA, et al., 2012).

The mean concentrations of each PAHs determined can be visualized in graphic form by figure 4 which shows the average concentrations obtained for each PAHs in both PM_{10} and $PM_{2.5}$ in the cities of Canoas and Novo Hamburgo.

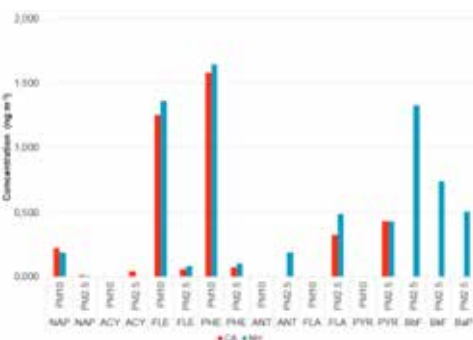


Figure 4. Mean of PAH bases detected in $MP_{2.5}$ and MP_{10} for the days discussed in both French points

Analyzing the obtained averages, it is verified that the highest concentrations remain of fluorene (FLA) and fenanthrene (PHE) in PM_{10} at the points in Canoas and Novo Hamburgo, followed by the concentration obtained for benzo(b)fluoranthene in $PM_{2.5}$ in which presented only one record, therefore its mean is represented only by the single determined concentration, as well as for benzo(k)fluoranthene (BkF) and benzo(a)pyrene (BaP), the most carcinogenic of the 16 PAHs found only in $MP_{2.5}$, which has a particle diameter capable of reaching the pulmonary alveoli (TEIXEIRA, et al., 2012; ALVES, et al., 2015).

At the same point in Canoas, Meincke (2018) also found fenanthrene, naphthalene, acenaphthylene, fluoranthene, pyrene and fluorene, in addition Meincke (2018) also detected anthracene and acenafteene. Comparing the concentrations obtained by Teixeira (2012) in the study period from 2006 to 2008 at the same point in Canoas, it can be observed that for $PM_{2.5}$ and PM_{10} the concentrations of PAHs remained below 1 ng m^{-3} , with the highest concentration obtained was 0.22 ng m^{-3} in $PM_{2.5}$ and

coincidentally also in MP_{10} . Teixeira (2012) also found anthracene, benzo(a)pyrene, acenafteene, benzo(a)anthracene, benzo(ghi)perylene, chrysene, dibenzo(a, h)anthracene, indene(1,2,3-cd)pyrene among others.

The origin of the PM was determined by the predominant wind direction in graphs plotted by the software WRPLOT View 8.0.0 software. As a result in Canoas the directions East and Southeast were the prevailing wind directions and coincide with the direction where the BR 116 is located and also with the Southeast direction that coincides with the direction where the Air Base of Canoas is located. In Novo Hamburgo, the predominant wind direction was East to West direction, where a residential area and shoe factories are located.

CONCLUSIONS

By means of the results obtained, only PM_{10} concentrations in Canoas and Novo Hamburgo were above that allowed by CONAMA Resolution 491/2018. In relation to that recommended by the WHO, only the $PM_{2.5}$ in Novo Hamburgo is within the standards. Ten of the 16 PAHs were identified as priority for monitoring by the US EPA. Because $PM_{2.5}$ gives better adsorption to the pollutants, the more toxic and higher molecular weight PAHs were found adsorbed on them.

It is also concluded that the PM concentration is not directly related to the concentration of adsorbed PAHs, but rather to the local activities where they originated and to the types of PAHs produced by the polluting sources. The meteorological factors also exerted influence on the quality of the air, since these phenomena, such as the direction of the wind, defined the origin of the pollutant sources that passed through the dichotomous samplers.

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DETERMINATION OF POLYCYCLIC AROMATIC HYDROCARBONS (PAHs) IN ATMOSPHERIC PARTICLES IN THE METROPOLITAN REGION OF PORTO ALEGRE, RS

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Abstract: The emission of Polycyclic Aromatic Hydrocarbons (PAHs) associated with particulate matter (PM) to the atmosphere in metropolitan areas is emitted mostly by anthropogenic sources. Therefore, this work had as objective to evaluate the concentration of 16 PAHs in samples of atmospheric particles in the metropolitan region of Porto Alegre-RS. Samples of PM_{2.5} and PM₁₀ were collected by the dichotomous sampler with PTFE filters in the cities of Novo Hamburgo and Canoas and their concentrations determined by gas chromatography coupled to mass spectrometry, which aimed to identify the 16 PAHs classified as priority by the United States Environmental Protection Agency (US EPA). As results greater concentration of PM₁₀ and PM_{2.5} in Canoas in relation to Novo Hamburgo. It was identified 10 PAHs from the 16 PAHs classified as priorities by the US EPA, in which the majority are associated with PM_{2.5}. The presence of benzo(a)pyrene in PM₁₀ was not detected. However, it was detected in PM_{2.5} along with benzo(b)fluoranthene, benzo(k)fluoranthene and naphthalene in Novo Hamburgo. The highest concentrations of PAHs were of fluorene and phenanthrene in PM₁₀. In Canoas the predominant wind direction comes from the east and southeast direction where the BR116 and Canoas Air Base are located. In Novo Hamburgo the predominant wind direction is the east direction where the residential area is located with small industries.

Keywords: Atmospheric monitoring, polycyclic aromatic hydrocarbons, atmospheric pollution, particulate matter.

INTRODUCTION

The urbanization, the industrialization and the extraction of natural resources around the world have been responsible for the high content of atmospheric pollutants (MARTINS, et al., 2017). The accumulation of pollutants into the atmosphere causes climatic changes and damages the health of humans, bringing short, medium and long term consequences mainly to children and the elderly (ILLI, et al., 2016).

Among these pollutants, the particulate matter (PM_{2.5} and PM₁₀) can be defined as a mixture of heterogeneous particles composed of dust, solid particles, liquid particles, smoke and soot that change in space and time according to the source emitted (GALVÃO, et al., 2017). In the PM are numerous pollutants associated with it, among them the PAH, composed only of carbon and hydrogen with two or more aromatic rings condensed in its structure (BAIRD, CANN, 2011).

According to its source, PAHs can be emitted into the atmosphere by the process of resuspension, volatilization and incomplete combustion (DIAS, et al. 2016). PAHs of lower molecular mass, formed by four or fewer benzene rings oxidize in the atmosphere, forming even more toxic compounds, such as oxy-PAHs and nitro-PAHs. Over four benzene rings, PAHs are found adsorbed to PM (GALVÃO, et al., 2017).

The main sources of these pollutants (PAHs) into the atmosphere in metropolitan areas are caused by

the burning of fossil fuels through the incomplete combustion of motor vehicles in major roadways and by the processing industries (PHILIPPI JR, et al., 2004).

The objective of this work was to identify and evaluate the concentration of 16 PAHs classified as priority by the US Environmental Protection Agency (EPA) in samples of atmospheric particles in the metropolitan region of Porto Alegre, RS.

METHODS

PM collection was performed in the city of Canoas (29°55'19.79"S and 51°10'43.05"W) and Novo Hamburgo (29°40'12.40"S and 51°7'15.73"W), both characterized by the proximity to the routes of intense traffic of vehicles. The collection of PM_{2.5} and PM₁₀ was done by the dichotomous sampler that fractionates the sampling flow in 900 m³ min⁻¹ for PM_{2.5} and in 100 m³ min⁻¹ for PM₁₀. The filter used was Millipore PTFE 47 mm diameter and 0.5 µm porosity previously weighed. The sampling period was from January 2018 to September 2018 every 15 days for 48 hours.

The procedure for extracting the PAHs retained in the PM filters was carried out in a soxhlett apparatus where the samples were extracted in laboratory with approximately 250 mL of dichloromethane (CH₂Cl₂), for 24 hours at 45°C.

After extraction, the samples underwent the Clean Up process to remove already in the first fraction with 20 mL of hexane the aliphatic

hydrocarbons that interfere in the sensitivity of the gas chromatograph detector. The second and third fraction of 20 mL of hexane and dichloromethane (1:1) and (3:1) were collected and concentrated with nitrogen gas (N₂) and injected into GC/MS mass spectrometry gas chromatograph. The mode of detection of PAHs used was Electron Ionization (IE) through Selective Ion Monitoring (SIM) scanning (SCAN). Samples were quantified in duplicates.

FINDINGS AND ARGUMENT

The PM₁₀ and PM_{2.5} samples were collected from January 9 to September 13, 2018. Their concentrations were determined and compared to the CONAMA Resolution 491/2018 that defines the emission standards of atmospheric pollutants in Brazil, and also with the quality standard recommended by the World Health Organization (WHO). The figure 1 shows the concentrations of PM₁₀ obtained in the city of Canoas and Novo Hamburgo and compares them with the emission standards of CONAMA Resolution 491/2018 (120 µg m⁻³) and also with the WHO standard (50 µg m⁻³).

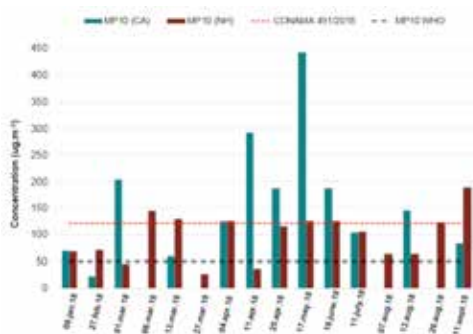


Figure 1. Concentrations of PM₁₀ obtained in the cities of Canoas and Novo Hamburgo

A total of 12 PM₁₀ samples were collected in Canoas and 16 samples in Novo Hamburgo.

As can be observed in Figure 1, the highest concentrations of PM₁₀ were obtained in the city of Canoas (CA), 441.53 µg m⁻³ concentration, where the sampling point is located a few meters from BR 116, about 50 m. Comparing the results obtained with the CONAMA Resolution 491/2018 and the quality standard recommended by the WHO, it is verified that seven samples of PM₁₀ in Canoas as well as in Novo Hamburgo obtained concentrations above the limit imposed by Resolution CONAMA 491/2018.

Regarding the WHO quality standard, 11 PM₁₀ samples had above-standard concentrations in Canoas and 13 samples in Novo Hamburgo also had concentrations above the recommended level.

The figure 2 shows the concentration results of PM_{2.5}.

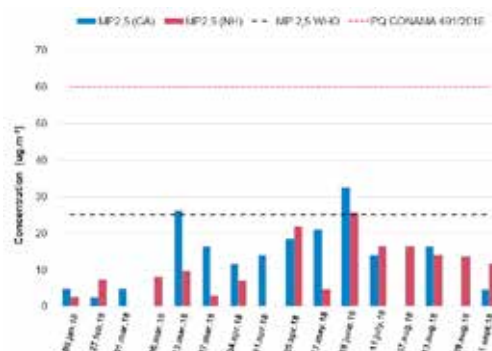


Figure 2. Concentrations of PM_{2.5} obtained in the cities of Canoas and Novo Hamburgo

Figure 2 shows the concentrations of PM_{2.5} obtained in the city of Canoas and Novo Hamburgo. In total, 13 samples of PM_{2.5} were collected in Canoas and 14 samples in Novo Hamburgo.

Analyzing the results of the PM_{2.5} concentrations expressed in figure 2, it is possible to observe that in relation to CONAMA Resolution 491/2018 in any sample there was a concentration above the quality standard (60 µg m⁻³), both at the sampling point in Canoas and in Novo Hamburgo. However, in relation to the standard determined by WHO (25 µg m⁻³), three samples had above-standard concentrations, two at the sampling point in Canoas and one in Novo Hamburgo.

From the total samples of PM₁₀ and PM_{2.5} collected, it was only possible to analyze the concentrations of PAHs present in PM from eight sets of filters (PM 10 µm and 2.5 µm) due to technical problems presented by GC/MS during the period of this study.

The Figure 3 shows the PAHs detected in the CG/MS and their respective concentrations found in PM₁₀ and PM_{2.5}.

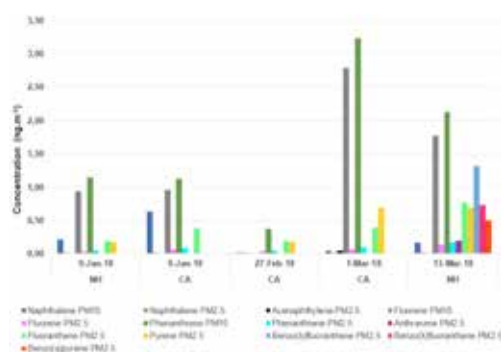


Figure 3. Concentration of the 10 PAHs determined according to the sampling date

Of the 16 PAHs classified as priority by US EPA, 10 were identified, Acenaphthylene (ACY) in MP_{2.5}, Anthracene (ANT) in MP_{2.5}, Benzo(a)pyrene (BaP) in MP_{2.5}, Benzo(b)fluoranthene (BbF) in MP_{2.5}, Benzo(k)fluoranthene (BkF) in MP_{2.5}, phenanthrene (PHE) in MP_{2.5} and MP₁₀, Fluoranthene (FLA) in MP_{2.5}, Fluorene (FLE) in MP_{2.5} and MP₁₀, Naphthalene (NAP) in MP_{2.5} and MP₁₀ and Pyrene (PYR) in MP_{2.5}. Not

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The mean concentrations of each PAHs determined can be visualized in graphic form by figure 4 which shows the average concentrations obtained for each PAHs in both PM_{10} and $PM_{2.5}$ in the cities of Canoas and Novo Hamburgo.

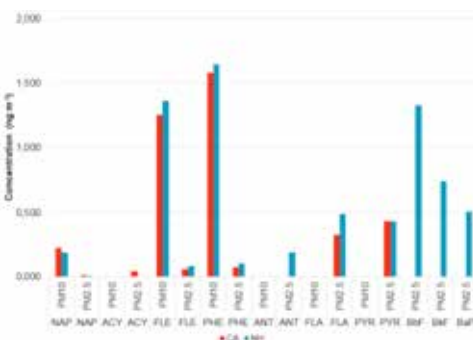


Figure 4. Mean of PAH bases detected in $MP_{2.5}$ and MP_{10} for the days discussed in both French points

Analyzing the obtained averages, it is verified that the highest concentrations remain of fluorene (FLA) and fenanthrene (PHE) in PM_{10} at the points in Canoas and Novo Hamburgo, followed by the concentration obtained for benzo(b)fluoranthene in $PM_{2.5}$ in which presented only one record, therefore its mean is represented only by the single determined concentration, as well as for benzo(k)fluoranthene (BkF) and benzo(a)pyrene (BaP), the most carcinogenic of the 16 PAHs found only in $MP_{2.5}$, which has a particle diameter capable of reaching the pulmonary alveoli (TEIXEIRA, et al., 2012; ALVES, et al., 2015).

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The origin of the PM was determined by the predominant wind direction in graphs plotted by the software WRPLOT View 8.0.0 software. As a result in Canoas the directions East and Southeast were the prevailing wind directions and coincide with the direction where the BR 116 is located and also with the Southeast direction that coincides with the direction where the Air Base of Canoas is located. In Novo Hamburgo, the predominant wind direction was East to West direction, where a residential area and shoe factories are located.

CONCLUSIONS

By means of the results obtained, only PM_{10} concentrations in Canoas and Novo Hamburgo were above that allowed by CONAMA Resolution 491/2018. In relation to that recommended by the WHO, only the $PM_{2.5}$ in Novo Hamburgo is within the standards. Ten of the 16 PAHs were identified as priority for monitoring by the US EPA. Because $PM_{2.5}$ gives better adsorption to the pollutants, the more toxic and higher molecular weight PAHs were found adsorbed on them.

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MULTI-ANGLE IMPLEMENTATION OF ATMOSPHERIC CORRECTION (MAIAC) AOD PRODUCT AS A PREDICTOR OF PM_{2.5} CONCENTRATIONS AT SÃO PAULO METROPOLITAN REGION

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Abstract: The spatial-temporal pattern of fine particulate matter (PM_{2.5}) is an important factor in predicting some health outcomes of inhabitants of an urban area. The concentrations of PM_{2.5} can be obtained through ground monitoring stations, which in general, are few and poorly distributed in space. However, satellite-derived estimates of aerosol optical depth (AOD) can be a key in leading models estimating PM_{2.5} at the ground level. We studied the relation between measures of the Multi-Angle Implementation of Atmospheric Correction (MAIAC) 1x1 km AOD product for Aqua and Terra satellites across the São Paulo Metropolitan Region (SPMR) versus collocated PM_{2.5} measures from 29 ground-based Environmental Company of São Paulo State (CETESB) stations over 6 years (2012-2017). The linear correlation (R) between daily PM_{2.5} mean concentrations (average of the 24 hours measurements), diurnal PM_{2.5} mean concentrations (average of the 6-18h period measurements) and PM_{2.5} concentrations at satellite overpass with MAIAC 1x1 km AOD were calculated. We found negative correlations between daily PM_{2.5} mean concentrations and MAIAC AOD (Aqua: -0.041; Terra: -0.047), over the six years period. The correlations between diurnal PM_{2.5} concentrations and MAIAC AOD were positive (Aqua: 0.078; Terra: 0.044), over the six years period. The correlation between PM_{2.5} concentrations at the satellite overpass and MAIAC AOD Aqua (Terra) was positive (negative): 0.213 and -0.011, over the six years period. Considering each year, the correlations were also positives or negatives, for both satellites, using daily PM_{2.5} mean, diurnal PM_{2.5} mean or PM_{2.5} at satellite overpass. The exception was MAIAC AOD Aqua data that provided positive and significant correlations in all the six years, when correlated with PM_{2.5} concentrations at Aqua overpass. In addition, the correlations were calculated considering the season of the year, dry and rainy seasons (May to August x September to April) and fires season (July to December). The correlations were slightly higher in spring, in rainy season and before fires season, but those differences were not statistically significant. The results suggested that MAIAC AOD potential to predict PM_{2.5} concentrations over SPMR needs further investigation.

Keywords: PM_{2.5}, aerosol optical depth (AOD), MAIAC, air pollution

INTRODUCTION

Elevated concentration of air pollutants and their associated health effects have drawn our attention in recent years in rapidly growing megacities, particularly in developing countries, (Kumar, 2007). A literature review relating particulate matter (PM) and different morbidity and mortality outcomes is presented in the World Health's Organization (WHO) report "Air quality guidelines: global update 2005: particulate matter, ozone, nitrogen dioxide, and sulfur dioxide". The harm of PM to human health is inversely related to particle size.

Ground-level PM_{2.5} (particles with size smaller than 2.5 µm) concentrations obtained by air quality monitoring networks are of great importance in exposures assessment studies, but their spatial coverage is limited and often insufficient for epidemiological studies (Chudnovsky et al, 2012). Satellite remote sensing is an important tool to retrieve aerosol information in areas where no ground monitoring stations are available (Wang and Christopher, 2003). The most common parameter derived from satellite observations is the aerosol optical depth (AOD), which is a measure of the extinction of electromagnetic radiation at a given wavelength due to the presence of aerosols in an atmospheric column. The AOD, from different

instruments and spatial resolutions, has been used in PM_{2.5} prediction models around the world. Chu et al. (2016) made a review on predicting ground PM_{2.5} concentration using satellite AOD. The AOD is one of the aerosol products from the sensor called Moderate Resolution Imaging Spectroradiometer (MODIS), on board of Aqua and Terra satellites. Recently, AOD at significantly higher spatial resolution (1x1 km²) is available by a new Multi-Angle Implementation of Atmospheric Correction (MAIAC) algorithm (Lyapustin et al., 2018) and those data were already validated across South America (Martins et al., 2017).

Studies relating satellite AOD and PM_{2.5} at São Paulo Metropolitan Region (SPMR) are rare (Natali, 2008). Therefore, in this study, we evaluated satellite AOD at a significantly higher spatial resolution (1x1 km²) as a predictor of the PM_{2.5} concentrations at SPMR. Also, we evaluated if MAIAC AOD-PM_{2.5} relationship vary seasonally.

METHODS

Spatial domain

Our spatial domain included the São Paulo Metropolitan Region (SPMR) (Figure 1).

AOD data

We used MAIAC AOD, at an wavelength of $0.55\mu\text{m}$, based on collection 6 MODIS Aqua and Terra data for the years of 2012-2017. HDF-EOS To GeoTIFF Conversion Tool (HEG, newsroom.gsfc.nasa.gov/sdptoolkit/HEG/HEGHome.html) was used to process the AOD data.

In the period of the study, Terra satellite overpassed SPMR between 9h-11h30 while Aqua satellite overpassed between 12h45-15h05 (local time).

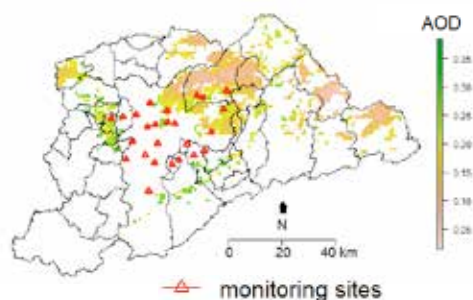


Figure 1. Map of the study area showing the location of CETESB monitoring sites and spatial variability of MAIAC AOD.

Monitoring data

At SPMR, $\text{PM}_{2.5}$ concentration corresponds to about 60% of PM_{10} concentration (CETESB, 2017). In the period of the study, there were 29 and 12 Environmental Company of Sao Paulo State (CETESB) air quality monitoring sites measuring PM_{10} and $\text{PM}_{2.5}$, respectively, not simultaneously. To increase the spatial cover of $\text{PM}_{2.5}$ CETESB sites, we used $\text{PM}_{2.5} = 0.6 \times \text{PM}_{10}$ when the $\text{PM}_{2.5}$ concentration was not available.

Statistical methods

All the analyses were done using the R statistical software version 3.5.0 (www.r-project.org). For each one of the 29 ground-based CETESB stations, we considered three averages types of $\text{PM}_{2.5}$ concentrations: (1) daily $\text{PM}_{2.5}$ mean concentration (average of the 24 hours measurements), (2) diurnal $\text{PM}_{2.5}$ mean concentration (average of the 6-18h measurements) and (3) $\text{PM}_{2.5}$ concentration at satellites overpass. The linear correlations (R) between $\text{PM}_{2.5}$ concentrations, for all three averages types, and the collocated MAIAC AOD (Aqua and Terra) data, during 2012-2017 period, were calculated.

We also estimated the correlations between the $\text{PM}_{2.5}$ concentrations, for all three averages types, and MAIAC AOD AQUA according to:

- four seasons: spring (September to November), summer (December to February), autumn (March to May) and winter (July to August);
- dry season (May to August) and rainy season (September to April) (www.estacao.iag.usp.br/seasons);
- and fires season (July to December), defined using Brazilian Institute for Space Research database (www.inpe.br/queimadas/bdqueimadas) (Figure 2).

FINDINGS AND ARGUMENT

The correlation between $\text{PM}_{2.5}$ concentrations, for all three averages types, and MAIAC AOD, for both satellites, were moderate or weak. MAIAC AOD Aqua and $\text{PM}_{2.5}$ concentrations at the satellite overpass (type 3) presented the highest correlations over the period of the study. Negative correlations were also found (MAIAC AOD Terra data, mainly) (Table 1). Natali (2008) studied the relationship between satellite AOD and the concentration of particulate matter (PM_{10} and $\text{PM}_{2.5}$) in the SPMR, between 2002 and 2005, and also found negative relationships. In addition, Terra retrievals got worse in quality in later years (DeVisser and Messina, 2013; Wang et al., 2012).

Since AOD is a value associated with the atmospheric column and $\text{PM}_{2.5}$ concentration measured in a monitoring site is a measure of dry particles near the surface, these two parameters are not expected to be highly correlated (Chudnovsky et al. 2012). The relationship between columnar AOD and ground-level $\text{PM}_{2.5}$ is not straightforward and depends on the vertical distribution and the optical, size distribution and hygroscopic properties of the aerosol. Also, the relationship depends on the season and the site location. (Boyouk, et al., 2010). AOD- $\text{PM}_{2.5}$ relationship can vary seasonally, because of the difference in the relative humidity (RH), an important factor to hygroscopic properties of the aerosols. The results were presented in Figure 3. Since the correlations between MAIAC AOD Terra and $\text{PM}_{2.5}$ concentrations were weak or negatives, even when $\text{PM}_{2.5}$ concentrations at Terra overpass were considered, the results will not be reported. Considering season of the year, dry/rainy season and fires season, the correlations were slightly higher in spring (Figure 3, top panels), in rainy season (Figure 3, middle panels) and before fires season (Figure 3, bottom panels). All differences were not statistically significant. The patterns discussed below are more evident when considering $\text{PM}_{2.5}$ concentrations at AQUA overpass.

Correlations between MAIAC AOD AQUA and $\text{PM}_{2.5}$ concentrations were higher in summer, autumn and spring, months that in general, present the highest mean relative humidity (www.estacao.iag.usp.br/seasons). Also, we can observe a lower (higher) variability in MAIAC AOD values in dry (rainy) season. That is expected due to hygroscopic growth of the aerosols.

Regarding to fires season, it has been shown that at higher altitudes there is the transportation of biomass burning, occurring in the North and Midwest of the Brazil or in the country of the state of Sao Paulo, to SPMR (Landulfo, 2009; Mariano et al. 2010). The presence of aerosols above the mixing layer, which are not measured by monitoring stations on the ground can impact the relationship between remote sensing AOD and $\text{PM}_{2.5}$.

Table 1: Linear correlations values (R) between satellite overpass time, daily and diurnal PM_{2.5} concentrations and MAIAC AOD

year	AQUA			TERRA		
	overpass	diurnal	daily	overpass	diurnal	daily
2012	0.349*	0.182*	0.08*	0.08*	0.169*	0.095*
2013	0.128*	-0.021	-0.18*	-0.154*	-0.128*	-0.268*
2014	0.161*	0.086*	0.004	0.048*	0.102*	0.012
2015	0.162*	0.022	-0.082*	-0.137*	-0.064*	-0.124*
2016	0.129*	-0.04	-0.171*	-0.055*	-0.001	-0.091*
2017	0.314*	0.224*	0.108*	0.03	0.054*	-0.038*
2012-2017	0.213*	0.078*	-0.041*	-0.011	0.044*	-0.047*

*statistically significant at a 5% significance level

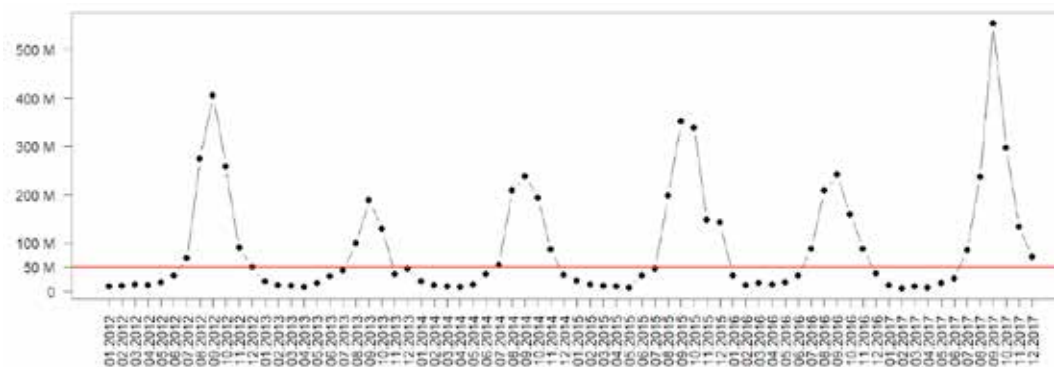


Figure 2. Fires number in Brazil between 2012 and 2017

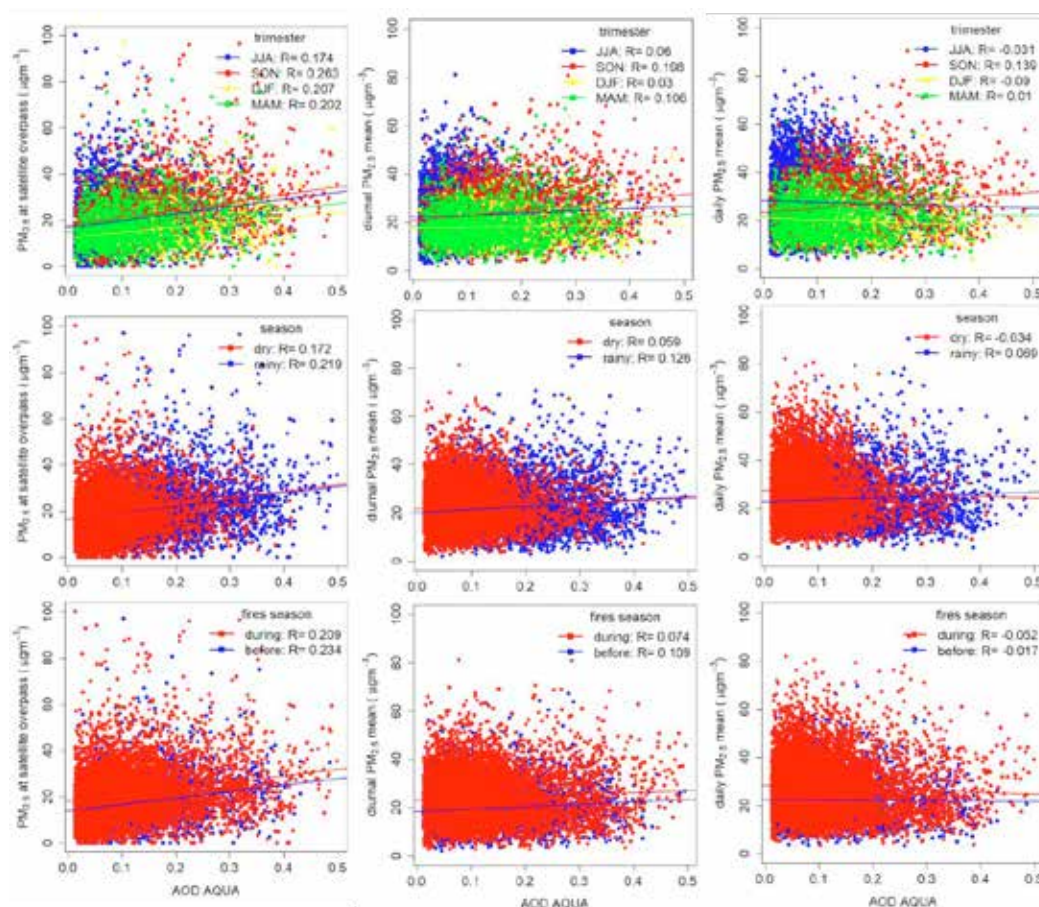


Figure 3: The relationship between MAIAC AOD Aqua and PM_{2.5} concentration at AQUA overpass (left column), diurnal PM_{2.5} mean (middle column) and daily PM_{2.5} mean (right column) according to season of the year (top panels), dry and rainy seasons (May to August x September to April) (middle panels) and fires season (July to December) (bottom panels), at the 29 sites in SPMR during 2012-2017. The correlation coefficients (R) are given in each subplot as well. The lines denote least squares fitting.

CONCLUSIONS

This study examined MAIAC AOD (Aqua and Terra) as a predictor of ground PM_{2.5} concentrations at SPMR during the period 2012-2017. Correlations between ground PM_{2.5} concentrations (overpass satellite time, diurnal and daily means) and collocated MAIAC AOD were calculated. The found correlations were moderate or weak. Our finds confirm the results found by Natali (2008). As indicated by others studies, MAIAC AOD-PM_{2.5} relationship can depends on the season. Considering the season of the year, dry and rainy seasons and fires season, the correlations were slightly higher in spring, rainy season and before fires season. However, those differences were not statistically significative.

Taking in count aerosol measures above the mixing layer seems important to better understand AOD-PM_{2.5} relationship at SPMR.

In others regions around the world, AOD from satellites has been used with success as a predictor of ground PM_{2.5} concentrations (Chudnovsky et al., 2012, Xiao et al., 2017, Just et al., 2015 and de Hoogh et al., 2018).

Promising results are found by adjusting for daily variability in the AOD-PM_{2.5} relationship and accounting for meteorological and land use variables (work in progress).

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PM₁₀ SOURCES IN THE METROPOLITAN AREA OF SÃO PAULO: THE ROLE OF BIOGENIC SOURCES

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Abstract: There has been great recent effort in São Paulo, Brazil, to determine the contributions from natural and anthropogenic sources to the particulate matter (PM) in the atmosphere. Airborne particles of biological origin (bioaerosols) can influence atmospheric processes such as ice and cloud condensation nuclei and cause adverse health effects as allergens. To better understand biogenic sources, ambient PM₁₀ (particulate matter with aerodynamic diameter smaller than 10 µm) was sampled in Metropolitan São Paulo. Twenty-four hour PM₁₀ samples were collected with Hivol (quartz-fiber filters) and Minivol samplers (Polycarbonate-membrane filters) on the rooftop of a campus building at the University of São Paulo, Southeast of the city. Polycarbonate-membrane filters were submitted to elemental analysis by energy dispersive x-ray fluorescence (XRF). Quartz-fiber filters were analyzed for ions (cations and anions) by ion chromatography (IC) and for organic and elemental carbon (OC and EC) by the thermal/optical IMPROVE_A protocol. Portions of the quartz filter samples were analyzed for carbohydrates (e.g., mannitol and arabinol, biomarkers of fungal spores, and levoglucosan, a tracer for biomass burning emissions) by IC-PAD and organic acids. The Positive Matrix Factorization (PMF 5.0) and Principal Component Analysis (PCA) were applied to the database to estimate PM₁₀ source contributions. The derived factors indicate a mixture of PM₁₀ sources. The main factor that contributed to 25% of the PM₁₀ mass concentration presented high loadings of crustal species (e.g., Al, Si, K, Ca, Ti, Mn and Fe) and carbon (OC and EC), consistent with geological source. The second main factor explained 20.6% of the PM₁₀ with high factor loadings of organic acids and crustal species (Al, Si, Ti and Ca). The third main factor explained 19% of the PM₁₀ with abundant NO₃⁻, S, P and NH₄⁺, pointing to vehicular emissions and secondary inorganic aerosols. The factor with high biomass burning loading had a probability of being transported from the northeast area, as calculated with the conditional bivariate polar plots (CBPF). PCA analysis presented similar results, consistent with biomass burning emissions from sugar-cane plantations and other agricultural areas in the Northwest region of São Paulo State and with the sea breeze impacting the city of São Paulo when Southeasterly winds prevailed.

Keywords: Bioaerosol, São Paulo aerosols, Brazil, PMF, PM₁₀ sources.

INTRODUCTION

Particulate matter (PM) is an air pollutant that causes harmful impact on air quality in Brazil, especially in São Paulo, and is important from a health perspective (Andrade et al., 2017). Airborne particles of biological origin (bioaerosols) can influence atmospheric processes such as ice and cloud condensation nuclei (Morris et al., 2011) and cause adverse health effects (Douwes et al., 2003). To better understand the contribution of biogenic sources to PM with aerodynamic size smaller than 10 µm (PM₁₀) a source apportionment study was conducted focusing on the biogenic source.

METHODS

Hivol and Minivol samplers were used to collect twenty-four hour PM₁₀ samples. Polycarbonate-membrane filters were used in the Minivol and were submitted to energy dispersive x-ray and fluorescence (XRF) analysis for trace-element determination. Quartz-fiber filters used in Hivol samplers were submitted to ion chromatography (IC) analysis for ion (cations and anions) determination; for organic and elemental carbon (OC and EC) determination by the thermal/optical IMPROVE_A protocol; and for carbohydrate and organic acid analysis by IC-PAD. All data equal or smaller than zero (including missing data) were replaced by half of the detection limit (MDL). The analytical uncertainty for ions, carbohydrates, OC and EC were calculated using the MDL (minimum detectable limit or method detected limit) and

precision (calculated with replicate analyses) adapted from Chow et al., 2017 (Equation 1). The uncertainty for the elements (XRF) and total PM₁₀ mass were calculated using the relative uncertainty (10% for PM₁₀) and the MDL, according to the equations indicated in the PMF 5.0 Fundamentals and User Guide.

$$CV = c_i > 10 \times MDL \text{ and } c_{i,r} > 10 \times MDL$$

$$> 10 \times MDL$$

$$\rightarrow \left| \frac{c_i - c_{i,r}}{(c_i + c_{i,r})/2} \times 100 \right|$$

$$CV = c_i < 10 \times MDL \text{ and } c_{i,r} < 10 \times MDL \rightarrow 10$$

$$Precision = \frac{\sum_i^N CV}{N}$$

$$AnalyticalUncertainty = \sqrt{(\hat{CV} \times c_i)^2 + \left(\frac{MDL}{3}\right)^2}$$

Equation 1. Calculation of precision and uncertainty (adapted from Chow et al., 2017). N is the number of replicates, c_i is the sample concentration, $c_{i,r}$ is the concentration of the replicate sample. i is each sample for each ion. MDL is the minimum detectable limit. CV is the coefficient of variation (Chow et al., 2017).

After that, the total uncertainty considering the sampler uncertainty were also calculated for all species (Equation 2).

$$uT = \sqrt{\frac{uC^2}{V^2} + \frac{c_i^2 uV^2}{V^4}}$$

Equation 2. Calculation of total uncertainty. uT is the total uncertainty in $\mu\text{g}/\text{m}^3$, uC is the analytical uncertainty of the sample ($\mu\text{g}/\text{filter}$), uV is the volume uncertainty of each sample (5%), c_i is the sample concentration ($\mu\text{g}/\text{filter}$), V is the volume (m^3).

PMF was configured to 20 runs with 6 factors; a 15% extra modeling uncertainty was added to the model. All S/N (signal-noise) values smaller than 3 were considered bad and those higher than 3 were considered strong, except those for Mg^{+2} and NO_3^- that were considered weak. Some elements were removed from the analysis or put as weak due to bad adjustment or similarity between element and ion. Principal component analysis was also used to reinforce the PMF analysis. For the PCA the normalized Varimax rotation was used, the explained cumulative variance percentage was 80.5%, the eigenvalues were higher than 1 and for most species the communalities were well explained. The final species used in PMF and PCA were: Na^+ , NH_4^+ , K^+ , Cl^- , NO_3^- , Mg^{+2} , Br^- , arabitol, glucose/xylose, levoglucosan, mannitol, mannosan, OC, EC, succinate, maleate, formate, methanesulfonate and oxalate, Al, Si, P, S, Ca, Ti, Mn, Fe, Cu, Zn and mass of PM₁₀ as a total variable. A conditional bivariate polar plots (CBPF) (Uria-Tellaetxe and Carslaw, 2014; Jeričević et al., 2019) were used to better explain the sources and identify their predominant wind direction considering the

wind speed. The polar plot to calculate the CBPF for the factors was run with a percentile of 75, $k=40$ (smoothing parameter), minimum number of points equals to 1, all values less than or equal to zero were set as missing data, and the statistic with CPF. Excel and RStudio (with the packages openair, dplyr, readxl, httr, magrittr, plyr, psych) were used to analyze the data and to do the CBPF.

FINDINGS AND ARGUMENT

For the PMF six factors were identified representing six sources for the PM₁₀. The identified sources are presented in the Fig. 1. Factor 1: Abundance of S, P, NO_3^- , NH_4^+ and Maleate indicating vehicular emissions with secondary inorganic aerosol (SIA). Factor 2: contribution mainly of organic acids (succinate, formate, methanesulfonate and oxalate), OC and crustal species (Al, Si and Ti); Factor 3: biomass burning (BB) tracers (levoglucosan, mannosan and K^+), OC, EC with Cu; Factor 4: a mixture of EC, OC, Cu, Zn, Br⁻ and biomarkers of fungi (arabitol, mannitol); Factor 5: Marine aerosol (MA) with the presence of Na^+ and Cl^- ; Factor 6: Abundance of crustal species (Al, Si, K, Ca, Ti and Fe), OC and EC; The main factors that contribute to the PM₁₀ mass were the Factor 6 (25.8%), Factor 2 (20.6%) and Factor 1 (19%).

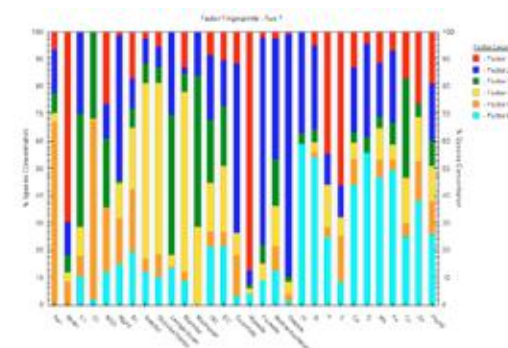


Figure 1. PMF factor fingerprint.

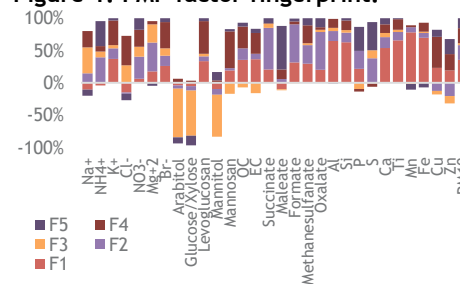


Figure 3. PCA factor loading.

With the PCA, five factors were found (Fig. 3). Factor 1 and 5 were similar to Factor 6 and 1 of PMF respectively; Factor 2: with high loading of S, P, NH_4^+ and NO_3^- indicated vehicular emissions and secondary inorganic aerosol mixture with organic acids (succinate, formate, methanesulfonate and oxalate). Factor 3, abundant Na^+ , arabitol,

mannitol, glucose/xylose. The biomarkers of fungi (mannitol and arabinol) and glucose/xylose had a negative loading in this factor, as opposed to Na^+ , probably due their negative correlation. Factor 4 has a high load of biomass burning tracers (levoglucosan, mannosan, K^+) and Cu. The factor scores calculated with PCA and the sources estimated by PMF were analyzed altogether with the wind direction by the application of the CBPF. The results from the CBPF are presented in Fig.5 (PMF).

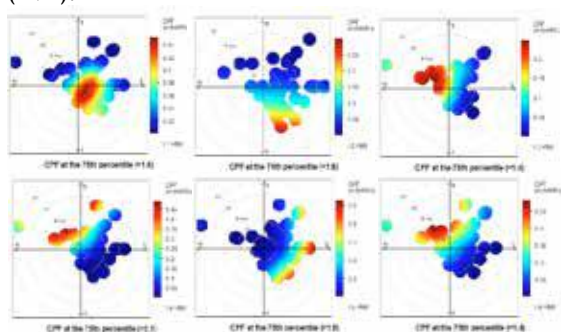


Figure 5. CBPF analysis for the factors obtained with PMF.

The CBPF analysis allows to better understand the origin of the sources when considering that 75 percentile of the factors scaled by the wind speed were related to the direction of the file. The F3 (PMF) and F4 (PCA) were transported from the northeast area. This factor has a high loading of biomass burning tracers (levoglucosan and mannosan). The fact that the northwest region of São Paulo State has biomass burning emissions from sugar-cane plantations and other agricultural areas explain this relation. F2 (PMF) and F2 (PCA) are very similar with the CBPF analysis, and both have high loadings of organic acids, and are influenced by Southeastern winds, where an industrial area is present. The secondary inorganic aerosol and vehicular emissions as indicated by F1 (PMF) are transported from the southeast region and could indicate a more local emission source since this factor is related with low wind speed. The influence of wind direction and wind speed on F3 calculated from the PCA (data not shown) is very similar with the factor F5 from PMF, which could indicate that even with the negative loading of biogenic aerosol, this factor is more strongly influenced by marine aerosol (Na^+). Specially when looking at CBPF from arabinol and manitol individually (Figure 7), it is possible to realise that there is a >40% probability that they are transported from the northwest and not from the east as F3 (PCA) and F5 (PMF) indicates. The F4 (PMF) that has a high loading of arabinol and manitol and from vehicular emissions shows a similar wind transport to the individual species arabinol and manitol (from the Northwest).

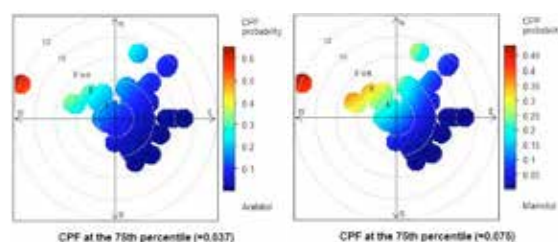


Figure 7. CBPF analysis for arabinol and mannitol.

CONCLUSIONS

This preliminary work indicated that is possible to concluded that: (1) The PMF and PCA analysis provide similar results in some way, and with the CBPF it is possible to describe the predominant wind direction and speed; (2) the biogenic emissions as represented by arabinol and mannitol seem to be transported mainly by the northwest winds and are related with high wind speeds. However, the PCA was not able to identify this source and PMF presents a mixture of sources. For a better identification of the sources, it would be necessary to have more biogenic and vehicular tracers, such as the total protein concentration. It could help to separate the factors and better explain the contribution of the biogenic sources to the PM_{10} mass concentration.

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Can biomonitoring be used to validate pollutant dispersion models? A case study of a petrochemical complex in São Paulo, Brazil

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Abstract: Pollutant dispersion models are based on emission inventories, geographic/topographic and meteorological data. They are widely applied in regulatory studies. Nevertheless, they rely on validation within situ pollutant concentrations samples. Biomonitoring is a low-cost sampling method mainly applied for particulate matter (PM) dispersion studies. Commonly, tree barks and leaves are used as sampling substrates. When compared to standard sampling methods, that use high precision equipment, the biomonitoring is inexpensive, but imprecise. The low cost enables datasets containing from tens to hundreds of locations, what could compensate the lack of precision.

This study shows a comparison between the PM concentration isolines derived from a dispersion model (AERMOD) with the biomonitoring samples around the biggest petrochemical complex in the Metropolitan Area of São Paulo (MASP).

The Polo Petroquímico do Grande ABC (PPABC) is an industrial complex located in the Southeast of the MASP, one of the largest metropolitan area in the world with more than 21 million inhabitants. The PPABC have an area of five square kilometers and emits about 15 g/s of PM. The principal products are fertilizers, gasoline, diesel, propene, liquefied petroleum gases and special solvents.

The annual average of PM, VOCs, SO₂, NO₂ and CO on the sampled points was calculated by the AERMOD dispersion model (American Meteorological Society (AMS)/United States Environmental Protection Agency (EPA) Regulatory Model Improvement Committee) with a 100 to 300 meters resolution (from the central to the marginal part of the mesh) in an area of 16 km². The AERMOD generates 3 outputs: the annual mean dispersion, the 1-hour max for each grid point (Max 1 h) and the 24-hours max for each grid point (Max 24 h).

To the biomonitoring sampling, barks of 44 *Tipuana Tipu* and 21 *Caesalpinia pluviosa* trees were collected. The barks' first 3 mm was grated and prepared to an elementary composition and magnetic proprieties analysis. Trace-elements and magnetic parameters were determined for each tree sample. A receptor model method was used to estimate the PPABC contribution to the pollution in the area using Factor Analysis, that point out 2 main sources of PM: the soil dust resuspension and anthropogenic sources (vehicular and industrial emissions). The sources profiles (scores) and the elements concentrations were compared to the AERMOD model concentrations.

As the processes governing the interactions between the tree barks and the PM are non-trivial, it was used an ordinal correlation between the data. The correlation method chosen to compare the data was the Spearman Correlation. The Spearman's coefficients show some correlation between the Anthropogenic factor and the Max 1 h (0.31) PM concentration, but did not present significant correlations with the other outputs. The Cu and Mn concentrations, which are tracers for industrial emissions, shows some correlation with the outputs also.

This work showed that biomonitoring cannot be used for dispersion model validation by itself, but it has a potential as complementary data to air quality stations-based validation.

Keywords: Pollutant Dispersion Model Validation, Industrial Pollution, Particulate Matter.

INTRODUCTION

The air pollution dispersion is a valuable information to the application of public health politics and regulation of industries impacts. The modelling of the atmospheric dispersion of pollutants is very complex, specially the case of the turbulent Planetary Boundary Layer. Models like the AERMOD dispersion model (American Meteorological Society (AMS)/United States Environmental Protection Agency (EPA) Regulatory Model Improvement Committee) considers the emission inventories, wind and surface data to calculate the dispersion plume of pollutants. These models rely on *in situ* samples to validation. The quality of the validation is proportional to the reliability, and spatial distribution of the samples. As the reference instruments are expensive, low-cost methods as bio monitors are used to atmospheric particulate matter (PM) dispersion studies.

Biomonitoring is the analysis of the response of individuals, in different levels of biological organization, to detect the effects of contamination in the human health (Markert et al., 2003). Biological samples as trees leaves and barks can be used to estimate the spatial distribution of the PM concentration (Moreira et al. 2016). Nevertheless, the interaction between the biological samples and the PM is not trivial nor linear. This entails in a non-accurate measure, however a relationship between the PM concentration and part of the proprieties of the samples is expected. The identification of this relation lies on multivariate statistics as the principal component analysis (PCA) or the factor analysis (FA) that uses the covariation of the sample's proprieties to identify groups of compounds with similar behaviour. Such methods can also distinguish different sources of PM and are utilised in the receptor modelling for PM

apportionment of common studies. Yet, as the substrate of the sampling is complex per se this apportionment needs tracers with good potential to distinguish the PM signals from the tree composition itself.

The use of magnetic proprieties analysis is becoming popular as this is proving to be valuable as an anthropogenic tracer (Hofman et al. 2017 and Maher & Thompson, 1999).

Once the PM target fraction (e. g. industrial emissions in a metropolitan context where are other PM sources) is found, the comparison between the spatial distribution of the target's fraction and the model's distribution can be made. The Pearson correlation coefficient is a standard method to compare the distribution of two sets of data, however as the interactions between the PM and the trees are not linear, this coefficient is not appropriate to this comparison. The Spearman's rank correlation coefficient (ρ) can be used in this scenario.

This study is situated on the Polo Petroquímico do Grande ABC (PPABC). This is an industrial complex (petrochemical + fertilizer industrial complex) located in the Southeast of the Metropolitan Area of São Paulo (MASP). The PPABC have an area of five square kilometers and emits about 15 g/s of PM. The principal products are fertilizers, gasoline, diesel, propene, turpentine, liquefied petroleum gases and special solvents.

This study shows a comparison between the PM concentration isolines derived from the dispersion model AERMOD with biomonitoring samples around the biggest petrochemical complex in the MASP. It's a continuation of the study performed by Kamigauti et al. (2018).

METHODS

To obtain a comparable data from the tree barks samples with the dispersion of pollutants calculated with AERMOD, several processes had to be done as shown in the Figure 1. The sampling consists in barks of 44 *Tipuana Tipu* and 21 *Caesalpinia pluviosa* trees (63 valid samples). The barks' first 3 mm was grated and prepared to an elementary composition and magnetic proprieties analysis. The elementary composition was obtained by X ray fluorescence. The sampling and the elementary analysis were made by the Laboratório de Poluição Atmosférica Experimental (LPAE) team. Trace-elements and magnetic parameters were determined for each tree sample.

The magnetic parameters measured were the initial magnetic susceptibility (Sus), anhysteretic remanent magnetization (ARM) and saturation

isothermal remanent magnetization (SIRM). A comprehensive explanation of these parameters can be found in Maher & Thompson (1999) and Evans & Heller (2003). The instruments used was the MKF1-FA Multifunction Kappabridge (Agico) susceptibilimeter for Sus, SQUID (super quantum interference design) magnetometer model RAPID (2G-Enterprises) for ARM and the 3900 Vibrating Sample Magnetometer (MicroMag) for SIRM. The operational parameters used in the measures was, for the Sus, an alternate magnetic field of 200 A/m with 976 Hz, for the ARM, an alternate magnetic field of 100 mT with a bias field of 0.01 mT and for the SIRM a 1T field.

A receptor model method was used to estimate the PPABC contribution to the pollution in the area using the factor analysis with the varimax raw rotation, that point out 2 main sources of PM: the soil dust resuspension and anthropogenic sources (mainly vehicular emissions). A third factor was found referent at the tree's bark itself.

The AERMOD model simulation used a 100 to 300 meters resolution grid (from the central to the marginal part of the mesh) in an area of 16 km². The wind data was obtained from a near airport and the emissions inventory was a mix of official data and information provided by the plant. The model generates 3 outputs: the annual mean concentration dispersion, the 1-hour max for each grid point (Max 1 h) and the 24-hours max por each grid point (Max 24 h). The model was operated by the Meteorologia Aplicada a Sistemas de Tempo Regionais (MASTER) and Laboratório de Análise dos Processos Atmosféricos (LAPAT) laboratory team.

The sources profiles (scores derived from FA) and the elements concentrations were compared to the AERMOD model concentrations.

The comparison between the model output and the sample data was made with the Spearman's Rank Correlation. It's compares the ordinality of two datasets using the formula:

$$\rho = R_{rg_x rg_y} = \frac{cov(rg_x, rg_y)}{\sigma_{rg_x} \sigma_{rg_y}}$$

Where the ρ is the Spearman's rank correlation coefficient, R is the Pearson correlation coefficient, σ the standard deviation and the rg_x and rg_y the rank-converted datasets X and Y.

Rank-converted datasets are a vector of 1 assigned to the lowest value and 63 to the highest.

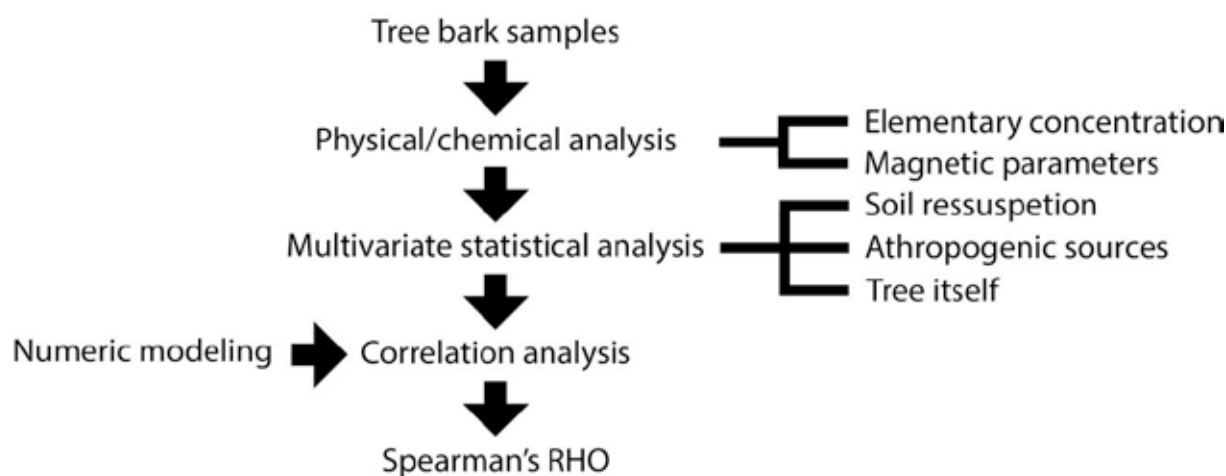


Figure 1. Flow chart of the methods.

FINDINGS AND ARGUMENT

The Spearman's rank correlation coefficients calculated can be found in the Table 1 and some rank distributions can be found in the Figure 2.

The correlations founded between the Anthropogenic Factor (Anthropo.) and the model outputs are relatively low, however the factor analysis could not separate the industrial and the vehicular fractions of the Anthro. Thus a low correlation as the 0.31 with the Max 1 h was expected. Nevertheless the low correlation between the Anthropogenic and the others model's outputs are not expected, yet it can indicate a relation of the intense industrial pollution events and the accumulation/absorption of the PM by the trees. It's indicate that the signals of the tree barks do not represent a extensive time period which is expected due the rain and wind washout effects.

Withal, the correlations between the Cu and Mn concentration and the model's outputs are noteworthy. They are potential tracers for industrial emissions.

The rank comparison can be seen in the Figure 2.

CONCLUSIONS

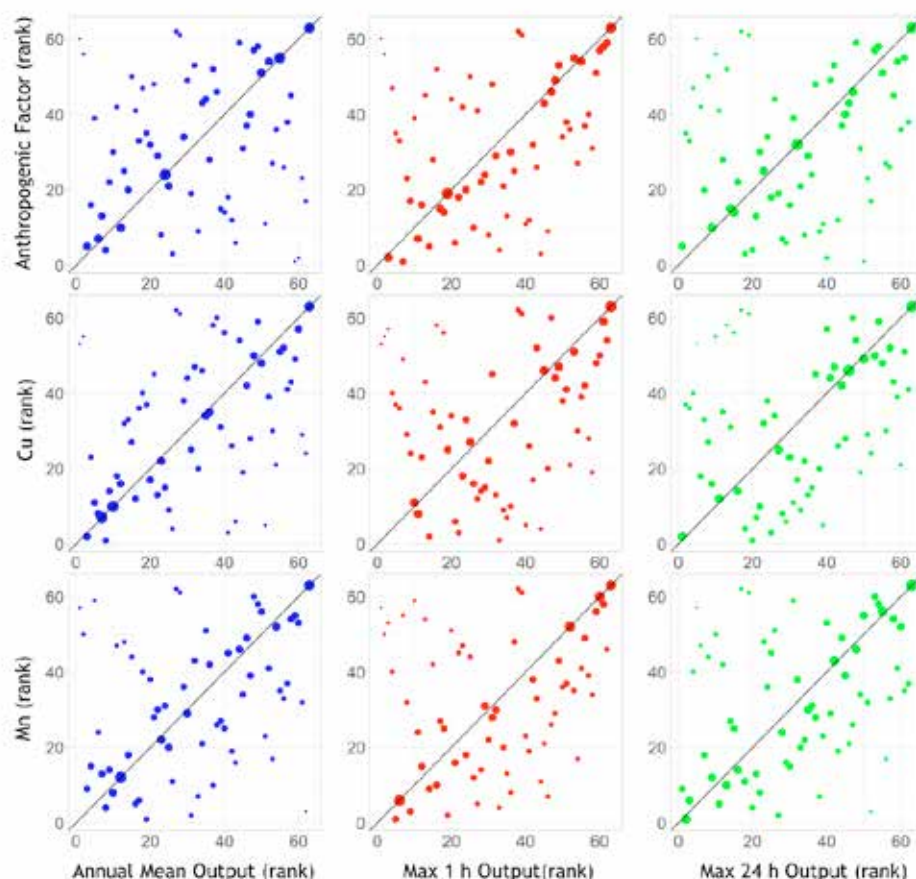
The use of biomonitoring data to validate the dispersion model is not conclusive due the natural complications of the method. Important aspects to consider are the time resolution of the bark's samplings, the impact of the industrial emissions and the vehicular emissions in the neighborhood. Two main avenues are located around the industrial

complex, so that the anthropogenic PM emissions are strongly related to the vehicular impacts. The industrial complex itself generate an internal traffic that cannot be neglected. As the biomonitoring do not generate direct reliable concentration data, the most used statistical methods can lead to invalid comparisons. This work showed that biomonitoring cannot be used for dispersion model validation by itself, but it has a potential as complementary data to air quality stations-based validation.

Table 1. Spearman's Rank Correlation Coefficients of the parameters analysed with the model's outputs.

	Annual Avg.	Max 24 h	Max 1 h
Soil Ress.	0.14	0.02	-0.09
Anthropo.	0.04	0.13	0.31
Al	0.16	0.06	-0.01
Ca	-0.22	-0.07	0.22
Cl	-0.13	-0.12	-0.21
Cu	0.36	0.22	0.12
Fe	0.16	0.09	0.01
K	0.01	-0.02	-0.12
Mg	0.06	0.10	0.00
Mn	0.25	0.28	0.17
P	-0.22	-0.19	0.12
S	-0.09	0.03	0.02
Sr	0.03	0.11	0.17
Sus	0.12	0.07	0.00
ARM	0.06	0.12	0.07
SIRM	0.11	0.04	-0.04

Figure 2. Ordinal comparison between the AERMOD output and the anthropogenic factor, Mn concentration and Cu concentration. In blue is the Annual Mean PM Concentration Output, red the Max 1 h PM concentration Output and in green is the Max 24 h PM Concentration Output. Note that the units are in ranks (1 to the lowest value and 63 to the highest) as the Spearman's correlation is based in rank comparisons.



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Evaluation of the air quality data from the monitoring network of the state of Espírito Santo - Brazil

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Abstract: The objective of this study was to evaluate the data of the monitoring networks of the Espírito Santo state in order to provide a diagnosis of local air quality and valuable analyzes that will be base for the scientific community and the Government. The pollutants analyzed were: particulate matter (PM_{2.5} and PM₁₀), total suspended particulates (TSP), nitrogen dioxide (NO₂), sulfur dioxide (SO₂), carbon monoxide (CO) and ozone (O₃). The study area covered 6 cities and 15 monitoring stations. The characteristics of each station were identified and the measured data were obtained with the environmental management entity. After data validation, were elaborated curves of the historical series of pollutants for the period from 2008 to 2018. In addition, were calculated the average concentrations of the pollutants in order to compare with the respective state legislation and the World Health Organization (WHO) guidelines, and were counted the exceedance events. It was observed that there are many data failures, with long periods without pollutant concentrations informations. For the average concentrations of short exposure, only pollutants PM₁₀ and SO₂ exceeded the standards. For the PM₁₀ average concentrations of long exposure, the two stations presented exceeded the standards in all years from 2008 to 2018. This is a work in progress and the next step will be to evaluate the quality of the data and to correlate them statistically with the meteorological data measured at the monitoring stations.

Keywords: Air pollution, air quality monitoring, Espírito Santo.

INTRODUCTION

Air pollution can be defined as the air contamination by any chemical, physical or biological agent that modifies the natural characteristics of the atmosphere, bringing environmental impacts and interfering with human health (WHO, 2019).

Urban areas are critical regions of air pollution. Due to the greater population density, a significant number of people are affected in the cities by the harmful effects of this environmental impact. In these regions, therefore, it is necessary to monitor air quality. One of the ways to carry out the monitoring is through direct measurements, with the installation of air quality monitoring networks. The monitoring information by the networks give supports air quality assessment and planning for improvement in urban environments.

Many authors have been dedicated to studying the various air quality monitoring networks, evaluating the characteristics of their stations (BARRERO et al., 2015), their special representativeness (JANSSEN et al., 2012; HAO and XIE, 2018; WANG et al., 2018) and the quality control of data (LIU, LI and LI, 2016).

The state of Espírito Santo, located in southeast Brazil, has two automatic air quality monitoring networks, located in urban areas: the network of Metropolitan Region of Greater Vitória (MRGV) and the network Southern Region (SR). Although not encompassing the entire state territory, they are positioned at strategic locations and provide the

data that supports scientific works and public decisions.

In this context, the objective of this study was to evaluate the data of the monitoring networks of the Espírito Santo state in order to provide a diagnosis of local air quality and valuable analyzes that will be base for the scientific community and the Government. In sequence, this work intends to perform an evaluation of the quality of data and correlate them statistically with meteorological data.

METHODS

The stations of Espírito Santo air quality monitoring networks are located in 6 municipalities, covering approximately 46% of the state population. The MRGV network, owned by the State Institute of Environment and Water Resources (IEMA), has 9 stations: Laranjeiras, Carapina, Cidade Continental, Jardim Camburi, Enseada do Suá, Vitória Centro, Vila Velha Centro, Vila Velha Ibes and Cariacica. The SR network, owned by the company Samarco Mineração S.A., has 6 stations: Meaípe, Parati, Castelhanos, Belo Horizonte, Maemba and Centro (Figure 1).

The period analyzed was the ten-year period covering the years 2008 to 2018. The pollutants considered were: respirable particles (PM_{2.5}), inhalable particles (PM₁₀), total suspended particulates (TPS), sulfur dioxide (SO₂), nitrogen dioxide (NO₂), carbon monoxide (CO) and ozone (O₃). Data processing and analysis were performed using Excel and Python softwares.



(a)



(b)

Figure 1. Automatic Air Quality Monitoring Network: a) Metropolitan Region of Greater Vitória (MRGV) and b) Southern Region (SR).

Initially, were calculated the average pollutants concentrations of short and long exposure according to State Decree n° 3463-R/2013 (Table 1).

Table 1. Average concentrations calculated for the analyzed pollutants.

Pollutant [$\mu\text{g m}^{-3}$]	Short exposure	Long exposure
PM _{2.5}	24-hour average	Annual average ¹
PM ₁₀	24-hour average	Annual average ¹
TSP	24-hour average	Annual average ²
SO ₂	24-hour average	Annual average ¹
NO ₂	1-hour average	Annual average ¹
CO	1 and 8-hour average	-
O ₃	8-hour average	-

¹ Arithmetic average

² Geometric average

The validation of the data was performed according to criteria established by the Environmental Company of the State of São Paulo (CETESB, 2013): hourly average: 75% of the measures valid in 1 hour; daily average: 75% of measures valid in 24 hours; annual average: 50% of the daily averages for the four-month periods.

Finally, the averages were compared to the air quality standards defined in the State Decree of Espírito Santo n° 3463-R/2013 and the World Health Organization (WHO) guidelines. The state decree has four types of standards: intermediate goals 1, 2 and 3, respectively (IG1, IG2 and IG3) and final standard (FS). The limits defined in the final

standards (FS) are the WHO guidelines, determined so that the population health is preserved to the maximum in relation to the damages caused by the air pollution.

FINDINGS AND ARGUMENT

The graphs (called violin plots) presented in the Figures 2 and 3 show the distribution of the average concentrations of monitored pollutants and their comparison with the relevant legislation and WHO guidelines. The violin plot include: a marker for the median of the data; a box indicating the interquartile range, and the probability density of the data at different values.

For the elaboration of the graphs, the Z-score technique was used for the elimination of outliers. The Z-scores were computed automatically based on the differences between the values of the individual components and the mean of the population, which were subsequently divided by the standard deviation of the population. The pollutant that had the highest number of deleted data, about 2%, was CO. The pollutants PM_{2.5}, NO₂ and O₃ had less than 1% of the deleted data.

It is worth mentioning that the data of the stations, besides the outliers, present many failures, with long periods without measurements or with indicatives of errors, mainly for the stations of the South Region (SR).

6 stations monitor the pollutant PM_{2.5} (Figure 2a), which corresponds to 40% of stations of the Espírito Santo monitoring networks. No exceedance were identified in the analyzed period. The highest concentrations were observed in the MRGV stations (Vila Velha Ibes and Enseada do Suã), with higher medians.

For pollutant PM₁₀ (Figure 2b), only one station does not perform monitoring (Castelhanos station). For all stations, the PF and IG3 were exceeded (except for the Belo Horizonte station that presented values at the IG3 limit, not exceeding it). The highest quantities of exceedance were in the stations Laranjeiras (362 days with exceedances compared to SF, most in 2012) and Cariacica (55 days with exceedances compared to SF, most in 2008), both of MRGV.

The TSP is monitored in 13 stations (87%) (Figure 2c). There were no exceedances in the studied period. MRGV stations with the highest concentrations, with the highest median values, were Cariacica and Laranjeiras. From SR, Anchieta and Meaípe stations presented higher concentrations.

It should be noted here that, according to the survey conducted by Melo (2015) in the Metropolitan Region of Greater Vitória from 2011 to 2014, 90% of the interviewed reported being annoyed by air pollution due to particulate matter emissions.

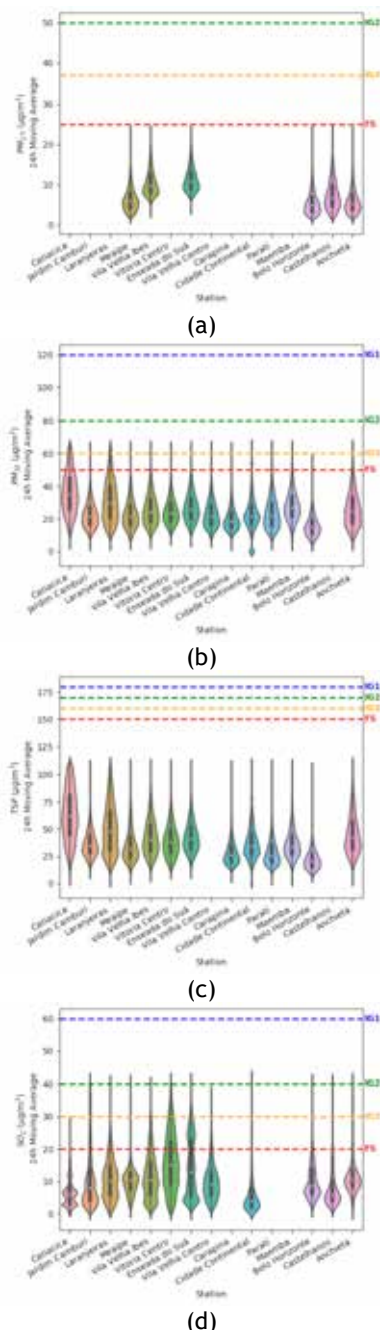


Figure 2. 24 hours average concentrations from 2008 to 2018, in $\mu\text{g m}^{-3}$. a) $\text{PM}_{2.5}$; b) PM_{10} ; c) TSP and d) SO_2 .

12 stations monitor SO_2 concentrations (Figure 2d). All of them has exceedances in the studied period. The stations with the highest number of exceedances were Vitória Centro (715 days with

exceedances compared to SF, most in 2010) and Enseada do Suá (876 days with exceedances compared to SF, most in 2010), in which the concentrations above the FS reached 75% of the data. All stations measured average concentrations above $40 \mu\text{g m}^{-3}$ (corresponding to IG2), with the exception of MRGV stations Cariacica and Vila Velha.

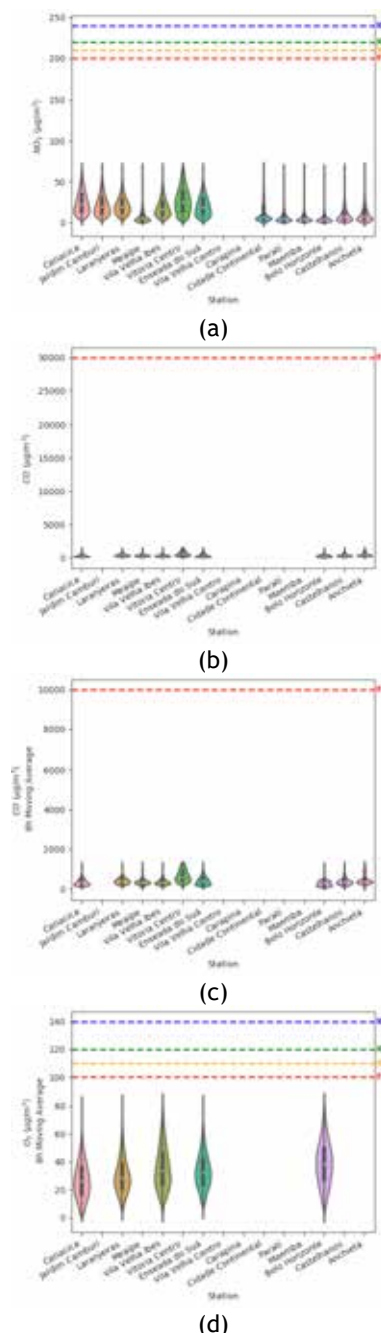


Figure 3. Average concentrations from 2008 to 2018, in $\mu\text{g m}^{-3}$. a) NO_2 (hourly average); b) CO (hourly average); c) CO (8 hours average) and d) O_3 (8 hours average).

13 stations measure NO₂ concentration (Figure 3a). In all of them, no exceedances of average concentrations were identified. The lowest median concentrations were identified for SR stations. But, for all stations the average concentrations are well below the limits established by legislation and WHO. The same is observed for the CO average concentrations (Figures 3b and 3c), in all 5 stations where there is monitoring of this pollutant. The distribution of the 1 and 8 hours average concentrations for CO in all stations was similar.

There were no exceedances for O₃ in all five stations where there is measuring of this pollutant. The highest mean concentrations for all stations pass 80 µg m⁻³ (coming close to the FS defined in the legislation). The highest median was for Belo Horizonte station, however, all stations presented a similar distribution of data.

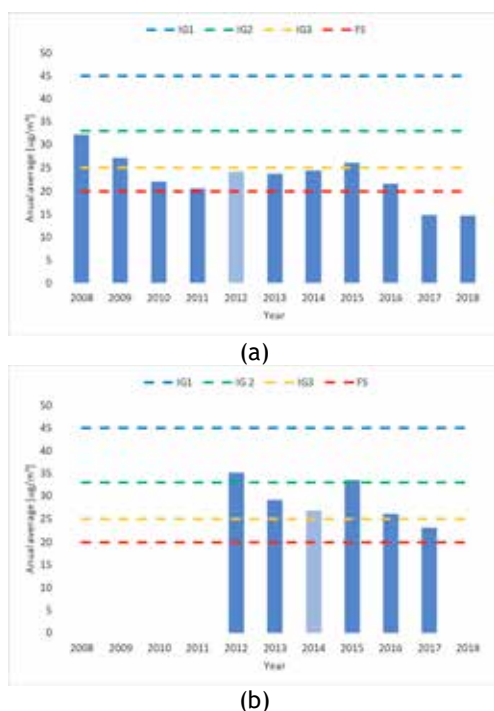


Figure 4. Annual average of PM₁₀ from 2008 to 2018: a) Jardim Camburi station; b) Maemba station. The bars in light blue indicate that annual average for those years is not representative.

According to the MRGV emissions inventory of 2015 (IEMA, 2019), approximately 26% of the PM₁₀ emitted in MRGV comes from the mining-metallurgical industries. Therefore, for completeness, annual average PM₁₀ data were analyzed for two stations: Jardim Camburi, near the ArcelorMittal Tubarão and Vale industrial park (MRGV), and the Maemba station, near the Samarco industrial park (SR) (Figure 1). The Figure 4 shows that the annual average exceeded the final standard (FS) in all years (2008 to 2018). The bars in light blue

indicate that annual average for those years is not representative, because it did not meet the validation criteria.

CONCLUSIONS

There is a lot of data failure (hours without measurements or with errors), especially in the South Region (SR) stations. In order to improve the quality of the data an anomaly detection technique was used (Z-score), however, a deeper analysis should be performed for the removal of these outliers.

The pollutants PM₁₀, TSP, SO₂ and NO₂ are monitored in a highest number of stations. On the other hand, there are few stations that monitor pollutants PM_{2.5} and O₃. Only pollutants PM₁₀ and SO₂ exceeded the standards established by legislation and the WHO for average concentrations of short exposure. As for the PM₁₀ annual averages (long exposure) for the stations presented (Jardim Camburi and Maemba), they exceeded the standards established in the legislation in all the period from 2008 to 2018.

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Compact air quality sensors in urban air quality monitoring - real life experiences and use cases in Helsinki, Finland

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Abstract: During the past 5 years the emergence of compact air quality sensors for ambient air monitoring has been rapid. Whilst the sensors are increasingly becoming available, the users and regulators are still learning about the different aspects on their use in practice, such as: a) how to benefit from their easy deployment and relatively low cost, b) how to optimally deploy and manage networks of such sensors and c) how to best interpret and make use of their data. In this presentation a brief overview of international standardisation activities for air quality sensor is presented as an introduction. After this we describe real life practical experiences from deploying and operating a pilot network of compact air quality sensors in Helsinki, Finland. For example the activities and learnings related to sensor colocation studies and sensor siting are presented. Finally we present a number of concrete examples of how the data from the network has been utilized in different aspects of air quality management work, such as community monitoring, pollution mitigation activities, studies for urban planning support and air quality modelling.

Keywords: compact sensors, urban air quality, air quality modelling.

INTRODUCTION

Outdoor ambient air pollution continues to be one of the most significant global health risks. In 2017 ambient air pollution contributed to 2.9 million deaths worldwide (HEI, 2019), and according to the World Health Organization air pollution represents the biggest environmental risk to people's health (WHO, 2016). Alarming the health burden is also heavy on children, of which 93% are exposed to fine particle levels higher than the WHO air quality guideline levels (WHO, 2018). Due to climate change effects on weather conditions also ozone levels and exposures have increased in recent years for example in the United States (American Lung Association, 2019). The health effects can also be converted into economic losses and account to 3.5 trillion USD for ambient PM_{2.5} exposure only (World Bank, 2016). These facts have underlined the need for new techniques and methodologies for local air quality management.

For the measurement of gaseous pollutants the amperometric electrochemical cell (EC) technology has traditionally been used in large quantities for industrial safety monitoring of toxic gases in ppm levels. During the past ten years this technology has taken leaps towards meaningful ppb level measurements making it feasible also for ambient

atmospheric air quality assessment (Baron, 2017; Alexandre, 2012)).

For the measurement of particulate matter the compact optical particle counter (OPC) technology has simultaneously been developed and applied to the measurement of respirable (PM₁₀) and fine (PM_{2.5}) particles (Jovasevic-Stojanovic, 2015; Holstius, 2014).

The performance and consequent practical usability of compact air quality sensors has been discussed in reports by for example World Meteorological Organisation WMO (WMO, 2018) and US EPA (EPA, 2018), which list a number of potential uses and applications for this technology. A related topic is performance testing and certification of the performance of compact sensors. In Europe the EU Air Quality Directive (EU, 2008) already acknowledges the use of "indicative" methods in air quality monitoring, and the preparation of the technical specification for sensor testing is under way (CEN, 2018). Similar efforts are under way in the US and China.

An obvious next step and a use case for compact air quality sensors is to construct dense networks of these sensors especially in urban areas where spatial variability of pollutant fields is high. Such networks have been piloted in a number of projects (Yi, 2015; Popoola, 2018).

METHODS

In this work results are presented from a pilot network consisting of 15 compact air quality sensors in Helsinki, Finland. Both practical experiences from designing and implementing the network and use cases for the network data in local air quality management will be shown and discussed.

The Helsinki Metropolitan Air Quality Testbed project (HAQT, 2019) is a joint project between local environmental and regional authorities, universities, research institutes, and industry to demonstrate a new paradigm in local air quality management. A network layout schematic is presented in Figure 1.



Figure 1. The HAQT network layout schematic

Data from the network was collected using data infrastructure developed in the Cityzer project (Cityzer, 2019), and utilized for local air quality management and high resolution air quality modelling using the ENFUSER model (ENFUSER, 2019). The model output was made available to the public on a public web site as well as displays on local metro and tramway. An example of the model output is presented in Figure 2.



Figure 2. Output from the ENFUSER high resolution model on a public web site

FINDINGS AND ARGUMENT

An example of the utilization of data from a compact sensor location for understanding and managing local air quality is from a residential street leading to a busy passenger port. Analysis of diurnal variations for a period of four months from a sensor installed on the street shows a specific pattern consisting of several brief peaks in NO_2 concentration superimposed on a normal daily traffic pattern (Figure 3.).

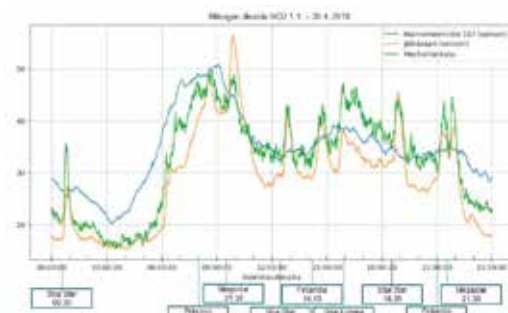


Figure 3. A four month diurnal average of NO_2 concentration in three sites at different distances from port.

On a closer analysis the peaks can each be associated with scheduled ferryboat arrivals and passenger traffic from offloading the ship. From this information the source, magnitude and temporal pattern of the nitrogen dioxide exposure from port operations can be determined.

Another example of sensor data utilization in local air quality management is related to PM_{10} particles and situational awareness on an hourly basis. One of the main air quality issues in Helsinki is spring time dust from studded winter tires. This is typically encountered in April-May, when the local authority is geared up for dust mitigation actions such as wetting/salting or cleaning the streets.

Figure 4. depicts a rare street dust event captured by the sensor network in January 2018, where the PM_{10} levels have been significant.

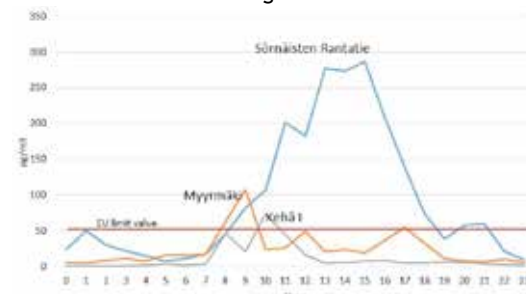


Figure 4. PM_{10} concentrations as identified by compact sensors in three network locations on 8th January, 2018.

These events may be local by nature, so a sensor network will provide a better coverage and detection efficiency for launching dust mitigation activities. Furthermore the sensor performance, although not reference level for accurate determination of concentrations, is well enough for spotting and reacting to this type of circumstances.

Support for high resolution air quality modelling is yet another benefit that a dense sensor network can provide especially in cities. In this example the cumulative 10 month data from a sensor location has been used to adjust model parameters in the FMI ENFUSER high resolution model (ENFUSER, 2019) to better take into account the wind shadowing effect of buildings on only one side of the street - a problem that typically requires heavy CFD processing to resolve.

Figure 5. depicts the comparison between modelled and observed wind dependent pollution roses for NO₂ in a one sided street canyon before and after the model adjustment. Once developed with data from one sensor site, the methodology can be applied to all locations with similar conditions in the modelled region to improve modelling throughout the area.

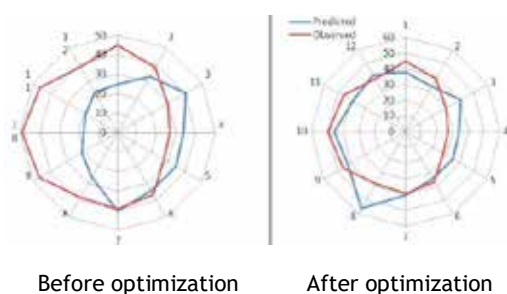


Figure 5. The pollution roses for nitrogen dioxide modelled and observed concentrations ($\mu\text{g}/\text{m}^3$) at the Sörnänen sensor site in the HAQT network

CONCLUSIONS

A new operational paradigm for air quality management based on a compact sensor network complementing a regulatory monitoring network and with a modern high resolution air quality model has been piloted. The feasibility of the network and data obtained from compact sensors for local air quality management and high resolution modelling has been demonstrated by a number of case examples.

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INTEGRATED AIR QUALITY ASSESSMENT WITH THE USE OF CHEMICAL AND BIOLOGICAL PARAMETERS

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Abstract: The Sinos River Basin (SRB), located in the state of Rio Grande do Sul, Brazil, has a high population, vehicular and industrial concentration and consequently pollutants that present characteristics such as toxicity and mutagenic and carcinogenic potential, such as polycyclic aromatic hydrocarbons (PAHs) and metals. The aims of this study were to evaluate the environmental quality in areas of the SRB, through an integrated assessment of the air quality associated with the quantification of PAHs and metals in the air gas fraction (GF) and in the *L. multiflorum* bioindicator. The sampling period was from June 2015 to May 2017. In the GF the most abundant PAHs were NAF, ACE, FLU, PIR and FLT. Regarding the metals in *L. multiflorum*, the presence of Al, Fe, Mn, Ba and Zn was observed in greater abundance. The integrated environmental assessments can contribute to the elaboration of a more in-depth environmental diagnosis, allowing a more complete characterization of the environmental scenario.

Keywords: Air pollution, Polycyclic aromatic hydrocarbons (PAHs), Metals, Integrated environmental, environmental diagnosis.

INTRODUCTION

In southern Brazil, in the state of Rio Grande do Sul, the Sinos River Basin (SRB) presents a high population concentration and is characterized by different typologies of stationary emission sources that contribute to declining air quality. Mobile sources are another important contribution to changing air quality in the region, as three major highways (BR116, BR448 and RS239) are located in the SRB, accounting for almost 40% of emissions from vehicles in the state (FEPAM, 2016; Costa; Petry; Droste, 2016).

The activities from these sources of pollution concentrate and release to the atmosphere a variety of pollutants, including polycyclic aromatic hydrocarbons (PAHs) and metals (Rodriguez *et al.*, 2010; Hassanvand *et al.*, 2015). Due to their toxicities and the serious health effects of their potential carcinogens and mutagens, and their increasing occurrence in the atmosphere, they make monitoring a priority task in programs to assess the risk to both health and the environment (Ares *et al.*, 2011).

Thus, the objective of this study was to evaluate the environmental quality in areas of SRB through an integrated assessment of the air quality associated with the quantification of PAHs and metals in the gas fraction (GF) and in the *L. multiflorum* bioindicator.

METHODS

Samplings were carried out in the municipalities of Canoas (CAN), São Leopoldo (SL) and Campo Bom (CB). The levels of urbanization in each of the municipalities are distinct, with CB being the least urbanized followed by SL and CAN (IBGE, 2016).

The definition of sampling sites followed the recommendations of ASTM D 5111 (ASTM, 2006). The sampling period was from June 2015 to May 2017.

The GF samples were collected in tubes of the XAD-2 adsorbent with the aid of a low volume active sampling pump model PAS500, brand Supelco, for 24 hours, monthly. Pump calibration was performed before and after collection and the volume of air sampled was calculated based on the average of the two flow values. The extraction of the PAHs from the adsorbent material occurred using toluene by constant stirring and the final extract was analyzed (Meincke, 2013).

The active biomonitoring method used the species *Lolium multiflorum* Lam. The seeds of *L. multiflorum* were sown in pots containing standardized substrate and later stored in a suitable place for the germination process. After 15 days, three pots containing the plants were exposed at each sampling site, remaining for 30 days (Klumpp; Ansel; Klumpp, 2004; Carminitti, 2008).

After sampling, the *L. multiflorum* of each vase was

divided into two equal parts for the determinations of metals and PAHs. For the metals, the leaves of the vegetable were cut into the substrate, washed with ultrapurified water and dried in a circulation oven for a period of four days. The extraction of metals (Al), barium (Ba), cadmium (Cd), copper (Cu), lead (Pb), chromium (Cr), iron (Fe), manganese (Mn), nickel (Ni) and zinc (Zn) was using microwave assisted digestion, according to protocol established in USEPA 3051 B (1994). The determination of the metals was carried out by flame atomic absorption spectrometry.

To quantify the PAHs, *L. multiflorum* was cut approximately 4 cm above the substrate, and a composition with the 3 pot plants from each sampled site was made. The extraction was in Soxhlet apparatus, using dichloromethane for 24 h (Teixeira *et al.*, 2011). The extracts were spin-evaporated, the wax and solvent phases were separated by centrifugation, and then the solvent phase was preconcentrated through the clean up procedure.

The PAHs studied were acenaphthylene (ACY), acenaphthene (ACE), anthracene (ANT), benzo[a]anthracene (BaA), benzo[a]pyrene (BaP), benzo[b]fluoranthene (BbF), benzo[k]fluoranthene (BkF), benzo[ghi]perylene (BP), chrysene (CHR), dibenzo[a,h]anthracene (DBA), phenanthrene (PHE), fluoranthene (FLT), fluorene (FLU), indene[1,2,3-cd]pyrene (INP), naphthalene (NAP) and pyrene (PYR). The gas chromatography coupled to mass spectrometry was used for the determination of the same.

RESULTS AND DISCUSSION

In the GF, were quantified the follow PAHs: NAP, ACY, ACE, FLU, PHE, ANT, FLT and PYR. The mean concentrations of PAHs that were detected above the LQ in the GF, according to Figure 1, ranged from 18.80 to 279.09 ng m⁻³ for CAN, 14.75 to 59.33 ng m⁻³ for SL and 18.28 to 48.11 ng m⁻³ for CB. Although FLT and PYR were identified in low samplings, their high average concentrations, which were almost as high as the average concentrations of other PAHs such as NAP, ACE and FLU, were detected with great frequency.

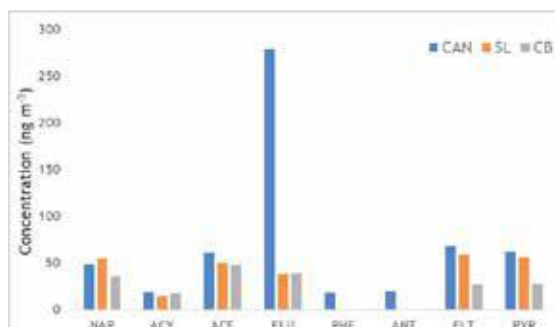


Figure 1. General mean of PAHs concentrations in GF.

In *L. multiflorum*, were quantified the PAHs NAP, ACY, ACE, FLU, PHE, ANT, FLT, PYR, BaA, CHR, BbF, BkF, BaP and BP. The mean concentrations of compounds that were detected above LQ (Figure 2) ranged from 0.72 to 22.67 ng g⁻¹ for CAN, 0.93 to 21.47 ng g⁻¹ for SL and 1.43 to 20.80 ng g⁻¹ for CB.

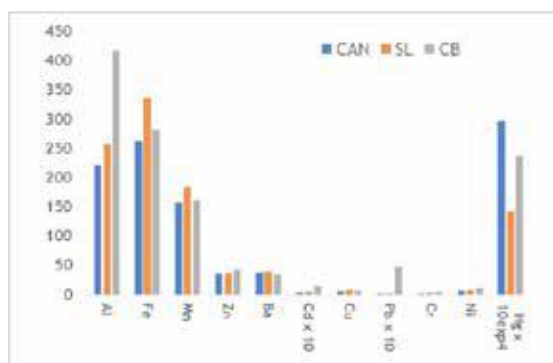
In relation to GF, in *L. multiflorum* it was possible to quantify a further six PAHs (BaA, CHR, BbF, BkF, BaP and BP), these being of intermediate to high molecular weight. In addition, other than GF, where the most polluted site was CAN, followed by SL and CB, in *L. multiflorum* a greater amount of pollutants was observed in SL, followed by CB and then CAN.



Figure 2. General mean of PAHs concentrations in *L. multiflorum*.

This profile may have occurred because, when associated with FG, PAHs do not move away from their emission sources, whereas when associated with PM, according to their size and the size of the particle to which they were adsorbed, can be transported over long distances, impacting places farther away from the main emission sources (Ravindra *et al.*, 2008), as well as CB, where a high concentration of these pollutants was not expected. In addition, another contributing factor for these differences in PAHs concentrations at the sampling points may be the exposure period of the two matrices, being that the FG samples were spotted for 24 hours on one day of each month and the *L. multiflorum* was exposed for a whole month.

Figure 3 shows the mean concentrations of metals accumulated in *L. multiflorum*. Significant mean concentrations of some elements such as Al (220.34 to 417.05 mg kg⁻¹), Fe (262.11 to 335.77 mg kg⁻¹) and Mn (156.75 to 183.58 mg kg⁻¹) and low or no detection of the other metals evaluated, were found.



Mean concentrations at the sampling points ranged from 0.003 mg kg⁻¹ (Pb) to 262.11 mg kg⁻¹ (Fe) in CAN, from 0.01 mg kg⁻¹ (Hg) to 335.77 mg kg⁻¹ (Fe) in SL and from 0.02 mg kg⁻¹ (Hg) to 417.05 mg kg⁻¹ (Al) in CB. The highest concentrations of metals predominated in the CB and SL points, followed by CAN.

As for PAHs in *L. multiflorum*, the possibility of higher concentrations of metals occurring at the CB sampling point, considered the least impacted by anthropogenic pollution, is probably related to the fact that metals are associated with PM in the atmosphere, they may be present in high concentrations away from their emission sources. The differences between the concentrations at the sampling points may also have been affected by the climatic and environmental conditions (Ng; Tan; Obbard, 2005).

CONCLUSIONS

Based on the results, it was verified that in the GF, the PAHs that presented higher concentrations were those of lower molecular weight, while in *L. multiflorum*, they were the ones with the highest molecular weight. In addition, in GF, the pollution by these compounds was higher in CAN, followed by SL and CB, already in *L. multiflorum*, SL showed higher pollution, followed by CB and then CAN.

Regarding the metals in *L. multiflorum*, the highest concentrations were detected in CB, SL and CAN, respectively.

These results evidenced the fact that probably higher molecular weight PAHs, as well as metals, are associated with particulate matter and not with GF.

In addition, these results highlight the importance of integrated environmental assessments, which contribute to the of a more detailed environmental diagnosis, allowing a more complete characterization of the Environmental scenario, since when used separately these pollutant quantification methodologies may not adequately reflect the ecosystem responses.

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HIPAE HELICOPTER-BORNE IN-SITU POLLUTION ASSESMENT EXPERIMENT: ALTERNATIVE PLATFORM FOR MEASURING CONTAMINANTS IN VERTICAL LAYERS

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Abstract:

The scientific initiative MAUI (Medellin Air qUality Initiative) brings several research projects and technological development, with the purpose to develop high-level scientific research dealing with problems on environment and sustainability, and impacts of air pollution in human health, agriculture, and ecosystems. In the mission named HIPAE (Helicopter In-situ Pollution Assessment Experiment), we developed a proof of a concept inside the aircraft from the Fuerza Aerea Colombiana (Colombian Air Force). In this first measuring campaign the metropolitan airspace of Aburrá Valley had been overflowed with the purpose to obtain input data to be used for the design of a Lidar 4D system, and to complement the TROPOMI (TROPOspheric Monitoring Instrument) satellite measurements for the assimilation of data with the LOTOS-EUROS model at high and low resolution, increasing the impact from local to national in terms of the capacity to forecast the transport of pollutants. In the aircraft, two kinds of PM particle counters were on board as well as two versions of the sensing platform named *Simple* for sensing meteorological variables (relative humidity, barometric pressure, temperature), altitude, geo-position and eight aerosol compounds (CO₂, H₂, NO₂, NH₃, C₂H₆OH, CH₄, C₄H₁₀, C₃H₈). Additionally, one experiment to test the capability of filters developed with nanomaterials to trap pollutants *in-situ* was validated. The analysis of the particulate matter captured on these filters offered valuable information on the composition, morphology, and chemistry via SEM-EDX (Scanning Electron Microscopy - Energy Dispersive X-ray spectroscopy) of the same material. From the data obtained it was possible to visualize high concentrations of aerosol compounds, especially compounds such as CO, NO₂, and CH₄, which shows the lowest concentration values in rural and forested areas compared with urban areas. The platform showed adequate behavior proving that the data delivered can be useful for modeling and monitoring the transport of pollutants.

Keywords: Helicopter-airborne, In-situ measurements, Air pollution, Chemical transport models, LOTOS-EUROS

INTRODUCTION

Airborne measurements deliver complementary *In-situ* information among the vast amount of measurements that is possible to perform of the atmosphere. The HIPAE was the proof of a measurement concept mission inside of the Colombian aircraft FAC4121 with the support of two groups of the Colombian Air Force (GRUCO/CETAD). This constitutes the first time that these kinds of measurements over Colombian territory were performed. Some references of airborne measuring campaigns come from the European project IAGOS (In-service Aircraft for a Global Observing System), a project that combines the expertise of two successful European research projects (Berkas et al, 2018), MOZAIC (Measurements of OZone, water vapor, CO, NO_x by in service Airbus aircraft) and CARIBIC (Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container) used in different scenarios to study the atmosphere composition. The work of Anthony et al., 2018 used Helicopter-borne electromagnetic measurements to derive a 3D resistivity model to study the permafrost carbon emission and compare a chemical transport model. In other case found in Shrivastava et al., 2019 the model prediction was assessed against aircraft measurements of organic aerosols. One example from North America is the

project from NOAA-ESRL named Tropospheric Aircraft Ozone Measurement Program focused on O₃ measurements (Boquet et al, 2015). Other project focus on aircraft measurements is named EMeRGe (Effect of Megacities on the transport and transformation of pollutants in the Regional and Global scales) which exploits the unique capabilities of the HALO (High Altitude and Long Range aircraft¹) to find out the impact of major population centers emissions on air pollution at local, regional and hemispheric scales by making dedicated airborne measurement campaigns, and coupled interpretation of modeling studies of short-live climate pollutants to compare ground measurements and aircraft measurement with the Sentinel 5 Precursor satellite instrument the TROPOMI (Griffing et al, 2019).

In the mission project HIPAE, we have the possibility of experimenting on topics such as nanomaterials, applied electromagnetism, atmospheric optics, environmental magnetism, biodiversity and conservation, mathematical modeling and meteorology. The data assessed constitute a valuable source necessary for data assimilation experiments with the LOTOS-EUROS to

¹ (<http://www.iup.unibremen.de/emerge/home/home.html>)

understand the dynamic of transport of contaminants in the region. The optical particle count and information retrieved from the 8 aerosol compounds of the Simple modules will enable valuable annotations to be used for the design of Lidar 4D systems; that will complement the TROPOMI ground and satellite measurements for the assimilation of data from the LOTOS-EUROS model at high and low resolution, increasing the impact from local to national in terms of the capacity to forecast the transport of pollutants.

METHODS

HIPAE combine 4 different experiments (Figure 1,a). The first consisted in a system of *in-situ* acquisition of pollutants from the environment using air pumps that sucked the material through the filters developed with nanofibers. The second was the test of a pair of remote sensing devices named Simple (Figure 1,c) which is a compact instrument that perform inertial (Inertial Measurement Unit, accelerometers), gasses and meteorological measurements as well as geolocation for spatially reference the other experiments. The third experiment was a particle monitor for use in high pollution urban environments (OPC-N3 (Figure 1,b)) and the fourth was the laser particle counter (AQ9600, Perfect Prime), both are capable to measure particulate matter (PM) 10, 2.5 and 1.0 size.

Nano-fibers and glass microfibers

Two types of filters were used: one manufactured at Universidad EAFIT based on PAN (PolyAcryloNitrile) nano-fibers, and the other, a commercial filter, based on glass microfibers. The nano-filters were manufactured by electrospinning technique, which consists of having a polymer solution in a syringe and, through the application of a high voltage, the polymer forms a small filament that travels to a collector system. To manufacture the nano-filters, a concentration of 12 wt% of PAN, a voltage of 8 [kV] and 120 mm needle-collector was used. The commercial filters evaluated were obtained from cassettes provided from Electron Microscopy Sciences (Hatfield, PA). The assembly of the filters was done using air cassettes and Air Sampling Pumps (GilAir 3, Gilian). The cassettes were connected by means of hoses to the pumps, which were programmed at a flow of 3 [L/min]. The filters were previously weighed in a microbalance (Mettler Toledo) and at the end of the test, they were again weighed to calculate the filtration efficiency of particulate material by gravimetry.

Simple modules

Simple module is a sensing device in CanSat (soda Can Satellite) form factor of a standard pico-satellite (0.1-1 [Kg] satellite classification by mass criterion) with a mass of 0.2 [Kg] and a volume of approximately 330 [mL]. It is a product of SimpleSpace Spin-off from Universidad EAFIT. This module contains the basic subsystems of a satellite:

EPS (Energy Power Supply), COMM (Communications Subsystems), CB&DH (Command On Board & Data Handling) and Payload Subsystem. The gasses that were measured and their respective concentration range in parts per million (ppm) were: Carbon monoxide CO (1 - 1000ppm), Nitrogen dioxide NO₂ (0.05 - 10ppm), Ethanol C₂H₅OH (10 - 500ppm), Hydrogen H₂ (1 - 1000ppm), Ammonia NH₃ (1 - 500ppm), Methane CH₄ (>1000ppm), Propane C₃H₈ (>1000ppm), Iso-butane C₄H₁₀ (>1000ppm).



Figure 1.a) Measurement instruments disposition: Particle counter OPC-N3, nanofilter experiments and GilAir 3 air pump disposition and Simple unit, b) Laser Particle counter, c) Simple CO&DH subsystem, d) Aircraft external load configuration.

Optical Counters

During the flight, the particulate material (PM_{2.5} and PM₁₀) was monitored using an optical particle counter (AQ9600, Perfect Prime). Different points of the Aburrá Valley were selected to perform the measurements of PM_{2.5} and PM₁₀. The frequency data measurement of the particle counter was of [1/50] Hz.

TROPOMI from Copernicus

Sentinel 5-Precursor (S5P) carried on board the instrument TROPOMI, a game changer instrument that closes the gap between the last instrument onboard satellites for atmospheric composition information retrieving, and the coming next-generation satellites focused on air quality measurements, in the future work the data collected from HIPAE is intended to be a way to compare and validate of this satellite instrument.

AIRBORNE FAC

The aircraft used was the Helicopter (Airborne) of the Fuerza Aerea Colombiana (Colombian Air Force), UH-60L FAC 4121, a utility helicopter made in the USA by Sikorsky Aircraft industries. The Capacity of 22.000 [lbs] under external load configuration, was used an external sling load of 60ft to avoid contamination from aircraft gas exhaust (Figure 1,d).

FINDINGS AND ARGUMENT

The HIPAE mission was held on the 12 of March 2019 from 9:30 AM to 12 PM at local time. Figure 2 shows the path where the helicopter flight above the city of Medellín. The designed pattern of the flight was at three different altitudes above ground: 600, 1200, and 1800 [ft]. The analysis of the Nanofibers and

Particle Matter chemistry and morphology via SEM/EDX validate the hypothesis that the designed nanomaterials capture more efficiently particulate matter than the commercial filters. Sigma substrates analysis offers valuable information on the composition, morphology, and chemistry via SEM EDX of the same material (Figure 4).

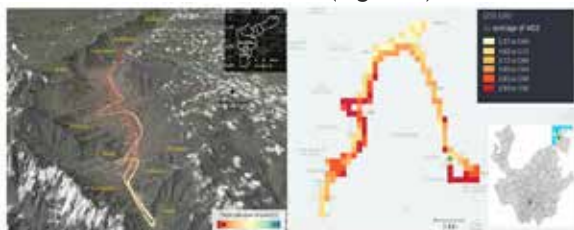


Figure 2. Map of the mission's flight route, departing from Air Force Base CACOM-5 and entering the Aburrá Valley through the municipality of Copacabana Northeast of Medellín. Land cover derived from pansharpened Landsat 8 image (2018-04-09). 3-D rendering based on JAXA's 30 m ALOS Global Digital the normalized concentration levels of NO₂.

Figure 3. shows the comparison of the altimeter from the Simple device against the PM counters. It is interesting here to notice how the concentration of the two fractions (PM₁₀ and PM_{2.5}) increase once the helicopter descended through the valley.

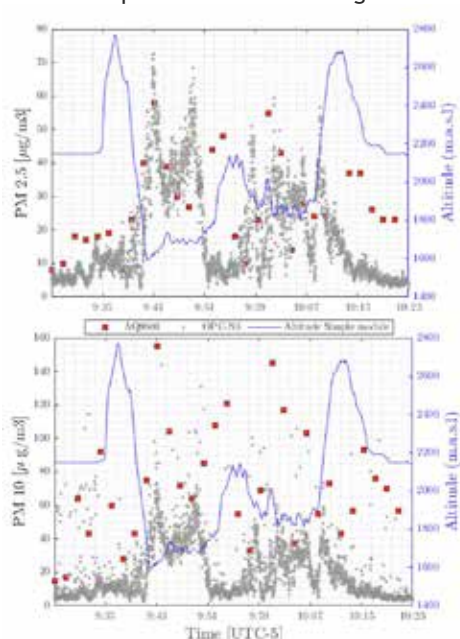


Figure 3. Aircraft altitude registered from the Simple unit vs PM_{2.5} and PM₁₀ concentrations measured by the particle counters

According to the gravimetric analysis (Figure 4.), the nano-filter managed to collect a particulate matter concentration of 96.2 [µg/m³]. while the commercial filter only collected 4.7 [µg/m³]. This shows the great efficiency of these nano-filters respect to commercial filters manufactured with microfibers, which makes them serious candidates for use in anti-pollution masks.

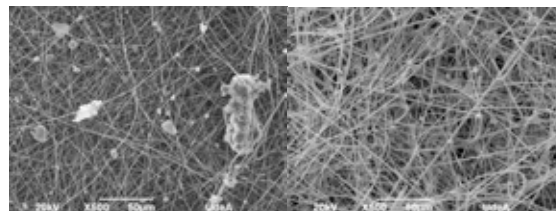


Figure 4. Images of collected particles on nano-fibers profiles

CONCLUSIONS

From *in-situ* aerosol measurements performed by HIPAE, a very clear picture about volume distribution of urban and rural pollutants in the Aburra Valley is retrieved with a good temporal and spatial resolution. A scanning Lidar will be designed taking into account this information to define the physical dimensions, its portability and, define the optimal channels to measure key particles i.e. wavelengths to detect, depolarization or Raman channels.

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ANALYSIS OF AIR POLLUTION DURING A TRUCKERS STRIKE IN BRAZIL, 2018

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Abstract: For a few days during May 2018, a Truckers Strike (TS) stopped several activities in Brazil. Due to the low circulation of vehicles during the TS, the event was an opportunity to evaluate the air quality. This study aims to investigate the behavior of air pollution before, during and after the TS, analyzing air pollutants datasets (O_3 , NO, NO_2 , NO_x and PM_{10}) of the city of Campinas, SP. It was used Principal Component Analysis (PCA), and Theil-Sen statistical analysis method. PCA indicated that May 23rd and May 24th were more affected by air pollution, while May 28th, May 29th and May 30th had lower concentrations in PM_{10} , NO_x and O_3 , during the TS. Trend analysis of PM_{10} and O_3 concentrations revealed that both decreasing day-on-day, an average rate of $2.21 \mu g \cdot m^{-3}$ per day and $5.35 \mu g \cdot m^{-3}$ per day, respectively. NO_x concentrations showed no significant trend. Finally, the results indicate that vehicular emissions are responsible for a great share of air pollution and investments in public policies for sustainable transportation are necessary.

Keywords: Principal Component Analysis, Trend analysis, Weekly cycle, Air pollution.

INTRODUCTION

High levels of air pollution emissions from vehicle traffic impact air quality in urban areas. Brazilian truckers went on a strike between 21 and 30 of May of 2018, with the most critical period between May 23rd and May 30th, that affected the population's routine, mainly because of the lack of fuel in most cities (BBC, 2018; G1, 2018). In these days there was a reduction of the fleet of vehicles in the streets, influenced, mainly, to the scarcity of fuel in gas stations. Thus, it is believed that the strike has directly influenced the air quality. The truck drivers' strike can be seen as an opportunity to evaluate the behavior of air pollutants. Thus, this study aims to evaluate the quality of the air during the period of that strike, in the city of Campinas, São Paulo, Brazil.

METHODS

Local and data characterization

The air quality data of this study was collected in Campinas, which is in São Paulo State, in Brazil. This city has an estimated population, in 2018, of 1,194,094 inhabitants and an area of 794.571 km^2 (IBGE, 2019). The air quality data analyzed was obtained online, at the QUALAR platform (QUALAR, 2019), which is a database of CETESB's (the Environmental Company of the State of São Paulo, Brazil) automatic station in Campinas, located in Taquaral Park (South latitude $22^\circ 52' 28''$ and West longitude $47^\circ 03' 3''$). The air pollution parameters analyzed, in $\mu g/m^3$, were nitrogen dioxide (NO_2), nitrogen monoxide (NO), nitrogen oxide (NO_x), ozone (O_3) and particulate matter with an aerodynamic diameter smaller than $10 \mu m$ (PM_{10})

concentrations. The meteorological data were temperature (temp) [$^\circ C$] and wind speed (WS) [m/s].

The truckers' strike was divided into three different periods in this study: Before the Truckers Strike (BTS), from 05/01/2018 to 05/22/2018; During the Truckers' Strike (DTS), from 05/23/2018 to 05/30/2018; and After the Truckers' Strike (ATS), from 06/01/2018 to 06/30/2018.

Statistical analysis

All analyses were performed utilizing the R software (R Core Team, 2018). In the first place, Principal Component Analysis (PCA) was performed with daily concentration pollutants and meteorological data, in order to identify days more polluted in DTS period. Varimax rotation was performed to reflect the better relationship between the PCs and the original variable (Dominick et al., 2012).

In the second place, the trend analysis for the daily average concentration of pollutants was performed using the TheilSen function of the Openair package (Carslaw and Ropkins, 2012; Carslaw, 2018) for BTS, DTS and ATS periods. The non-parametric method of Theil-Sen is used in nonnormal and heterocedastic data series, and even in presence of outliers (Ancelet et al., 2015; Font and Fuller, 2016; Cho et al., 2017; Mateus and Gioda, 2017). In this analysis, the data series were deseasonalized (Mateus and Gioda, 2017; Gama et al., 2018). Bootstrap sampling was used to get the 95% confidence intervals and p-values (Font and Fuller, 2016; Cho et al., 2017; Mateus and Gioda, 2017).

FINDINGS AND ARGUMENT

Figure 1 shows the biplot of PC (Principal Component) for first and second components obtained from PCA. PC1 and PC2 explained 96% of the total variance after varimax rotation. Notice that May 23rd and May 24th were separated from the other days (Fig. 1). This occurred because these days were the most affected by truckers strike when the population began to realize the effects of the first of strike and started looking for gas stations to fuel their cars (BBC, 2018; G1, 2018). In the others days, population avoided getting out by car, in order to save fuel, and consequently, in these days (especially May 28th, May 29th and May 30th), there was a low circulation of vehicles and reduction of air pollutants concentrations.

Table 1 shows trend estimate and 95% confidence interval for trend estimate for air pollutants (PM₁₀, O₃, NO_x, NO and NO₂), during BTS, DTS and ATS periods based in Theil-Sen method. Notice that only PM₁₀ and O₃ presented trends significant. PM₁₀ concentration presented negative trend in DTS period, as O₃ concentration.

Table 1. Trend estimate (before brackets) and 95% Confidence Interval (between brackets)

	Period	Estimate [95% CI]
PM ₁₀	BTS	-0.59 [-1.44, 0.56]
	DTS	-2.21 [-3.89, -1.61]**
	ATS	0.33 [-0.57, 1.31]
O ₃	BTS	-1.66 [-3.13, -0.50]**
	DTS	-5.35 [-8.89, -3.17]***
	ATS	0.32 [-0.02, 0.88]+
NO _x	BTS	0.37 [-0.49, 1.22]
	DTS	-0.55 [-2.47, 1.98]
	ATS	0.32 [-0.82, 1.26]
NO	BTS	0.14 [-0.07, 0.51]
	DTS	-0.08 [-0.39, 0.43]
	ATS	0.14 [-0.42, 0.67]
NO ₂	BTS	0.49 [-0.81, 1.18]
	DTS	-0.95 [-4.21, 2.80]
	ATS	0.36 [-0.52, 1.04]

$p < 0.001 = ***$; $p < 0.010 = **$; $p < 0.050 = *$; $p < 0.100 = +$.

Figures 2 and 3 details trend analysis based on the Theil-Sen method for the PM₁₀ and O₃ daily averages data, respectively, during DTS period. The trend was for PM₁₀ concentration to decrease, showing a reduction of 2.21 µg/m³ ($p < 0.010$) per day in this period (Figure 2). The PM₁₀ concentration average reduced from 36.85 µg/m³ to 16.00 µg/m³. The ozone concentration presented a reduction of 5.35 µg/m³ ($p < 0.001$) per day in DTS period, and the

concentration average reduced from 74.0 to 40.2 (Fig. 3).

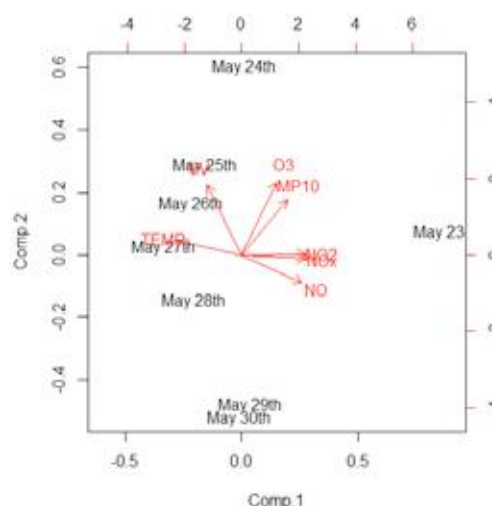


Figure 1. Biplot of days during DTS period

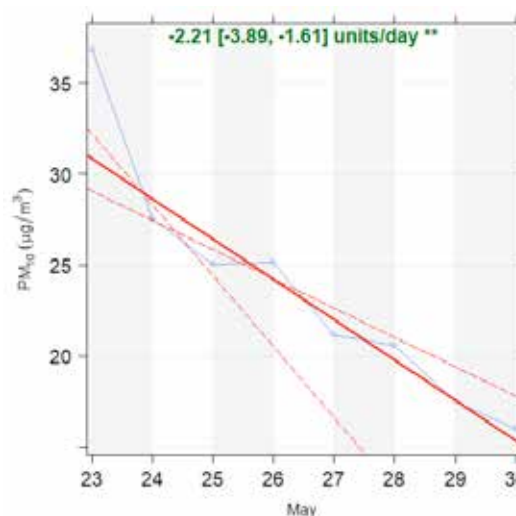


Figure 2. Trend analysis for PM₁₀ concentrations in DTS period

The PM₁₀ reduction (Fig. 2) may be explained to a reduction in the fleet of vehicles during this period. With the low circulation of vehicles in the streets, it was expected lower NO_x concentrations, but this behavior was not observed in the analyzed period (Table 1). In the other hand, occurred O₃ concentration reduction (Fig. 3). For ozone reduction, there are two possibilities, being a reduction in NO_x or in VOC (Volatile Organic Compounds) (Sillman, 1999). Reduction in NO_x will be effective if NO_x-sensitive chemistry predominates, and, reductions in VOC will be effective in reducing ozone if VOC-sensitive chemistry predominates (Sillman, 1999). So, we

believed that the atmosphere of Campinas had a reduction in VOC concentrations (ie, VOC-sensitive chemistry), and consequent, reduction in ozone concentration during DTS period. Unfortunately, the relation O_3 - NO_x -VOC are so complex, and lack of VOC concentration did not allow us to conclude this.

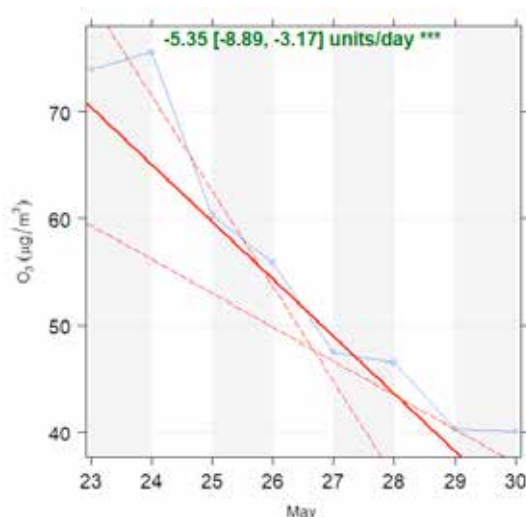


Figure 3. Trend analysis for O_3 concentrations in DTS period

CONCLUSIONS

The truckers strike was an opportunity to evaluate the air pollution caused by vehicles emissions. The DTS period, the results obtained in PCA indicated that May 23rd and May 24th were more affected because the population was searching for fuel in the gas station, increasing the traffic and the emissions. In the other hand, May 28th, May 29th and May 30th showed lower concentrations in PM_{10} , NO_x and O_3 , due to the reduction of the fleet of vehicles in the streets. The Theil-Sen analysis indicated on PM_{10} and O_3 concentrations decreasing day-on-day during DTS period. Finally, the results indicated that vehicular emissions are responsible for a great share of air pollution. Thus, investments in public policies for transportation are important to improve air quality.

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AEROSOL OPTICAL PROPERTIES IN THE ATMOSPHERE OF NATAL/BRAZIL BY AN AERONET NETWORK SUN-PHOTOMETER

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Abstract: The study of atmospheric aerosols contributes to the understanding of radiative forcing and global warming. In addition, aerosols may influence atmospheric chemistry, visibility, precipitation and human health. Since 2016, Natal (capital of Rio Grande do Norte, Brazil) has a Sun-photometer (CIMEL) of the RIMA-AERONET network that can identify the presence of biomass burning aerosols and desert dust from Africa. For this identification, it is aimed to characterize the optical properties of these aerosols present in the atmosphere of Natal. The level 1.5 data (version 3) provided by AERONET provide information on some aerosol characteristics such as Aerosol Optical Depth (AOD), Ångström Exponent (α), Single Scattering Albedo (SSA), Asymmetry Factor (g), Complex Refractive Index (N) and Volume Size Distribution (VSD). The analysis period was from August 2017 to March 2018. Aerosols were classified according to global climatologies and their optical properties were described. In addition, backward trajectories were modeled using the HYSPLIT model (version 4.8) to identify the predominant air masses origins. Aerosols present in the atmospheric column of Natal showed monthly mean AOD (500 nm) in the range of 0.10 to 0.40 (representing ~40%), monthly means of α (440-670 nm) between 0.6 and 0.8 (representing 30%), bimodal VSD with dominant coarse mode, SSA (440 nm) about 0.80, real part around 1.500, imaginary part ranging from 0.0125 to 0.0437 and g above 0.74. The classification showed mixed (60.4%), marine (30.7%) and mineral dust (8.9%) aerosols. The backward trajectories identified that, in about 51% of the cases, are originated from Africa.

Keywords: Sun-photometer, desert dust, AERONET, HYSPLIT.

INTRODUCTION

One of the main components of the atmosphere are the aerosols. These atmospheric components can influence radiative forcing, global climate, visibility (Seinfeld and Pandis, 2016), human health (Fuzzi et al., 2015), cloud formation (Koren et al., 2008), precipitation, air quality (Orza and Perrone, 2015) and carbon cycle, modifying the land and ocean uptake of anthropogenic CO₂ (IPCC, 2018). Among the atmospheric aerosols, there is desert dust, focus of this study, is an important component in biogeochemical cycles (Abouchami et al., 2013) and fertilization of the Amazon rainforest and oceans, contributing with micro- and macro-nutrients (Kaufman et al., 2005; Kumar et al., 2014).

A detailed knowledge of their optical and microphysical properties and distributions, is required in studies on the Earth's climate and its temporal variations (Hamill et al., 2016). Consequently, this reduces the uncertainties about the impact of aerosols on climate (IPCC, 2013). Thus, there is a need of monitoring and studying both anthropogenic and natural aerosols. Among other techniques, the monitoring and observation of atmospheric aerosols can be performed by remote sensing. In the last decades, remote sensing networks were created worldwide to improve our knowledge on aerosols such as Global Atmospheric

Watch (GAW), European Aerosol LIDAR Network (EARLINET), Latin American LIDAR Network (LALINET) and Aerosol Robotic Network (AERONET). The last one represents the efforts to reduce the uncertainties in the estimation of the radiative forcing of aerosols (Holben et al., 1998). Along the years, AERONET retrieving algorithm has evolved from the the Version 1 algorithm based on the inversion code of Dubovik and King (2000), to the Version 2 code developed by Holben et al. (2006), which improves the inversion products and, recently, the Version 3 algorithm, which provides quality cloud scanning and fully automatic instrument anomaly controls (Giles et al., 2019). In order to study atmospheric aerosols, Natal (capital of Rio Grande do Norte (RN) in Brazil) has joined AERONET through RIMA (Red Ibérica de Medida fotométrica de Aerosoles) in 2016. Natal is located in a region where the long-range transport of mineral dust from the African continent occurs under strong influence of the trade winds during December, January and February, when the Intertropical Convergence Zone (ITCZ) is positioned further South (Talbot et al., 1990; Swap et al. 1992; Landulfo et al., 2016).

Some studies prove the presence of desert dust from the African continent in the atmosphere of southern hemisphere regions, such as Ascension Island (Smirnov et al., 2002), Amazon basin (Ben-

Ami et al., 2010; Baars et al., 2011) and eastern Brazil (Wang et al., 2016). These findings were possible due to the characteristics of the aerosols observed. It is important to accurately characterize the optical properties of representative types of ambient aerosol particles to assess its impact on the Earth's energy budget and climate change (Rizzo et al., 2013). Indeed, the aerosol features are needed to incorporate aerosol particles into global climate models and evaluate climate forcing effects produced by aerosols of different origin and composition (Perrone et al., 2005).

This paper focuses on the characterization of optical properties of the aerosols present in the atmosphere of Natal, making it a pioneer study at the region due to the use of a CIMEL Sun-photometer to obtain the optical properties of aerosols.

The paper has the following structure: the measurement site, the Methods section, which the instrumentation and methodology are described, Findings and Argument section, where the results for each optical property of aerosols are presented and discussed and, finally, the conclusions.

METHODS

Measurement site

Natal is the capital of Rio Grande do Norte (RN), one of the states of the Northeastern Region of Brazil (NRB) (Figure 1). It is a coastal city ($05^{\circ}47'42''$ S, $35^{\circ}12'34''$ W, 30 m asl) and its climate is tropical with a rainy season that extends from Southern autumn to winter (Alvares et al., 2014), with months of May to July with the highest rainfall. According to the National Institute of Meteorology, the average temperature is 26°C , solar irradiation produces around 3,000 hours of sunshine per year and the average rainfall is 1465 mm/year.

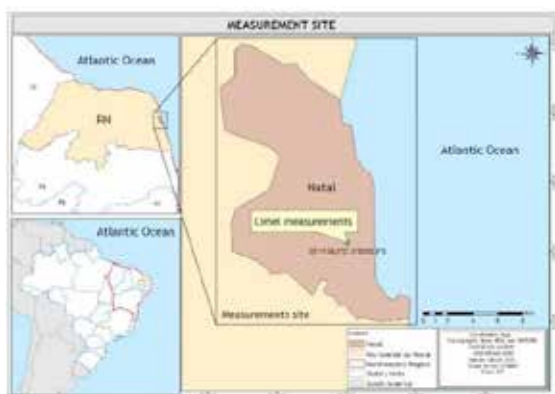


Figure 1. Location of the measurement site, Natal capital of Rio Grande do Norte (Brazil).

The ITCZ, Easterly Wave Disturbances (EWDs), Upper Tropospheric Cyclonic Vortex (UTCv) and sea-breeze circulation favor NRB precipitation (Cavalcanti et al., 2009) and, consequently, the precipitation in Natal. Another feature is that the evaporation of the sea forms a series of low clouds

(cumulus and fractocumulus types) throughout the year (Motta, 2004).

Instrumentation

The instrument used for the measurements was the CIMEL Sun-photometer, standard model CE-318. It provides retrievals from direct Sun measurements of aerosol and water vapor content (940 nm), in addition to aerosol properties from inversion of spectral sky radiances (Holben et al., 1998). The CIMEL makes two protocols of measurements, either direct Sun or sky ones, both within several programmed sequences. The direct Sun measurements are made in eight spectral bands channels (between 340 nm and 1020 nm, being 440, 670, 870 and 940 nm the standard channels) and sky measurements are performed at 440, 670, 870 and 1020 nm in two sky observation sequences (almucantar and principal plane) to acquire aureole and sky radiances observations through a large range of scattering angles from the Sun through a constant aerosol profile to retrieve size distribution, phase function, and aerosol optical thickness (AOT) (Holben et al., 1998). See Holben et al. (1998) for more details.

Calculation of aerosol optical properties

Optical Aerosol Depth (AOD), Ångström Coefficient (α), Single Scattering Albedo (SSA), Asymmetry Factor (g), Complex Refractive Index (N) and Volume Size Distribution (VSD) were the optical properties used in the characterization of the aerosols in the atmospheric column of Natal.

In this study, the wavelength 440 nm was used for the optical properties VSD, SSA, N and g with AOD (440 nm) values > 0.4 (Holben et al., 1998; Prats et al., 2008) and the wavelength 500 nm was used for the calculation of AOD, provided by AERONET with accuracy of ~ 0.015 (Fuzzi et al., 2015), because the mineral dust absorbs significantly in the wavelengths blue and UV, due to the iron oxide impurities (Sokolik et al., 1999; Kaufman et al., 2002; Olmo et al., 2008; Valenzuela et al., 2010), with 500 nm being a well-used standard wavelength (O'Neill et al., 2000; O'Neill et al., 2001; Smirnov et al., 2002). Moreover, the 440 nm was insufficient due to the large amount of negative values and the few days with data for AOD. Therefore, the range of 440-670 nm was used for the α calculation. Currently, Natal makes its measurements with a second CIMEL (#752) and provides data at level 1.5, since the instrument has not been calibrated and therefore does not provide the level of quality assured (2.0) yet.

In January 2016, Natal joined the RIMA-AERONET network (the city's first CIMEL and the second in the NRB). It was brought to the Federal University of Rio Grande do Norte through a partnership between the Institute of Energy and Nuclear Research (IPEN-São Paulo), the Research Group on Atmospheric Chemistry Modeling and Observation (GP-MOQA,

UFRN) and the University of Granada (Spain). An analysis of the temporal evolution was made for AOD and α from August 2017 to March 2018 and for other properties until January 2018. On other hand, the aerosol typing was based on the main climatologies developed in AERONET (Eck et al., 1999; Holben et al., 2001; Smirnov et al., 2002). The optical depth data were at level 1.5 of the new version of AERONET (Version 3) as well as aerosol inversion data (VSD, SSA, N and g). However, inversion data is only available until January 2018, because, in order to have a good inversion, the sky must be free of clouds at a low Sun angle. This resulted in the number of days with inversion data to decrease.

HYSPPLIT

The HYbrid Sigle-Particle Lagrangian Integrated Trajectory (HYSPPLIT) can be used to attribute a type of aerosol to the origin of the air masses. According to (Toledano et al., 2009), when analyzing the back trajectories, the main assumption is that there is a link between the origin of the air mass and/or path and the aerosol observations at the receiving site. The back trajectories were calculated within 10 days and for each day that had available level 1.5 AERONET observations of (V 3), totaling 102 days with modeling and five back trajectories per day (500, 1500, 3000, 4000 and 6000 m agl). It was possible, then, to know how many back trajectories came from the African continent and from other origins.

FINDINGS AND ARGUMENT

Figure 2 shows the monthly average of AOD (500 nm) for almost every month and these values are close to those found by Smirnov et al. (2002) for coastal areas and continental seas (AOD (500 nm) > 0.12). February 2018 (~0.20) was the unique month whose average was above 0.15, probably due to the transport of dust from the African continent most present this month. AOD on the Natal atmosphere was mostly between 0.05 to 0.15 (~70%) and only 20% of the values are between 0.15 and 0.20. These values are attributed to the presence of marine aerosols (Knobelspiesse et al., 2004) and values between 0.20 and 0.50 to the desert aerosols (Holben et al., 2001). However, AOD (500 nm) < 0.20 can also be attributed to biomass-burning aerosols (Sena and Artaxo, 2015).

Figure 3 shows a subtle seasonality for the Southern hemisphere summer (averages between 0.6 and 0.8 from December 2017 to March 2018), the lowest monthly average was in September 2017 (0.38) and the maximum in March 2018 (0.76).

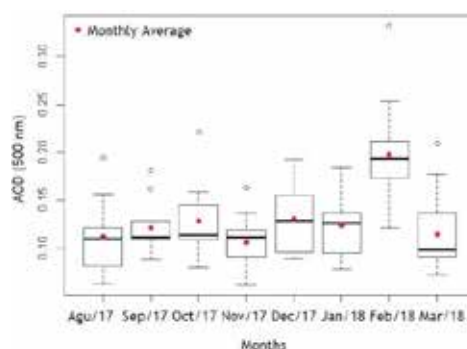


Figure 2. Boxplot of monthly AOD (500 nm) from August 2017 to March 2018. The base of the boxes represents the first quartile, the center lines represents the median, the top of the boxes represents the third quartile and the red points the monthly average.

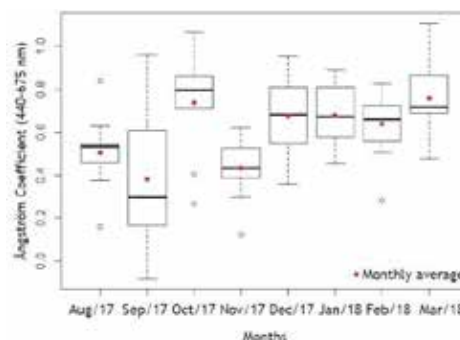


Figure 3. Boxplot of Ångström Coefficient (440-675 nm) from August 2017 to March 2018.

The high variability in September may be related to the contribution of biomass burning aerosol from the burning of sugarcane in the regions near Natal, but also may be related to low number of datapoints. Close values (around 0.6-0.7) were found in Cuiabá (Brazil) (Holben et al., 2001). More than 60% of the α (440-670 nm) values were between 0.4 and 0.8 and more than 20% were between 0.8 and 1.0. The results over Natal resemble those of Smirnov et al. (2002) for Ascension Island with dominant values typically below 1.0, under scenarios with predominance of coarse particles.

Figure 4 shows that the aerosol over Natal is bimodal with a dominant volume in coarse mode for the months of December 2017 ($0.036 \mu\text{m}^3/\mu\text{m}^2$), September 2017 ($0.034 \mu\text{m}^3/\mu\text{m}^2$) and November 2017 ($0.028 \mu\text{m}^3/\mu\text{m}^2$) with the largest distributions. The fine mode stands out in the months of December 2017 (0.008), October 2017 ($0.007 \mu\text{m}^3/\mu\text{m}^2$) and January 2018 ($0.005 \mu\text{m}^3/\mu\text{m}^2$).

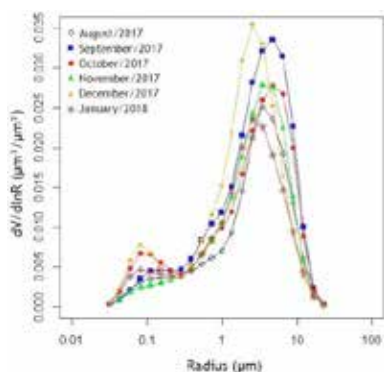


Figure 4. Monthly average of the Volume Size Distribution ($\mu\text{m}^3/\mu\text{m}^2$) from August 2017 to January 2018.

The fine mode is probably related to fuel-burning or biomass-burning aerosols. However, there was no discernible relationship between the aerosols of fine mode and the months under review, which leads to reinforcing the need for a more accurate statistic. The radius that separates coarse mode and fine mode is $0.33 \mu\text{m}$ which was a value close to those found by Smirnov et al. (2002) on five islands around the globe ($0.40 \mu\text{m}$) and by Taylor et al. (2015) for the dust cluster ($0.35 \mu\text{m}$).

Aerosol microphysical properties

Table 1 reports the aerosol microphysical properties found in this period. SSA (440 nm) remains around 0.80 for the period of observations. This result is close to what was found by Dubovik et al. (2002) for biomass burning in African Savannah (Zambia - 0.88 ± 0.015) and by Prats et al. (2008) for a range of 0.82 to 0.97 in characteristic of desert dust (Huelva - Spain).

The real part of N remains around 1.500 with the lowest value in December 2017 (1.444 ± 0.05) and the imaginary part is very variable over the measurement period, with a monthly maximum in August 2017 (0.0437 ± 0.03) and the minimum in September 2017 (0.0125 ± 0.01). The observations of the real and imaginary part of complex refractive index are similar to those found by Dubovik et al. (2002) for mixed and industrial urban aerosol in Greenbelt (USA) (1.47 ± 0.03 ; 0.014 ± 0.0006), for biomass burning in the Brazilian Cerrado (1.52 ± 0.01 ; 0.015 ± 0.004) and the African Savannah (Zambia) (1.51 ± 0.01 ; 0.021 ± 0.004), for desert dust and oceanic aerosol in Bahrian (Persian Gulf), Solar (Saudi Arabia) and Cape Verde (1.55 ± 0.03 , 1.56 ± 0.03 and 1.48 ± 0.05 respectively). However, Perrone et al. (2005) classified the days with values of 1.46 ± 0.09 and 1.50 ± 0.07 (real part) as urban industrial aerosols in Lecce (Italy).

The asymmetry factor (g) also did not change significantly over the period, with values above 0.74, whose maximum occurs in November 2017 (0.78 ± 0.02) and the lowest occurs in October 2017

(0.75 ± 0.06). These values agree with those of Dubovik et al. (2002) for desert dust and oceanic aerosol found in Cape Verde and Lanai, Hawaii, (0.73 ± 0.04 , 0.75 ± 0.04 , respectively), as well as Taylor et al. (2015) who found values of $g = 0.74$ for mineral dust.

Aerosol typing

The aerosol classification in Natal atmosphere (Figure 5) shows a mixture aerosol between mineral dust and marine aerosol (60.4%), marine aerosol (30.7%) and mineral dust (8.9%) based on climatologies of Holben et al. (2001) and Smirnov et al. (2002).

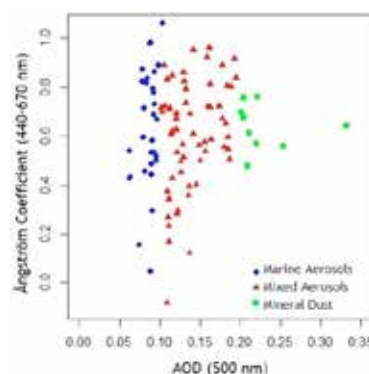


Figure 5. Scatter plot of daily averages of AOD (500 nm) vs. Ångström Coefficient (440-675 nm). The colors indicate the aerosol type.

The high percentage of mixed aerosols is due to the difficulty in distinguishing sea salt aerosols from those of dust, since both are associated with low Ångström exponents (Holben et al., 2001), having characteristics of both. The predominance of aerosols classified as mineral dust occurred in February 2018, possibly due to the ITCZ most displaced to the South in this period. A summary of the classification is shown in Table 2. These data are compatible with those used by Knobelspiesse et al. (2004) for AOD (50 nm) in North America (dust: 0.17, marine: 0.08) for the Pacific (maritime: 0.09) and for South Asia whose values for marine aerosol were in the range of mixed aerosol (0.14).

Origin of air masses

The Figure 6 shows the number of modeled back trajectories arriving from the African continent in Natal (261) and the quantity arriving from other regions (249). The amount of trajectories coming from the African continent is around 1500 to 4000 m above ground level, with the majority at 3000 m (70), validating the results found in previous studies (Swap et al., 1992; Holben et al. 2001; Toledano et al., 2009; Bem-Ami et al., 2010; Kumar et al., 2014; Orza and Perrone, 2015; Landulfo et al., 2016; Wang et al., 2016) for transatlantic air masses at 3000 m high.

Table 1. Monthly average and standard deviation for Single Scattering Albedo (SSA), Complex Refractive Index (real part and imaginary part) and Asymmetry Factor (g) at 440 nm from August 2017 to January 2018.

Aerosol property (440 nm)	August 2017	September 2017	October 2017	November 2017	December 2017	January 2018
SSA	0.75 ±0.10	0.86 ±0.05	0.81 ±0.05	0.81 ±0.08	0.83 ±0.10	0.77 ±0.07
Real part (N)	1.519 ±0.07	1.517 ±0.04	1.501 ±0.04	1.506 ±0.01	1.444 ±0.05	1.512 ±0.08
Imaginary part (N)	0.0437 ±0.03	0.0125 ±0.01	0.0231 ±0.01	0.0152 ±0.009	0.0153 ±0.02	0.0315 ±0.03
g	0.77 ±0.04	0.77 ±0.04	0.75 ±0.04	0.78 ±0.02	0.76 ±0.02	0.75 ±0.06

Reference: Oliveira (2019).

Table 2. Mean AOD (500 nm), standard deviation of AOD (σ_{AOD}), mean of α (440-670 nm), standard deviation of α (σ_α) for their respective classifications.

AOD (500 nm)	σ_{AOD} (500 nm)	α (440-670 nm)	σ_α (440-670 nm)	Classification
0.09	0.01	0.65	0.25	Marine Aerosol
0.14	0.03	0.61	0.22	Mixed Aerosol
0.23	0.04	0.64	0.09	Mineral Dust

Reference: Oliveira (2019)

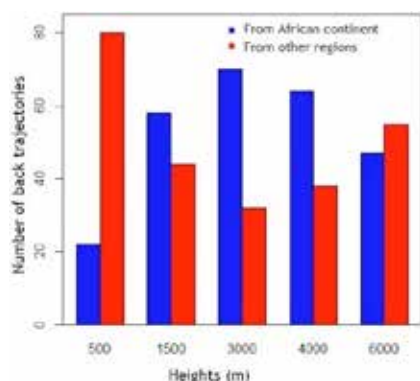


Figure 6. Bar graph for the back trajectories from Africa (blue color) and from other directions (red color) in five different height levels from August 2017 to March 2018.

CONCLUSIONS

For the first time it was possible to characterize the aerosol optical and microphysical properties present in the atmospheric column of Natal by a CIMEL Sun-photometer of AERONET.

The AOD, α , VSD, SSA, N and g showed predominant characteristics of desert dust and marine aerosols. Thus, the coarse mode was predominant, with a radius of 0.33 μm between modes. The classification of aerosols confirmed the predominance indicated by the optical properties (marine, dust and mixed aerosols), having February 2018 the highest number of days classified as mineral dust. In addition, the back trajectory modeling by HYSPLIT identified that half of them originated in the African continent (51%), especially at 3000 m agl (70 trajectories).

This study is the initial step to (i) generate a future climatology of aerosols properties for Natal; (ii) new studies with other aerosol properties (phase function, geometric radius, effective radius and others); (iii) future studies linking optical properties

and chemical composition of aerosols; and (iv) other studies relating local sources of aerosols and the characteristics provided by the CIMEL Sun-photometer.

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BULK ATMOSPHERIC DEPOSITION AND THE INFLUENCE OF AIR MASSES TRAJECTORIES IN SOUTHERN REGION OF MINAS GERAIS, BRAZIL

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Abstract: The aim of this study is to evaluate the atmospheric deposition chemical composition and pollutants long-range transport in the southern region of Minas Gerais, Brazil. The monitoring system consists of a bulk deposition collector, exposed to open air for collection of rainwater (wet deposition) and particulate matter (dry deposition) in defined periods. After the collection, the samples were analyzed in laboratory through physical-chemical methods and ion chromatography analysis. Deposition monitoring started on 10/10/2017. For this work, samples were analyzed until the month of April, 2018 (19 samples). As a result it was observed that the estimated atmospheric deposition flux for 12 months obeyed the following order $\text{Ca}^{2+} > \text{NO}_3^- > \text{C}_2\text{H}_3\text{O}_2^- > \text{NH}_4^+ > \text{SO}_4^{2-} > \text{CHO}_2^- > \text{Cl}^- > \text{Mg}^{2+} > \text{Na}^+ > \text{K}^+ > \text{C}_2\text{O}_4^{2-} > \text{H}^+$, with calcium being the highest flow chemical species ($18.3 \text{ kg ha}^{-1} \text{ ano}^{-1} \sim 40\%$). Inorganic nitrogen compounds (NO_3^- and NH_4^+) and sulfur (SO_4^{2-}) represented 23% and 8%, respectively, and the N and S contribution was 4.57 and $1.20 \text{ kg ha}^{-1} \text{ ano}^{-1}$. The back-trajectory analyzes indicated a significant fraction of the air masses influencing the samples in November, March and April were of local origin (16.7%, 60% and 26.6%, respectively). In October more than 70 % of the air masses came from the south of the Atlantic Ocean and in December, about 80% came from the north and northeast quadrant of the state.

Keywords: Bulk deposition, Back-trajectory analysis, Sources apportionment, Ionic composition, Monitoring.

INTRODUCTION

Air pollution is closely related to human activities emissions and to meteorological factors, which influence the emissions rate from local sources and photochemical reactions in the atmosphere (AVILA; ALARCO, 1999; CHENG *et al.*, 2019; PIHL *et al.*, 2016). In addition, such air pollution processes are considerably modified by long-range transport of the air masses, enriching the complex interaction between air pollutants and their environmental fate (MAHAPATRA *et al.*, 2018). Such atmospheric pollutants are subjected to atmospheric recirculation processes and may be redistributed through atmospheric deposition (TOSITTI *et al.*, 2018).

Regarding the deposition processes, which may occur through dry-only, wet-only and bulk deposition. Bulk deposition refers to the scavenging process of pollutants by both wet and dry deposition. Wet deposition results from cloud droplets nucleation and precipitation as rainwater, haze, graupel or fog. In addition, dry deposition refers to aerosol dry-scavenging through complex physical-chemical mechanisms such as gravitational settling, turbulence driven collision and adhesion.

Furthermore, atmospheric deposition exerts a key role in terrestrial and aquatic biogeochemical processes, since it is a main cycling pathway for both primary chemical species (Cl^- , Na^+ , K^+ , Mg^{2+} , Ca^{2+}), derived directly from aerosols, as well as secondary chemical species (SO_4^{2-} , NO_3^- , NH_4^+),

which originate from gaseous emissions and subsequent reactions into the atmosphere (ARAUJO *et al.*, 2015; DE SOUZA *et al.*, 2006; XING *et al.*, 2017). These nutrients and pollutants may be carried out into environmental compartments causing significant impacts, such as eutrophication and soil acidity due to atmospheric deposition (DUAN *et al.*, 2016; ZHAN *et al.*, 2017).

Therefore, considering bulk atmospheric deposition as main mechanism of removal and atmospheric pollutants inputs, highlight that studies on this theme are practically absent in southern region of Minas Gerais. In this context, the aim of this study is to evaluate the atmospheric deposition chemical composition and pollutants long-range transport.

METHODS

The atmospheric deposition monitoring began on October 2017 in the southern region of Minas Gerais, Brazil. Both bulk and dry deposition were collected of a high-density polyethylene bucket (NALGON) of 10L that was installed in the Universidade Federal de Lavras (UFLA) campus. The sampler was placed inside a PVC structure attached in a wood stand with 1,50 meters above ground level, also covered with a nylon screen to prevent litter fall. The sampling period was of 7 days in general, however specific shorter sampling times were recorded for intense rainfall events. After sampling *in situ*, potentiometric and conductimetric measurements were performed in an atmospheric deposition sample aliquot. Also,

another sample aliquot was filtered and stored in rinsed polyethylene bottles and kept at -18°C prior ion chromatography (IC) analysis. The species quantified by IC were Ca^{2+} , NO_3^- , $\text{C}_2\text{H}_3\text{O}_2^-$, NH_4^+ , SO_4^{2-} , HCO_2^- , Cl^- , Mg^{2+} , Na^+ , K^+ , $\text{C}_2\text{O}_4^{2-}$ with detection limit of $1\mu\text{molL}^{-1}$.

FINDINGS AND ARGUMENT

In this study, bulk atmospheric deposition 19 samples were evaluated, which 4 are referred to dry deposition (samples 1, 16, 18 and 19) and 15 are bulk atmospheric deposition (wet and dry), in the period between October 2017 and April 2018. In order to analyze the atmospheric inputs of the major ionic compounds, table 1 was constructed.

Table 1. Bulk atmospheric deposition fluxes segregated per month, in kg ha^{-1} from October 2017 to April 2018

Month	H^+	Na^+	NH_4^+	K^+	Mg^{2+}	Ca^{2+}	$\text{C}_2\text{H}_3\text{O}_2^-$	CHO_2^-	Cl^-	NO_3^-	SO_4^{2-}	$\text{C}_2\text{O}_4^{2-}$
out/17	0.0006	0.1210	0.3035	0.0781	0.0788	1.5107	0.2204	0.8003	0.1303	0.7465	0.2616	0.1052
nov/17	0.0005	0.1412	0.5812	0.1462	0.1991	3.4297	0.1504	0.1614	0.2408	0.8383	0.4853	0.1735
dez/17	0.0008	0.0964	0.4909	0.0632	0.1401	1.1793	1.3963	0.0048	0.1706	0.6424	0.4880	0.0087
mar/18	0.0002	0.0429	0.2587	0.0925	0.0904	1.3008	0.2850	0.1041	0.1088	0.4651	0.2336	0.0470
abr/18	0.0001	0.0403	0.0063	0.0322	0.0111	0.2093	0.0080	0.0015	0.0787	0.0890	0.0355	0.0033
Total	0.0022	0.4417	1.6404	0.4124	0.5193	7.6297	2.0601	1.0721	0.7293	2.7814	1.5040	0.3377
Total Annual	0.0052	1.0600	3.9370	0.9898	1.2464	18.3114	4.9443	2.5731	1.7503	6.6752	3.6095	0.8105

For all months calcium had the highest deposition, with maximum in November (3.4 kg ha^{-1}), however in December the acetate surpassed calcium deposition ($29.8\% \sim 1.4 \text{ kg ha}^{-1}$). The ammonium ion kept its relative contribution constant for all months, except for April, in which its deposition flux was minimal (0.006 kg ha^{-1}). Nitrate and sulphate also showed constant relative contribution over the evaluated period, with 15% and 8% respectively. The chloride and sodium species had a low relative contribution over the months, around 3.5% and 2%, respectively. However, in April, there was a significant increase in the deposition of these ions, about 4 times more than the previous months, with chloride representing 15.3% and sodium 7.8%. From the data obtained from to five months evaluated, the deposition was estimated for the period of 12 months, whose species abundance obeyed the following order: $\text{Ca}^{2+} > \text{NO}_3^- > \text{C}_2\text{H}_3\text{O}_2^- > \text{NH}_4^+ > \text{SO}_4^{2-} > \text{CHO}_2^- > \text{Cl}^- > \text{Mg}^{2+} > \text{Na}^+ > \text{K}^+ > \text{C}_2\text{O}_4^{2-} > \text{H}^+$. Highlighting that the inorganic nitrogen compounds (NO_3^- , NH_4^+) contributed 23% and the sulfur compounds (SO_4^{2-}) 8%. During the five months of collection, the accumulated nitrate flux (2.78 kg ha^{-1}) was 1.7 times higher than ammonium (1.64 kg ha^{-1}). The flux of these two species together was about 3 times greater than the accumulated sulfate flux. In addition, the cumulative flux for the nitrogen compounds (N- NH_4^+ , N- NO_3^-) and sulfur (S- SO_4^{2-}) were calculated for one-year values were 4.57 and 1.20.

In order to better understand the profile observed in table 1, air mass back-trajectories were constructed for the period evaluated. Also, cluster analyzes were also performed as a way to verify the contribution of air masses (figure 1).

In October, figure 3 (a), air masses predominated in the northeast and northwest quadrant of the

Minas Gerais state, where 70% of the trajectories came from the South Atlantic Ocean. For the month of November figure 3 (b), the influence of frontal systems at the sampling point were observed, showing contribution from the countryside of the state (23.3%), besides a trajectory that indicates local influence (16.7%). In In December (Figure 3 (c)) there are similarities with the month of October, which reflects similar depositions in both periods. However, the month of December had greater participation of organic species in the deposition, noting that the air masses were predominantly from the north and northeast of the state. March presented a pattern similar to that observed in November, but with a lower influence of oceanic masses, figure 3 (d). In addition, we can indicate that in that month about 60% of the days of the month the air masses were local, with little contribution of transport of long distances. The most atypical pattern can be seen in figure 3 (e), April, when there was greater influence of air masses east of the sampling point, and a significant fraction of local contribution (26.6%).

CONCLUSIONS

In this study, bulk deposition chemical composition monitoring at Lavras provided valuable information on air quality and apportion pollution sources.

As a result, it was observed that the estimated atmospheric deposition flux for 12 months followed the order of $\text{Ca}^{2+} > \text{NO}_3^- > \text{C}_2\text{H}_3\text{O}_2^- > \text{NH}_4^+ > \text{SO}_4^{2-} > \text{CHO}_2^- > \text{Cl}^- > \text{Mg}^{2+} > \text{Na}^+ > \text{K}^+ > \text{C}_2\text{O}_4^{2-} > \text{H}^+$, with calcium leading the chemical species deposition ($18.3 \text{ kg ha}^{-1}\text{ano}^{-1} \sim 40\%$). The relative contribution of N and S inputs presented small variability over the period evaluated and their annual deposition estimates were 4.57 and $1.20 \text{ kg ha}^{-1}\text{year}^{-1}$. In addition, a significant fraction of the air masses influencing the samples in November, March and

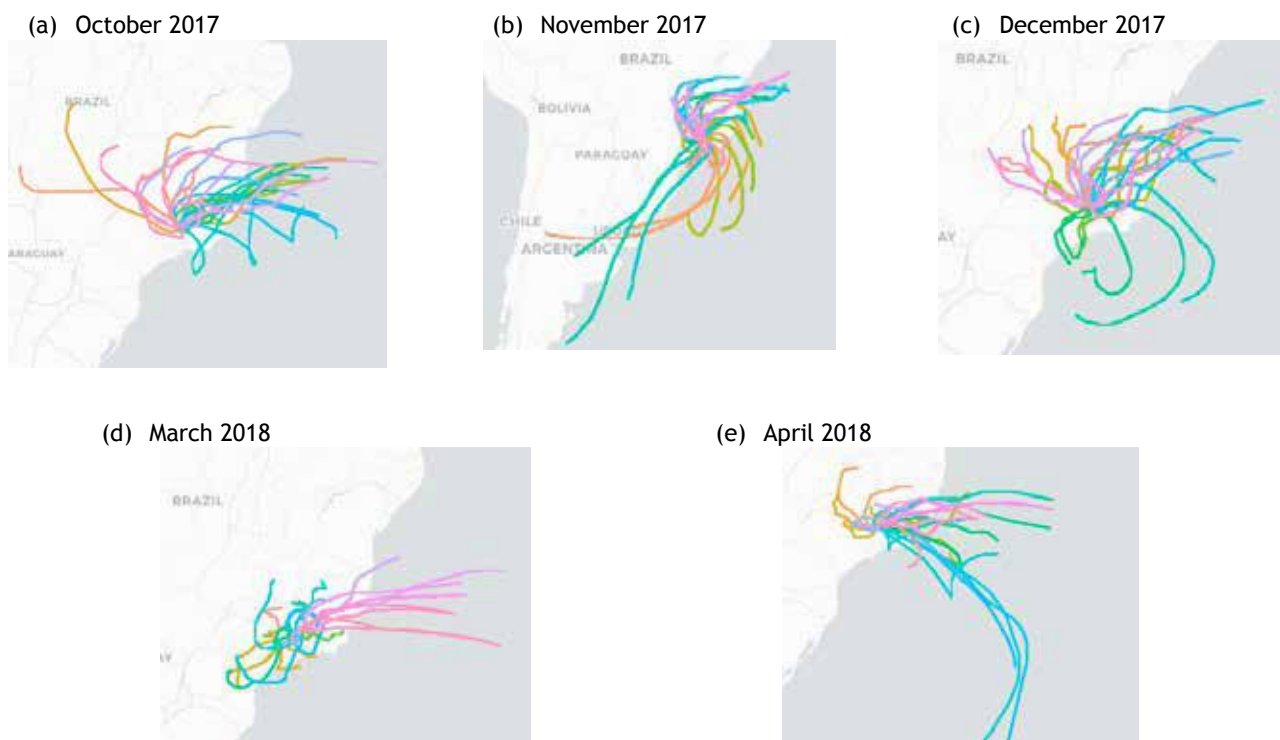


Figura 1. Back-trajectories of air masses from the sampling point (-21.23, -44.97) with a duration of 72 hours for the months: a) October 2017, b) November 2017, c) December 2017, d) March 2018 e) April 2018.

April were of local origin (16.7%, 60% and 26.6%, respectively). With respect to October, more than 70% of the air masses came from the south of the Atlantic Ocean and in December, about 80% came from the north and northeast quadrant of the state.

Therefore, attention must be given to the role of atmospheric deposition of the majority species, mainly N and S. There is also a need to mitigate the emission of pollutants such as NO_x and SO_x in the region, since the main air masses that influenced the samples are of short or medium range and the contribution of these compounds can cause impacts on the environment such as eutrophication and acidification of soils.

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Atmospheric Aerosol Behavior Study in Natal City through LIDAR Backscatter Profiles and Random Errors Propagation Analysis by Monte Carlo Method

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Abstract: The physical and optical interaction of aerosols in atmospheric processes are complex and have high temporal and spatial variability, representing uncertainties as, for example, the aerosol particles influence on the atmosphere energetic balance. The Duster is a LIDAR system (Light Detection and Ranging) located in Natal / RN, capable of working with four detection channels (355 nm, 532 nm p, 532 nm s and 1064 nm). Duster sends pulses of laser light to the atmosphere and detects the return signal that results from the interaction of light with aerosol particles in the atmosphere. The signal detected by the system is represented by the LIDAR equation, which describes the optical properties and the system geometric parameters. The solution for this equation is obtained by the Klett-Fernald-Sasano Inversion Method (KFS), which extracts the inverted optical properties as backscattering (B) and extinction (α) profiles. The present work brings the result of analysis in backscatter profiles of the LIDAR signal in channel 532 nm during the aerosol Monitoring Campaign Long-Range Transportation Over Natal II (MOLOTOV II) that occurred from November 2017 to February 2018. We applied the Monte Carlo method for the analysis of the error in DUSTER measurements, which employs random numbers sequences. Two days of signal measurements were selected, to deal with four groups files, within approximately 30 min each group (frequency acquisition every 10 seconds). N synthetic profiles, as height function, with a random number generator, were created. Algorithms were performed, which removed the measurements clouds, the dark profiles, the background noise and generated the Range Corrected Signal (RCS). The KFS was applied to the synthetic profiles to obtain a set of N solutions (backscatter and extinction coefficient profiles). The results show that the N optical property profiles presented a considerable variability, characterized by their standard deviation. This variability, calculated as the height function, is the random error estimate of the LIDAR signal associated with the inversion procedure. The observed aerosols, according to information from the Hysplit trajectory model, were originated from the Sahara desert.

Keywords: LIDAR, Backscattering, Error Propagation

INTRODUCTION

As propriedades físicas e ópticas dos aerossóis nos processos atmosféricos são complexas e tem uma alta variabilidade temporal e espacial, representando incertezas quanto à influência das partículas de aerossóis nos processos na atmosfera, como, por exemplo, no balanço radioativo da Terra (RUIZ-ARIAS, et al., 2013; ORZA; PERRONE, 2015), de forma direta, espalhando e absorvendo a radiação solar que chega à atmosfera, e de forma indireta, modificando as propriedades das nuvens (KAUFMAN et al., 2002; CORTÉS-HERNÁNDEZ et al., 2014; TOMASI et al., 2015), que pode alterar o perfil de temperatura na camada da atmosfera, uma vez que o aerossol é variável no tempo e no espaço. Os aerossóis podem prejudicar a saúde humana, a qualidade do ar, a visibilidade, o balanço da radiação do planeta, causando efeitos danosos à sociedade, o que implica

em um assunto de grande importante a ser estudado.

O Brasil é um país de escala continental onde existem, atualmente, apenas três sistemas Lidar realizando o monitoramento das propriedades ópticas de aerossóis na troposfera do território brasileiro: um instalado em São Paulo-SP, outro em Manaus-AM e o mais recente em Natal-RN.

No Brasil, o monitoramento das propriedades ópticas dos aerossóis na atmosfera é aplicado nas seguintes áreas:

The physical and optical properties of the aerosols in the atmospheric processes are complex and have a high temporal and spatial variability, representing uncertainties as to the influence of the aerosol particles in the processes in the atmosphere, such as in the Earth's radioactive balance (RUIZ-ARIAS, (1998), directly by spreading and absorbing the incoming solar radiation to the atmosphere, and indirectly modifying the properties of the clouds

(KAUFMAN et al., 2002; CORTÉS-HERNANDEZ et al., 2014; TOMASI et al., 2015), which can alter the temperature profile in the atmosphere layer, since the aerosol is variable in time and space. Aerosols can harm human health, air quality, visibility, and the planet's radiation balance, causing harmful effects to society, which implies a major issue to be studied.

Brazil is a continent-wide country where there are currently only three Lidar systems monitoring the optical properties of aerosols: one installed in São Paulo-SP, another in Manaus-AM and the most recent in Natal -RN.

In Brazil, the aerosols optical properties monitoring in the atmosphere is applied in the following areas:

- (a) transportation of dust from the Sahara desert and from burning emissions from the sub-Saharan region to the South American continent;
- (b) study of optical and physical properties and formation of Cirrus clouds, which are formed at the international flights altitude;
- (c) validation and comparison of measurements of satellite and solar photometer of the AERONET Network data, which measure the vertical distribution of aerosols in the atmosphere;
- d) calibration, alignment and optimization of the atmosphere optical properties measurements, for application in the validation of the EARTHCaré satellite.

These applications are being developed with national and international cooperation, such as the Institute of Energy and Nuclear Research - IPEN / Brazil, University of Granada / Spain, Langley Research Center-NASA / USA, National Institute for R & D for Optoelectronics in Romania, Ludwig Maximilians University, in Germany, Spain and the European Space Agency under the project Assessment of atmospheric optical properties during biomass burning events and Long-range transport of desert dust - APEL and the project ADM-Aeolus CAL / VAL of the ESA, for the validation of the satellite EARTHCaré.

In order to monitor the transportation of dust from the Sahara desert and the emission of fires from the sub-Saharan region to the South American continent, and to study the properties of the aerosols in the atmosphere, a Duster Light Detection and Ranging (Duster /

LIDAR) remote sensing system and a CIMEL solar photometer from the AERONET network were installed in the Brazilian northeast (city of Natal / RN), which is located in a strategic geographic position for this study (5th S).

METHODS

The signal detected by the system is represented by the LIDAR equation, which describes the optical properties of the aerosol particles in the atmosphere, generating information from the backscatter profiles, according to (Weitkamp, 2005):

$$P(R, \lambda) = P_0 \frac{c\tau}{2} A \eta \frac{O(R)}{R^2} \beta(R, \lambda) \left[-2 \int_0^R \alpha(r, \lambda) dr \right]$$

Where:

$P(R, \lambda)$ is the Laser energy flux backscattered at wavelength λ , at distance R ; P_0 is the mean power of the laser unit pulse; c is the speed of light; τ is the pulse duration; A is the area of the primary receiver, which receives the light backscattered back; η is the overall efficiency of the system; $O(R)$ is the overlap function; $\beta(R, \lambda)$ is the backscatter coefficient at wavelength λ , at distance R , and is given in $\text{m}^{-1}\text{sr}^{-1}$; λ is the backscattered light wavelength; $\alpha(r, \lambda)$ is the extinction coefficient [m^{-1}].

According to theoretical and observational studies, the extinction and backscattering coefficients may be related to the LIDAR ratio:

$$RL_{\text{aer}}(R) = \beta_{\text{aer}}(R) / \alpha_{\text{aer}}(R).$$

The solution of the Lidar Equation is obtained through the Klett-Fernald-Sasano Inversion Method (KFS), which extracts the coefficients $\beta(R, \lambda)$ and $\alpha(R, \lambda)$ from the measurements performed with the Lidar system.

We applied the Monte Carlo method for the error analysis of in DUSTER measurements, which employs random numbers sequences (Rascado, 2008). Two days of signal measurements were selected, to deal with four groups files, within approximately 30 min each group (frequency acquisition every 10 seconds). N synthetic profiles, as height function, with a random number generator, were created. Algorithms were performed, which removed the measurements clouds, the dark profiles, the background noise and generated the Range Corrected Signal (RCS). The KFS was applied to the synthetic profiles to obtain a set of N solutions (backscatter and extinction coefficient profiles).

RESULTS AND DISCUSSION

In this section we show results using two days of signal measurements: 19 and 27 December 2019.

For 19 December, we present Figure 1 with the particulate backscatter profile in wave length, as below.

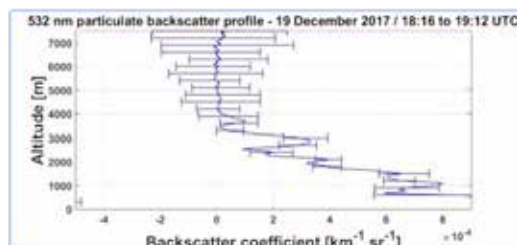


Figure 1. Backscatter Profile

Figure 2 shows the Quicklooks figures, where we can observe aerosols as light blue stripes.

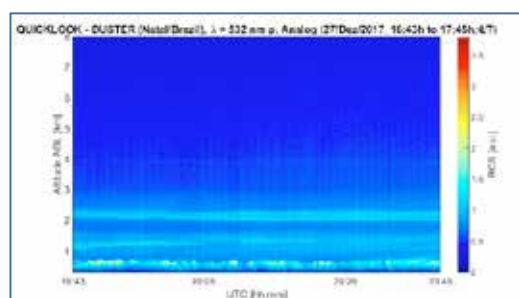


Figure 2. Quicklooks figures

And Figure 3 shows aerosols originated from the Sahara desert.

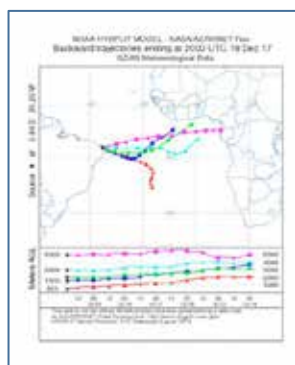


Figure 3. HYSPLIT model backtrajectories
For 27 December, we present sim19 December day.

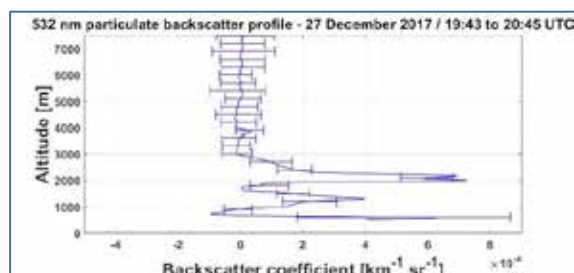


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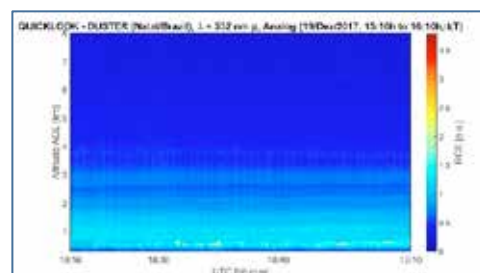


Figure 5. Quicklooks figures

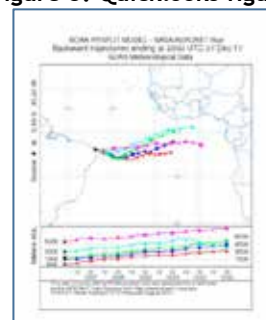


Figure 6. HYSPLIT model backtrajectories

The error bars considering both days characterize the random error estimate of the LIDAR signal associated with the inversion procedure.

CONCLUSIONS

This preliminary study shows that the N optical property profiles presented a certain variability that is characterized by their standard deviation (Particular Backscatter Profile figure). This variability, calculated as the height function, is the random error estimate of the LIDAR signal associated with the inversion procedure. According to the HYSPLIT model backtrajectories, the observed aerosols, as shown by the Quicklooks figures, were originated from the Sahara desert.

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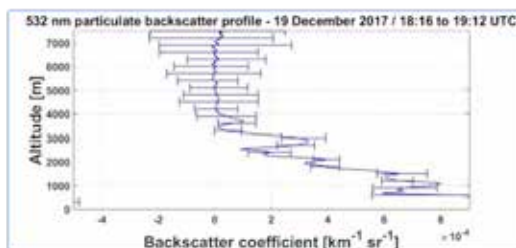


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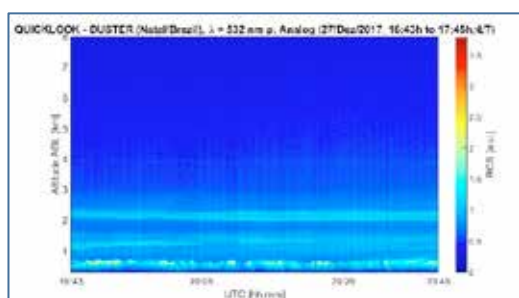


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And Figure 3 shows aerosols originated from the Sahara desert.

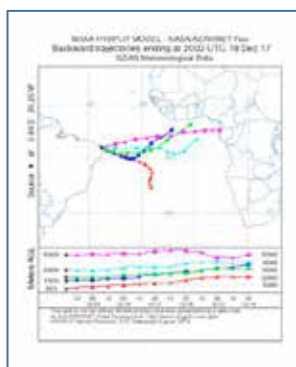


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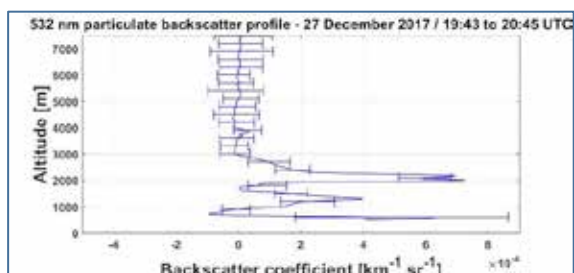


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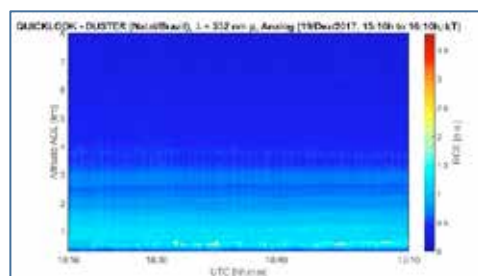


Figure 5. Quicklooks figures

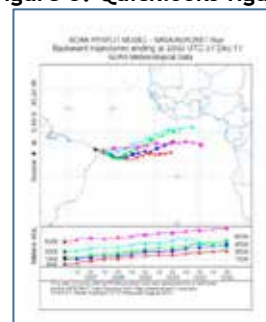


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CONCLUSIONS

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LOW-COST AIR QUALITY MONITOR TO QUANTIFY CO IN URBAN AREAS

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Abstract: Carbon monoxide (CO) may be present in outdoor and indoor environments, and exposure to this substance can cause symptoms from simple nausea to death. Low-cost sensors are becoming increasingly popular for urban air quality monitoring, since most of the monitors used nowadays has a high cost. In this work, we developed a low-cost air quality monitor that couples CO, temperature and humidity sensors. We used MQ-7 sensors for CO and DHT22 for temperature and humidity. The sensors were installed in a mini wind tunnel built in acrylic, where a fan maintains a continuous airflow. An ATmega8 microcontroller board captures data from these sensors. To validate the proposed monitor, tests were performed using a commercial equipment (3M™ EVM 7) and the obtained results have shown equivalent performance, with a cost reduction higher than 99%.

Keywords: Air quality monitoring, Carbon monoxide, Low-cost sensor.

INTRODUCTION

Currently, air pollution is one of the main environmental risk factors. Exposure to air pollutants can directly affect human health in many ways, leading to both increased mortality and morbidity of the population. Epidemiological evidence on the effects of air pollution on health is growing and evolving rapidly (WHO, 2016).

One of the main pollutants that directly affects the health of the population in large urban centers is carbon monoxide (CO). This compound is generated largely from the incomplete burning of fossil fuels and carbon-forming materials. The effects caused by CO exposure to human health may go undetected and cause tissue hypoxia, generated by the stable binding of CO to hemoglobin in the red blood cells, leading to a range of acute symptoms including convulsion, disorientation, visual disturbances, headache, weakness and nausea (Fleig et al., 2016).

Due to the harmful effects of CO, it is necessary to monitor this pollutant. The monitoring of air pollution can be included as part of the technologies used in smart cities, which promotes the improvement in the quality of life of the population, attending to present and future needs, regarding economic, social, environmental and cultural aspects.

An economically viable technology that can facilitate the expansion of monitoring areas and the

availability of air quality data are platforms that use low-cost sensors. The accessibility of these data allows the development of new strategies for health and the environment.

There are numerous proposals to spread the use of low-cost sensors for monitoring air quality in real time. Some of these works use commercial sensors that costs around US\$100 dollars and compares capabilities and limitations between them (Marques, G., Pitarma, R, Piedrahita et al., 2014, Rai et al., 2017, Sun et al., 2016).

This work explores a sensor of the MQ family, which costs less than US\$10, lower than those mentioned previously. In addition, this prototype includes a mini wind tunnel to provide a constant flow in order to improve the performance of the measurement.

METHODS

This study consists of assembling a prototype of an air quality monitoring device using sensors to monitor CO concentrations, temperature and humidity. The materials used in this prototype, including their average price in Brazil, follows:

- 1) ATmega328 Development Board (US\$ 15,00)
- 2) DHT22 Temperature and Humidity sensor (US\$ 5,00)
- 3) Acrylic (US\$ 7,50)
- 4) Fan (R\$ 3,75)
- 5) Two MQ-7 CO sensors (US\$ 10,00)

The developed system uses a development board based on the ATmega328P microcontroller. This platform enables the interface with the external sensors included in this project. The microcontroller features a low-power Atmel® AVR® 8-bit, 16 MHz external clock, 32 KB flash ROM and 2 KB SRAM; In addition, it has AD converters and general purpose digital input and output pins.

There are several sensors available for the application proposed in this work. Existing commercial sensors are mostly metal oxide or electrochemical. The device chosen was the MQ-7, which is widely used for the detection of CO concentration. Inside, there is a metal oxide semiconductor sensor, consisting mainly of SnO₂. To perform the detection, the device operates under two conditions: high and low temperature. During high temperature, the existing gases around the sensor surface evaporates, cleaning it for the measurement. During low temperature, the CO is absorbed on the sensor surface, when the measurements are made. Its operation is based on conductivity, such that conduction is higher in proportion to the increase in gas concentration. The MQ-7 sensor depends on the humidity and temperature conditions, which are also being monitored. The CO sensor detection range is from 20 to 2000 ppm. According to the datasheet, an adjustment curve presented in Eq. 1 was determined.

$$CO(ppm) = 100 \cdot \left(\frac{V_{sensor}}{5 - V_{sensor}} \right)^{1.532} \quad (1)$$

Where V_{sensor} is the voltage read by the Microcontroller in volts.

This project includes a temperature and humidity sensor of DHT type, which are composed by a capacitive sensor to measure the humidity and by a thermistor to measure the temperature. The last one is an electrical sensor that has its electrical resistance thermally altered linearly, which makes it possible to determine the temperature. The DHT22 allows to measure temperatures from -40°C to 80°C with an accuracy of $\pm 0.5^\circ\text{C}$, and humidity in the range of 0 to 100% with an accuracy of 2 to 5%. Together with these components, an alphanumeric LCD display was used to facilitate the presentation of measured data in loco.

Fig. 1 shows the top view of the first version of the prototype of the air quality monitoring system. In red is highlighted the two MQ-7 sensors, called “A” located in lateral and “B” in the top. The DHT22 sensor is highlighted in yellow. The fan is highlighted in blue. The display is in the left corner and the ATmega328 board is in the lower center of the acrylic piece.

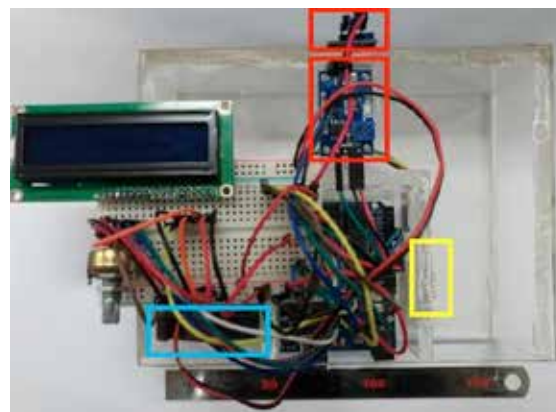


Figure 1. Top view of the prototype.

Regarding the commercial equipment used as a reference for the performance evaluation of the prototype, 3M™ EVM7 was chosen. The CO detection range is from 0 to 1000 ppm, with 1 ppm resolution and $\pm 5\%$ accuracy. The temperature range is from 0°C to 60°C with 0.1°C resolution and $\pm 1.1^\circ\text{C}$ of accuracy. Finally, the relative humidity range is from 0% to 100% with 0.1% resolution and $\pm 5\%$ of accuracy.

FINDINGS AND ARGUMENT

To test the performance, the data provided by the sensors in the developed prototype were simultaneously collected with those of the commercial equipment. The data obtained in an interval of 1 hour, measured in an internal environment, were selected.

Fig. 2 compares the temperature measurement performed by both devices. Overall, the prototype sensor recorded a temperature close to the commercial equipment. The difference between the measurements was up to 0.9°C.

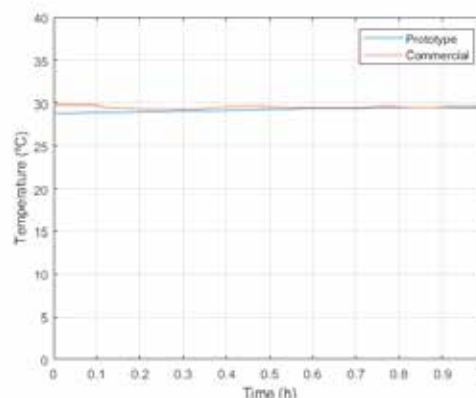


Figure 2. Temperature

Fig. 3 compares the measure of relative humidity, where the sensor recorded a value slightly above than that detected by the commercial equipment.

The maximum humidity difference between both equipment was 3.0%.

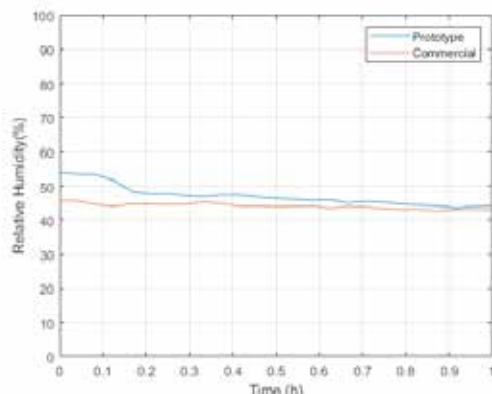


Figure 3. Humidity

Fig. 4 compares the concentrations of CO, in ppm, of the sensors and commercial equipment. The EVM has an accuracy of 1 ppm, while the measurements of the prototype perform a conversion, according to Eq. 1, presenting values in a smaller magnitude. Thus, if the measured value is rounded for integer values, it is understood that the measured values between the prototype and the equipment are in the same order of magnitude.

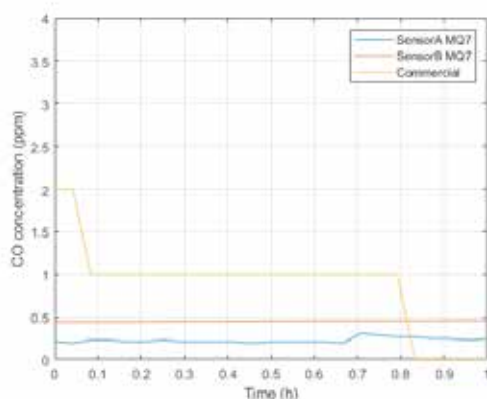


Figure 4. CO concentrations

CONCLUSIONS

Due to the characteristics of the used sensor, it has been observed that there is a difference with the absolute values measured in relation to the commercial equipment. Nevertheless, it is understood that the device provides enough qualitative data for observing the behavior of the parameters in general.

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ANALYSIS OF EVAPOTRANSPIRATION, PRECIPITATION, AND NDVI DYNAMICS USING REMOTE SENSING DATA IN THE UPPER PARANÁ RIVER BASIN

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Abstract: This study aims to evaluate the spatial and temporal behavior of evapotranspiration (ET) in different land covers of the Upper Parana River Basin (UPRB) during 13 years (2001 - 2013), as well as its correlation with precipitation and NDVI (Normalized Difference Vegetation Index) data, using TRMM (Tropical Rainfall Measuring Mission) and MODIS (Moderate-Resolution Imaging Spectroradiometer) data sets. The results showed that ET presents higher values in areas with a higher amount of biomass on the surface, such as those covered by forests and grassland. However, considering the entire ET time series, forest areas present higher ET loss when compared with grassland areas. Moreover, ET was directly related to NDVI, especially for Cropland ($R^2 = 0.92$) and Savanna ($R^2 = 0.91$). The relationship between ET and precipitation was more consistent for Savanna ($R^2 = 0.84$) and Cropland ($R^2 = 0.79$) classes. Thus, the results of this study suggest that it is necessary to take into account the influence of the type of coverage in the water balance of the UPRB.

Keywords: MODIS, TRMM, Evapotranspiration, Upper Paraná River Basin.

INTRODUCTION

The Upper Parana River Basin (UPRB) is Brazil's most intensively exploited region, producing the most food and electricity in the country. This scenario has led to intense land use and land cover changes over the last few decades. Studies have shown that these land cover changes have the potential to affect water and energy balance, with direct effects on the evapotranspiration.

The evapotranspiration (ET) that occurs on the surface of the planet is central to the cycles of the climatic and biogeochemical system in terrestrial ecosystems, acting as a dominant component in the global water balance, especially in semi-humid to arid areas (MO et al., 2015). It consists in the transfer of water to the atmosphere by evaporation of water present in the soil, free surfaces or wet vegetation, and transpiration in plants. Thus, it's important monitoring the ET space and time, mainly in tropical areas, since they exert strong control in the processes of atmospheric circulation at regional and global scales (KUSTAS & NORMAN, 1996). In addition, ET has strong implications for climate modeling and the hydrological cycle, as well as assessing environmental stress in natural and agricultural ecosystems (JOINER et al., 2018). In addition, methodologies that use remote sensing in monitoring ET have been highlighted (MICHEL et

al., 2015; YANG et al., 2015; NOURI et al., 2016; compared to traditional physical and empirical methods, as these limit their estimation (OLIVEIRA, et al 2017).

The UPRB has undergone major changes in its vegetative cover over the last century. The forest cover of São Paulo and Paraná states, located in the center of the basin, decreased from approximately 70% in 1907 to less than 8% in 1990 (TUCCI, 2003). These changes, along with soil compaction due to increased agricultural mechanization, have been attributed as the main propellant in increments in the flow regime of the basin (TUCCI, 2002; DOYLE & BARROS, 2011). This context of land cover changes may have a direct impact on hydrological cycle variables, such as precipitation and ET. Thus, the objective of this study was to analyze the spatiotemporal behavior of ET between 2001 and 2013 in different types of vegetation cover in Upper Parana River Basin, using remote sensing data. In addition, the relationship between ET, precipitation and Normalized Difference Vegetation Index (NDVI) was evaluated.

METHODS

In data processing, firstly the MODIS products (MOD16A2, MOD16A3, MOD13A3, and MCD12Q1)

obtained in the Hierarchy Data Format (HDF) were converted to the Tagged Image File Format (TIFF) using the Modis Reprojection Tools (MRT). Then, Monthly and annual values of ET, NDVI, and precipitation were analyzed for each aggregate class of the land cover data (MCD12Q1). Information regarding the satellite, product and ancillary data used in this study are listed in Tab. 1. All MODIS products were purchased for scenes h12v10, h12v11, h13v10 and h13v11.

Table 1. Summary of the characteristics of data sets.

Product	Information	Satellite/ RADAR	Spatial Resolution	Reference
MOD16A2	Monthly ET	Terra/Aqua	500m	MU; ZHAO; RUNNING, 2011
MOD16A3	Annual ET	Terra/Aqua	500m	MU; ZHAO; RUNNING, 2011
MOD13A3	NDVI	Terra/Aqua	1km	DIDAN <i>et al.</i> , 2010
MCD12Q1	Land Cover	Terra/Aqua	500m	FRIEDL <i>et al.</i> , 2010
3B43	Monthly Rain	TRMM	0,25°	HUFFMAN <i>et al.</i> , 2007

The land cover products between 2001 and 2013 were extracted from the MCD12Q1 product, which contains 5 classification schemes (Friedl *et al.*, 2010). The primary scheme, defined through the International Geosphere-Biosphere Program - IGBP, was used for class association. The file contains 17 thematic classes (12 vegetation classes), which were aggregated into 5 vegetation classes, as described in Tab. 2.

Table 2. Vegetation classes aggregated from the IGBP classification.

	IGBP
Forest	Evergreen Needleleaf Forest (1) Evergreen Broadleaf Forest (2) Deciduous Needleleaf Forest (3) Deciduous Broadleaf Forest (4) Mixed Forest (5)
Cropland	Croplands (12) Cropland/Natural Vegetation Mosaic (14)
Grassland	Grasslands (10)
Shrubland	Closed Shrublands (6) Open Shrublands (7)
Savanna	Woody Savannas (8) Savannas (9)

Correlations between variables (in the monthly context) were verified through the application of the Spearman correlation test. The Kruskal-Wallis test was used to evaluate the difference in the vegetation classes for the monthly ET and precipitation. When applicable, the pairwise multiple comparison tests were conducted with Dunn test, which was used to discern which of the pairs have significant differences. All statistical indicates that considered 5% significance.

FINDINGS AND ARGUMENT

Based on an annual analysis of ET in UPRB (Fig. 1), it can be observed that the lowest ET values recorded (mm.year⁻¹) are observed in the upper and the right bank of the basin, regions defined as

Cerrado Biome. The regions of Cerrado Biome are essentially defined as areas of savanna in MCD12Q1 data, with variations in the area over the 13 years.

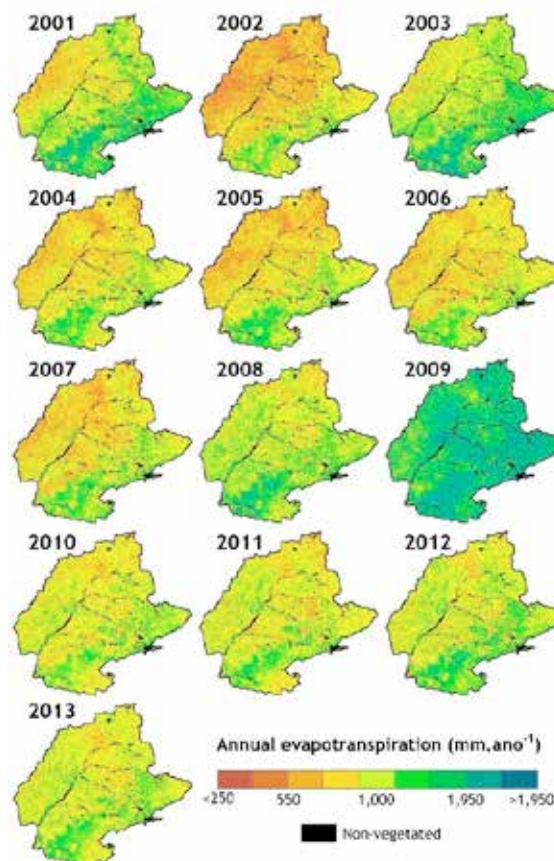


Figure 1. Annual evapotranspiration (mm.year⁻¹) in the Upper Paraná River Basin.

To the south of the basin, the highest ET values are observed annually. This area is characterized by remnant areas of the Atlantic Forest Biome (left bank of the basin). The highest ET values in Forest areas are shown in Figure 2a.

The year 2009 was the most atypical, presenting the highest ET values (Fig. 1 and 2). This change can be observed mainly in the right bank of the UPRB, which presented the highest ET values throughout the historical series. High values of precipitation and NDVI were also observed for this year (Fig. 2b and 2c). In this period, the Sea Surface Temperature (SST) in the equatorial Pacific region 3.4 was in the El Niño period (NOAA/CPC, 2019). The southern and southeastern regions of Brazil tend to have high precipitations during the El Niño period. The correlation between the precipitation variables - ENSO is greater as the latitude in the South of Brazil increases. In this region, El Niño produces positive anomalies of rainfall and La Niña negative anomalies, mainly in the spring and early summer of the year of beginning of the phenomenon, due to the higher temperatures and the intensification of the

convective systems and mesoscale convective complexes - MCCs (BERLATO et al., 2005; BRITO et al., 2008; NÓIA JUNIOR; SENTELHAS, 2019; CALDANA et al., 2019).

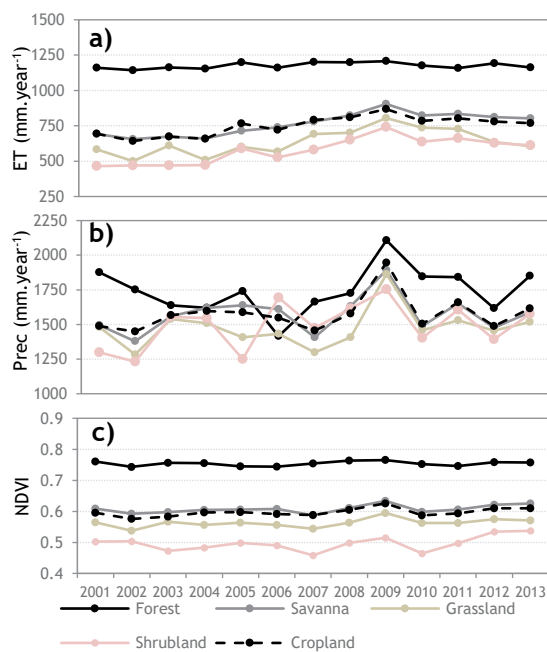


Figure 2. Profiles of ET (a), precipitation (b) and NDVI (c) by vegetation class.

It is also worth noting the year 2013 with high rainfall heights, observed under conditions of SST neutrality. In these periods, high precipitation can occur in the Center-South of Brazil, as there is a reduction in the atmospheric blocks in the subtropical strip, while in the tropical region of South America the air that ascends to the west (low atmospheric pressure) tends to descend on the cold waters to the east (high atmospheric pressure). As a consequence, there is an absence of clouds and precipitation in this region (BERLATO, 2005; ANDERSON et al., 2017). This justifies the highest rainfall heights in the subtropical or transitional of the Paraná River Basin.

The analysis of the correlation between ET and NDVI indicates that NDVI has a good linear correlation with ET (in the monthly context), as shown in Table 3. These results are in agreement with previous studies (SZILAGYI et al., 1989; ROSSATO et al., 2005; MAO et al., 2010; ISLAM & MAMUN, 2015). Analyzing by class, it is observed that Cropland and Savanna classes have more consistent correlations, with correlation values of 0.92 and 0.91, respectively. Oliveira et al. (2017) indicate that the high correlation in these cases may be related to high variation within these vegetation types. The Cropland cover, for example, varies from the exposed soil to the soil completely covered with the crop (OLIVEIRA et al.,

2017). On the other hand, the forest class had the lowest correlation values (0.56).

Table 3. Correlation coefficient values (R^2) between ET vs. NDVI and ET vs. Precipitation, for each class of vegetation.

Class	ET vs. Precipitation		ET vs. NDVI	
	R^2	p-value	R^2	p-value
Forest	0.492	6.88E-11	0.559	3.43E-14
Savanna	0.837	3.74E-42	0.912	1.74E-61
Grassland	0.721	2.50E-26	0.898	1.07E-56
Shrubland	0.703	1.36E-24	0.878	4.68E-51
Cropland	0.792	7.98E-35	0.921	6.60E-65

As for NDVI, significant correlations were observed between precipitation and ET for analysis by vegetation type. However, correlations did not have the same magnitude as that presented between ET vs. NDVI, which may be related to the lower resolution of precipitation data (3B43 - spatial resolution of 0.25°). By class, it is observed that Savanna and Cropland presented the highest values of correlation, 0.92 and 0.91, respectively.

From Table 3 it is clear that the NDVI has a strong correlation with the total ET than the precipitation rate. Figure 3 shows the monthly profiles of ET, precipitation, and NDVI for the Cropland class. It is observed that the NDVI index has a good correlation with ET data, indicating that NDVI may be an effective tool for estimating ET a help modelers for model estimation by providing reference values of ET on regional scale (SZILAGYI et al., 1989; ISLAM & MAMUN, 2015).

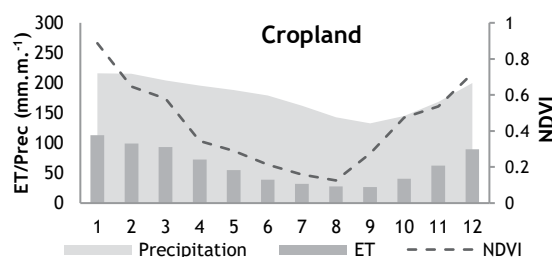


Figure 3. Profiles of mean monthly ET, mean monthly precipitation and NDVI for Cropland class.

Based on the application of the Kruskal Wallis test it is concluded that there are differences between the medians, both for ET and for precipitation. Through the multiple comparisons test, it can be concluded that for ET, most of the vegetation classes presented statistical difference between them (Tab. 4). Savanna and Cropland showed no significant difference, as well as Grassland and Shrubland.

Table 4. Dunn p-values for the vegetation classes, considering ET data.

	Forest	Savanna	Grassland	Shrubland
Savanna	1.59E-15			
Grassland	1.82E-27	0.003873		

Shrubland	9.74E-33	0.000079	0.290125	
Cropland	8.59E-17	0.724251	0.011227	0.000326

As for precipitation, the Forest class is different from all other vegetation classes (Tab. 5), with the exception of Cropland, for $\alpha = 5\%$. This shows that, in general, the amount of precipitation in forest areas is significantly higher than in other areas.

Table 5. Dunn p-values for the vegetation classes, considering precipitation data.

	Forest	Savanna	Grassland	Shrubland
Savanna	0.024867			
Grassland	0.006359	0.627533		
Shrubland	0.001283	0.328911	0.623351	
Cropland	0.065761	0.686644	0.374209	0.167672

CONCLUSIONS

This study evaluated the behavior of the ET in different grading classes, as well as monthly comparing them with precipitation data and NDVI. ET was strongly controlled by seasonality, as well as vegetative cover (expressed by NDVI) and water availability.

The analysis of the correlation between ET and NDVI indicates that NDVI has a good linear correlation with ET. This shows that NDVI may be an effective tool for estimating evapotranspiration on regional scale. The Cropland and Savanna classes had the highest ET correlation values for both NDVI and precipitation.

A significant difference was observed in the Rain Forest class, indicating that there are higher rainfall heights recorded in these areas.

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ECOPM: DEVELOPMENT AND PERFORMANCE EVALUATION OF A PARTICULATE MATTER CONTINUOUS MONITOR

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Abstract: Pollution is the largest environmental factor of disease and premature death in the world. Among diverse forms of environmental pollution, air pollution stands out as the cause of the most severe effects on human health. Atmospheric particulate matter (PM) is considered the most toxic component of air pollution and is a key factor in a number of effects on the environment, ecosystems and health of exposed populations. There are many papers reporting that air pollution affects human health and environment. There is a strong growth in the number of publications from the 1990s, coinciding with technological advances and greater diffusion of methods of monitoring air quality and increasing environmental awareness on a global scale. In recent decades, a large number of epidemiological and toxicological studies have demonstrated associations between increased PM concentrations and increased morbidity and mortality caused by cardiopulmonary diseases. Knowledge about air quality is often scarce and limited by how air quality data are obtained. Conventional monitoring stations allow the knowledge of air quality with a high level of metrological quality and data reliability. However, due to their high cost and mobility limitations, only conventional stations are not able to describe all the complexity of air quality, which presents high variability spatial and temporal. Therefore, to increase knowledge and control populations exposure (not only human), it is necessary to develop monitoring technologies and strategies that allow short-term responses, mobility and resource use in a more flexible and less costly way to increase the density of air quality monitoring networks. The technological advances, mainly with the application of metrological techniques based on the use of laser, have enabled the development of a new generation of low cost and portable PM sensors. The development of these sensors is providing the opportunity to use this technology for a wide range of applications in addition to regulatory monitoring. Among monitoring alternatives, these sensors can be used for the monitoring emitting sources, industrial environments, indoor air quality, personal exposure, scientific research, toxicological studies, among others. With focus on the improvement of the technologies and amplification of the density and capacity of monitoring PM concentrations we developed ECOPM, a continuous monitor for TSP, PM₁₀, PM_{2.5} and PM_{1.0}. ECOPM also allows the continuous measurement of the deposition flux of settleable particulate matter (SPM), an important variable for places with problems related to dustfall. This article presents the results obtained with ECOPM and intercomparison with another reference equipment used in conventional air quality stations. ECOPM calibration and intercomparison with standards such as High-Volume Air Sampler Method (Hi-Vol) and Beta Attenuation Monitor (BAM), both included in the List of Desired Reference and Equivalent Methods published by United States Environmental Protection Agency, has shown results correlated very well (r^2 higher than 0.99, for TSP, PM₁₀ and PM_{2.5}) in the TSP concentration range of 0 - 1400 µg/m³. Development of portable and low-cost PM monitors, like ECOPM, are aligned to the forefront of air quality instruments technology. Therefore, we have sought to combine the high levels of metrological quality and data reliability with portability and feasibility to improve the knowledge about air quality, emission control and prevention to PM exposure.

Keywords: air quality, low-cost sensor, monitoring, optical particle counter, portable monitor, PM₁₀, PM_{2.5}, TSP.

INTRODUCTION

Pollution is the largest environmental factor of disease and premature death in the world (Landrigan, 2017). Among diverse forms of environmental pollution, air pollution stands out as the cause of the most severe effects on human health. Atmospheric particulate matter (PM) is considered the most toxic component of air pollution (World Health Organization, 2006) and is a key factor in a number of effects on the environment, ecosystems and health of exposed populations. There are many papers reporting that air pollution affects human health and environment.

There is a strong growth in the number of publications from the 1990s, coinciding with technological advances and greater diffusion of methods of monitoring air quality and increasing environmental awareness on a global scale. In recent decades, many epidemiological and toxicological studies have demonstrated associations between increased PM concentrations

and increased morbidity and mortality caused by cardiopulmonary diseases (Curbani et al., 2019). Knowledge about air quality is often scarce and limited by how air quality data are obtained (Austin et al., 2015; Kumar et al., 2015).

Conventional monitoring stations allow the knowledge of air quality with a high level of metrological quality and data reliability (Schneider et al., 2017). However, due to their high cost and mobility limitations, only conventional stations are not able to describe all the complexity of air quality, which presents high variability spatial and temporal (Austin et al., 2015; Kumar et al., 2015). Therefore, to increase knowledge and control populations exposure (not only human), it is necessary to develop monitoring technologies and strategies that allow short-term responses, mobility and resource use in a more flexible and less costly way to increase the density of air quality monitoring networks.

The technological advances, mainly with the application of metrological techniques based on the use of laser, have enabled the development of a new generation of low cost and portable PM sensors (Austin et al., 2015). The development of these sensors is providing the opportunity to use this technology for a wide range of applications in addition to regulatory monitoring. Among monitoring alternatives, these sensors can be used for the monitoring emitting sources, industrial environments, indoor air quality, personal exposure, scientific research, toxicological studies, among others (Williams et al., 2019).

Focusing on the improvement of the technologies and amplification of the density and capacity of monitoring PM concentrations we developed ECOPM, a continuous monitor for suspended particles concentrations (TSP, PM_{10} , $PM_{2.5}$ and $PM_{1.0}$) and deposition flux of settleable particulate matter (SPM). Here we described the results of performance tests with intercomparison of ECOPM and other monitors reference equipment used in conventional air quality stations. ECOPM calibration and intercomparison with standards such as High-Volume Air Sampler Method (Hi-Vol), Beta Attenuation Monitor (E-BAM Plus), both included in the List of Desired Reference and Equivalent Methods (United States Environmental Protection Agency, 2019).

METHODS

ECOPM is an optical particle counter able to simultaneously measuring PM concentrations at 2 s period, with integration and recording averages of 1 to 60 min. ECOPM measurement principle is based on counting particles suspended in the airflow through a laser beam and its size is determined by the signal perceived by the detector positioned at 90° from the laser beam. A microprocessor fully dedicated to the sensor is capable of detecting millions of particles per liter of air. An integration algorithm of the sampled particles determines the concentrations of the fractions measured. A heated sampling probe, controlled according to air humidity and temperature, ensuring adequate conditioning of the sampled airflow and reducing the interference of air humidity.

Due to the low power consumption, ECOPM can be powered by a common power supply, battery or solar panel. ECOPM was designed to be robust, compact, lightweight, high-portable and user-friendly, being able to be quickly repositioned in different localities, returning to the measurements in a few minutes. ECOPM operates directly indoor (low PM concentrations) and outdoor (exposed to rain, sun, wind and high PM concentrations), providing readings for a long-term period without any intervention. The equipment can be calibrated with reference in conventional monitoring stations

and monitors, as well as using other comparative methods. ECOPM can receive various optional features such as GPS, connection with other sensors (meteorological sensors for wind speed, wind direction, air temperature, relative humidity, solar radiation, precipitation gauges, etc.), simultaneously operating as a datalogger, 915 MHz radio and GPRS modem for data transmission (Figure 1).

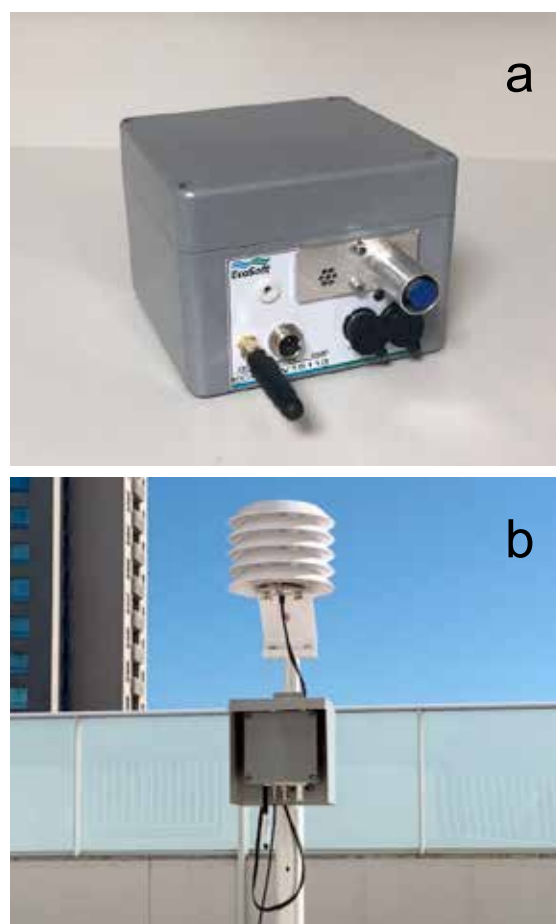


Figure 1. ECOPM (EcoSoft®) continuous PM monitor for measurement of TSP, PM_{10} , $PM_{2.5}$ and $PM_{1.0}$ concentrations and SPM deposition flux. (a) ECOPM monitor, (b) ECOPM operating and receiving data from meteorological sensors (air temperature and relative humidity).

We tested ECOPM with two different approaches. In the first one we performed the ECOPM tests in the laboratory under different concentrations of TSP, PM_{10} and $PM_{2.5}$ generated in a PM generation chamber. Concentrations ranged from zero to values greater than $1000 \mu\text{g}/\text{m}^3$ to ensure a wide application measurement range. In this approach we used an E-BAM Plus analyzer (Met One Instruments Inc.) as the reference standard. E-BAM Plus is an equivalent method as defined by the

USEPA (Equivalent Method: EQPM-1215-226). After the exposures the series of the analyzers were tested statistically by linear regression model and performance tests according to metrics (Schneider et al., 2017) usually applied for comparison between measurement methods. We used R 3.5.3 software (R Core Team, 2019) to perform statistical analyses. A p-value less than 0.05 was considered significant.

The second approach was carried out in a field test at Serviço Nacional de Aprendizagem Industrial (SENAI), state of Santa Catarina, Brazil. SENAI is an institution accredited by the Instituto Nacional de Metrologia, Qualidade e Tecnologia (INMETRO) to provide proficiency testing under ISO/IEC 17043:2010. Proficiency tests are a requirement for ISO/IEC 17025:2017 certification. The statistical planning adopted by the SENAI for the evaluation of data from each interlaboratory comparison proficiency round is based on the robust statistical principles of ISO/IEC 13528:2015 - Statistical methods for use in proficiency testing by interlaboratory comparisons. In this approach SENAI used High-Volume Air Samplers as the reference standards.

FINDINGS AND ARGUMENT

Laboratory tests (ECOPM vs. E-BAM Plus) indicated very good agreement between ECOPM and the standard reference (E-BAM Plus) (Table 1, Figure 2). These results are compatible with the performance required for the application aiming to improve density (supplement) of air quality monitoring networks, monitoring of emitting sources among other applications in research and monitoring of air quality, mainly considering applications where conventional PM monitors are unsuitable or incompatible. Results obtained by the linear regression model are presented in Table 2.

Table 1. Metrics of comparison of ECOPM and E-BAM Plus (EQPM-1215-226) PM monitors.

Metric	TSP	PM ₁₀	PM _{2.5}
MB ($\mu\text{g}/\text{m}^3$)	54.52	20.36	3.01
MGE ($\mu\text{g}/\text{m}^3$)	55.23	24.62	9.62
NMB	0.16	0.11	0.02
NMGE	0.16	0.13	0.08
RMSE ($\mu\text{g}/\text{m}^3$)	85.20	45.15	17.88
NMSE	0.05	0.05	0.02
MFB	0.11	0.15	-0.04
r	1.00	1.00	1.00
IOA	0.99	0.99	1.00

MB indicates the mean bias, MGE the mean gross error, NMB the normalized mean bias, NMGE the normalized mean gross error, RMSE the root mean squared error, MFB the mean fractional bias, r is the Pearson correlation coefficient and IOA is the index of agreement.

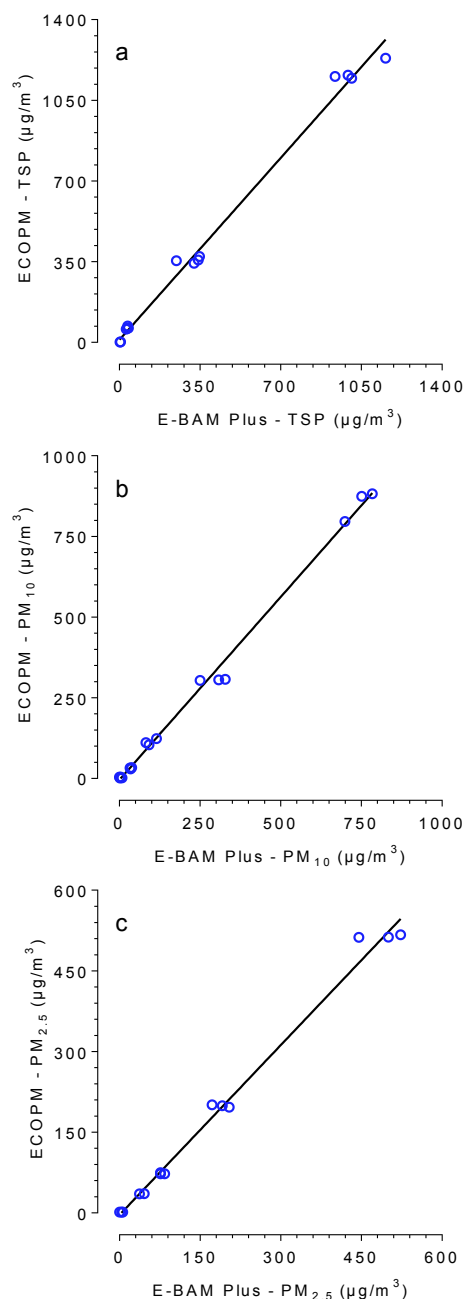


Figure 2. Scatterplots of concentrations measured by ECOPM versus E-BAM Plus (EQPM-1215-226) in PM exposure chamber and linear regression lines. (a) TSP, (b) PM₁₀, (c) PM_{2.5}.

We emphasize that within the laboratory tests we force the reading ranges to values above 1000 $\mu\text{g}/\text{m}^3$ in order to promote tests under severe conditions. It is known that under ambient conditions the measurement ranges may be reduced to the expected ranges. In these conditions of more restricted ranges the indicators can be even better

considering the amplitude and sensitivity adjustments of ECOPM.

In field tests (proficiency tests) promoted by SENAI the results were satisfactory and ECOPM was approved in all evaluations, according to the Proficiency Testing Program 07/2018, conducted on August 28-30, 2018. The participation in Proficiency Testing Programs allows continuous evaluation of laboratory work, guiding errors detection, improving the operational techniques and improving the quality of measurements. Good results in these programs ensure greater reliability for customers and play an important role in accepting the laboratory by accrediting or certifying bodies.

Table 2. Results from linear regression model applied to laboratory performance test (ECOPM vs. E-BAM Plus).

Metric	TSP	PM ₁₀	PM _{2.5}
r ²	0.99	1.00	0.99
F	2018	3892	2331
p	< 0.001	< 0.001	< 0.001
df	16	19	19

CONCLUSIONS

Development of portable and low-cost PM monitors, like ECOPM, are aligned to the forefront of air quality instruments technology. It is imperative to apply monitoring solutions that increase the capacity to obtain information, at low cost, combining quality and portability so that air quality data can be measured more comprehensively. In this way, the whole society can benefit from the monitoring systems currently restricted to a few specialists and academics.

Therefore, we have sought to combine the high levels of metrological quality and data reliability with portability and feasibility to improve the knowledge about air quality, emission control and prevention to PM exposure. ECOPM is suitable equipment for applications in the most diverse, including: air quality monitoring (indoor and outdoor), supplementing existing monitoring, PM sources monitoring (identification and characterization), control measures efficiency evaluation, research, mobile monitoring, personal monitoring, education, information/awareness.

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RAMP: A MONITORING NETWORK TO IMPROVE KNOWLEDGE, MANAGEMENT AND CONTROL OF PARTICULATE MATTER DIFFUSE EMISSION SOURCES

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Abstract: Diffuse sources of particulate matter (PM) exist in different industrial and urban sectors, and are very common in sectors such as mining and steel plants, due to the existence of transport circuits and storage of materials (such as conveyor belts, silos, storage yards, piles, roads, wind erosion, etc.). Quantification of the emission rates of PM diffuse sources and their continuous knowledge and control are hard tasks that sometimes challenge those who study atmospheric emissions and the managers responsible for the control of atmospheric emissions. Since 2009, we have been working on the development of integrated solutions (sensors, PM monitors, software, communication systems) that are capable of obtaining reliable data on PM concentrations, wind conditions and PM emission rates from diffuse emission sources. RAMP is an automatic network for the monitoring fugitive PM emissions, composed of a set of measuring stations strategically placed (upwind and downwind) around the particular emitting source of interest, that measures the vertical profile of total suspended particles concentrations in the atmosphere. From the variations in dust concentrations detected upwind and downwind of the source of interest, in addition to the measurement of air flow passing by the source (wind direction and wind speed), RAMP continuously measures the PM emission rates generated by the monitored sources. RAMP particle concentration monitors are calibrated by intercomparison to traceable standards, based on United States Environmental Protection Agency (USEPA)-approved PM concentration analyzers (as published in USEPA's List of Designated Reference and Equivalent Methods). The calibration guarantees the metrological quality of the RAMP system. Monitors are protected from interference from air humidity, temperature, lightness, mists, rain and vibration. The data is generated at scheduled short time intervals (1, 5, 10 or 15 min) and sent to SSED (Supervisory System of Diffuse Emissions) for processing. The SSED is an application that can interpret and integrate the information received from the RAMP, calculating PM and wind fields, and PM emission rates generated by each emitting source monitored continuously. The emissions of the monitored sources can be displayed continuously by web-based application (Ambion or Atmos). Under dust emission events beyond a certain pre-set value, the RAMP can send alerts to the responsible for the affected area, making it possible to take immediate action to neutralize the causes of the problem, at the time of occurrence or when it is about to occur. All the equipment that make up a RAMP are designed and built to withstand harsh operating conditions of the production area for a long period of continuous operation. This is an innovative solution that has helped companies in one of the most difficult environmental management tasks, which is effective control of fugitive dust emissions in mining, roads, materials storage yards, handling dry bulk materials, civil construction other activities. In addition to improving the management of atmospheric emissions in the short term, the RAMP allows establishing the real gains from the implementation of control actions by evaluating the long-term evolution of the emission rates of the monitored areas. This paper presents the results of RAMP measurements applied to the environmental management of an Industrial Complex containing several PM diffuse emitting sources.

Keywords: continuous measurement, dust control, management tool, real-time monitoring, PM profile.

INTRODUCTION

Dust is a primary cause for air quality deterioration, as well as a potential health hazard (Jia, 2014). Fugitive dust was defined as dust that could not reasonably pass through a stack, chimney, vent, or other functionally equivalent opening (Western Regional Air Partnership's and Countess Environmental, 2006). Thus, fugitive dust is equivalent to the particulate matter (PM) emitted by diffuse emission sources.

Diffuse sources of PM exist in different industrial and urban sectors, and are very common in sectors such as mining and steel plants, due to the existence of transport circuits and storage of materials (such as conveyor belts, silos, storage yards, piles, roads, wind erosion, etc.) (Cui et al., 2019; Jia, 2014; Watson et al., 2000). Quantification of PM emission rates from diffuse sources and their continuous knowledge and control are complex

tasks that sometimes challenge those who study atmospheric emissions and the managers responsible for the control of atmospheric emissions (Cui et al., 2019).

Since 2009 we have been working on the development of integrated solutions (sensors, PM monitors, software, communication systems) that can obtain reliable data on PM concentrations, wind conditions and PM emission rates from diffuse emission sources. In this context, we developed RAMP, an automatic network for the monitoring fugitive PM emissions, composed of a set of measuring stations strategically located (upwind and downwind) around the emitting sources of interest, that measures the vertical profile of total suspended particles concentrations in the atmosphere.

Here we described the main results in terms of PM emission rates from an Industrial Complex (IC) that

has used RAMP as an integrated environmental management tool and monitoring network to improve control of PM diffuse emission sources.

METHODS

The Industrial Complex monitored by RAMP (located in Vitória, ES, Brazil) is an important logistic hub to international distribution of iron ore, grains and other products. Regarding the huge quantities of materials transferred and stored, PM diffuse sources are important issues to control in order to obtain improvements in air quality.

RAMP in IC is composed by 37 profiling towers. Each tower (up to 20 m high) is composed by three PM monitors (optical particle counters) located to obtain a vertical concentration profile. Nine towers are equipped with wind sensors to provide information about wind direction and speed in real-time along IC (Figure 1).



Figure 1. RAMP: Automatic network for the monitoring fugitive PM emissions installed in an Industrial Complex (Vitória, ES, Brazil). Circles indicate profiling towers. Blue circles indicate stations equipped also with wind sensors.

We combine exposure-profiling and upwind-downwind methods (Cowherd et al., 1974; Kolnsberg, 1976; Western Regional Air Partnership's and Countess Environmental, 2006) to obtain a measurement system and computational algorithm that allow calculation of the PM emission rates for different weather and operational conditions, covering several PM sources. From the variations in

dust concentrations detected PM profile upwind and downwind of the source of interest, in addition to the measurement of air flow passing by the source (wind direction and wind speed), RAMP continuously measures the PM emission rates generated by the monitored sources.

All the equipment that compose a RAMP were designed and built to resist harsh operating conditions in field/industrial site for a long period of continuous operation. The data is generated at scheduled short time intervals (1, 5, 10 or 15 min) and sent to a Supervisory System of Diffuse Emissions (SSED) for processing. The SSED is an application that process and integrate the information received from the RAMP sensors, calculating PM and wind fields, and PM emission rates generated by each emitting source/area monitored continuously. PM emissions of the monitored sources are recorded and can be displayed continuously by web-based application (Ambion® or Atmos®) (Figure 2).



Figure 2. PM concentration and wind field generated by RAMP/SSED.

RAMP particle concentration monitors are calibrated by intercomparison to traceable standards, based on United States Environmental Protection Agency (USEPA) approved PM concentration analyzers (as published in USEPA's List of Designated Reference and Equivalent Methods). The calibration guarantees the metrological quality of the RAMP system.

Data analyzed comprises a timeseries of PM emission rates generated by RAMP system from April 1st, 2011 to June 18th, 2019. To evaluate the trend in PM emission rates we applied Mann-Kendall trend test and a linear regression model. We used R 3.5.3 software (R Core Team, 2019) to perform statistical analyses. A p-value less than 0.05 was considered significant.

FINDINGS AND ARGUMENT

Since April, 2011 the PM emission rates from diffuse emission sources measured by RAMP system have

been decreased Mann-Kendall trend test ($S = -1872006$, $Z = -658.87$, $p < 0.001$, $n = 2956$).

The decreasing trend in PM emission rates was a result of many control measures to reduce and mitigate fugitive dust sources. Figure 3 shows the decreasing trend, in terms of 30-day moving average and PM linear regression model ($r^2 = 0.24$, $F_{1,2954} = 911.5$, $p < 0.001$, slope $\beta = -0.03551 \text{ kg h}^{-1} \text{ day}^{-1}$, intercept $\alpha = 125.8 \text{ kg h}^{-1}$) obtained considering the data measured by RAMP system as 15-min PM emission rates.

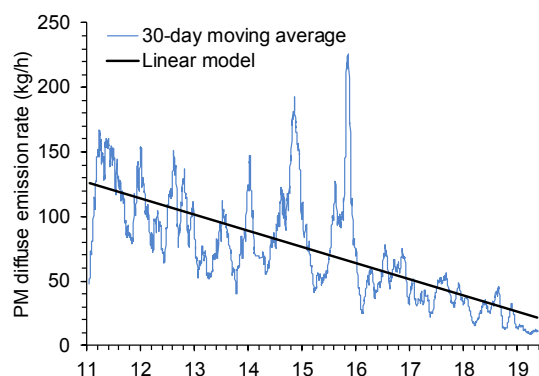


Figure 3. Fugitive PM emission rates from an Industrial Complex (Vitória, ES, Brazil) including storage piles, industrial wind erosion and materials handling. Data measured by RAMP from April 1st, 2011 to June, 18th, 2019.

RAMP system is an innovative solution that has helped companies in one of the most complex environmental management tasks, which is effective control of fugitive dust. The monitoring that has been carried out through the RAMP has shown to be an important instrument of environmental management of the referred IC. The implementation of RAMP has provided improvements in how to deal with the control and reduction of PM emissions, leading to a search for continuous improvement to reduce fugitive dust emissions, either by adopting new solutions or even by improving operational practices.

Associated with the possibility of monitoring fugitive dust emissions in the short-term, the knowledge improvements about PM emissions in diffuse sources have great importance. This knowledge can be applied to atmospheric emissions inventories so that PM emission factors and models are gradually improved to obtain better input data for atmospheric dispersion models, such as CMAQ, AERMOD, and others. RAMP and its data history enable the substitution of more simplified assessments and inventories, based on emission factors and models, as it allows to include a wider range of information that can significantly change PM emission rates.

Indeed, RAMP is an unprecedented project, developed with the following main functionalities/objectives:

- Continuous knowledge of the levels of dust in the IC;
- Continuous and improved knowledge of surface wind conditions (direction and speed) at strategic points in IC;
- Continuous detection and indication of the productive sectors in the IC with PM emissions above the pre-established limits, allowing immediate action to be taken, with a view to restoring adequate control or mitigation of emissions;
- Immediate (every 15 minutes) identification of cause and effect, i.e. the relationship between PM emissions in the IC and the short-term effects on the air quality of its nearest environment;
- Real time quantification (every 15 minutes) of the order of magnitude of the global PM emission by diffuse sources in the IC, with recording of timeseries in a database;
- Monitoring of the evolution of the control of PM emissions in the IC, as well as its short and long-term effects on the air quality.

CONCLUSIONS

The generalization and improvement of exposure-profiling and upwind-downwind methods with the application of RAMP enabled the creation of an important instrument for the management of atmospheric emissions and air quality. Thus, RAMP has become a tool for the internal management of particulate matter emissions, subsidizing the decision on the adoption of corrective measures in real time, allowing monitoring of the evolution of dust emissions in the IC. In addition, the measured concentrations have aided in calculating the emission rates of various diffuse sources, as an alternative to the emission factors estimated by EPA AP-42. RAMP allows for several gains including: monitoring fugitive PM emissions in the short-term; implementation of control and mitigation actions; long-term evaluation and history of PM emission rates; improvement of the data used in atmospheric emissions inventories; evaluation of PM emissions control measures.

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AIR QUALITY ASSESSMENT DURING COPACABANA'S REVEILLON

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Abstract: Fireworks are an ancient tradition started in China about 2000 years ago. Throughout the centuries the western cultures also adopted the fires as a form of celebration in special dates. During the New Year's Eve in Copacabana in Rio de Janeiro city occurs the largest fireworks display in the world. On this day, the city takes several actions to ensure the safety of the event, such as reducing vehicles traffic and allow only pedestrians mobility, hours before the fireworks, which start at 0h on January 1st and lasts about from 12 to 17 minutes. This work aims to assess the impacts on air quality caused by the burning of fires during Copacabana's Reveillon. For this, the data from 2015 to 2018 will be evaluated at Arcoverde monitoring station located in Copacabana, operated by the government of Rio de Janeiro city. At this station, particulate material up to 10 μ m (PM₁₀), ozone (O₃), sulfur dioxide (SO₂) and carbon monoxide (CO) are monitored. Among the first results, it was observed that during the first hour of January 1st the CO, PM₁₀ and SO₂ concentrations were higher than the average of December at the same time. These results were similar to those seen in other pyrotechnic celebrations, such as in India during the Diwali festival, where the daily PM₁₀ level was 2 to 6 times higher than those found on regular days, and SO₂ increased almost 10 times. As in the Chinese New Year, where concentrations of PM_{2.5}, PM₁₀, SO₂, NO₂ and CO were about 1.25 to 4.5 times greater than on the eve of the celebration.

Keywords: : Fireworks, short-time exposure, Copacabana, air quality.

INTRODUCTION

Fireworks are an oriental tradition which started in China about 2000 years ago. Throughout the centuries, the western cultures also adopted the fires as a celebration form in special dates (Breitenecker, 2009). Around the world many celebrations with the extensive burning of firecrackers occur, such as the Lantern Festival and Spring Festival in China, Diwali Festival in India, and New Year's Eve celebrations throughout the world (Yang et al., 2014). On the evening(s) at 1st January is celebrated the denominated 'Reveillon' in Copacabana, in Rio de Janeiro city, Brazil, where about 2 millions of people meet in Copacabana beach. It is considered the largest pyrotechnic show in the world (Riotur, 2018). During 14 to 17 minutes after 0h is burned massive amount of firecrackers, from 17 to 25 tons (Riotur, 2019; Riotur, 2018; Riotur, 2017; Riotur, 2016; Riotur, 2015).

Fireworks or crackers, which are commonly set off during celebrations and vacations, are unique anthropogenic sources that generate massive quantities of air pollutants within a short span of time (Li et al., 2017). According to Barman et al. (2009), this kind of celebration is often characterized to fill with trace gases and particulates into the atmosphere, giving rise to thick smoke clouds. The crackers are reported to have significant adverse effect on environment as well as human health (Barman et al., 2009).

Burning of fireworks is responsible for elevated levels of pollutants gaseous and particles (e.g., SO₂, NO_x, O₃, PM₁₀ and PM_{2.5}) in short span of time causing degradation in air quality (Godri et al., 2010; Singh et al., 2010; Thakur, 2010; Beig et al., 2013).

As firework displays emit massive amounts of NO_x and organic compounds, secondary processes between gasphase and particle-phase compounds may lead to production of secondary air pollutants after firework displayed (Li et al., 2017). Tropospheric ozone (O₃) is a secondary air pollutant formatted from photochemical reaction, when its precursor are on atmosphere, which are nitrous oxide (NO_x) and volatile organic compounds (Atkinson, 2000; Martins et al., 2015).

Burning of firecrackers are associated ecological impacts (Sijimol and Mohan, 2014) and with serious health hazards, such as chronic lung diseases, cancer, neurological and hematological diseases (Shi et al., 2011; Godri et al., 2010). Exposure assessments have associated firework events with negative impacts on respiratory and cardiovascular health (Godri et al., 2010; Beig et al., 2013). The pollution generated by the burning of firecrackers has recently received attention in the scientific community. However, most of the studies were located at China and Indian. The objective of the present study is to assess criteria air pollutants such as PM₁₀, SO₂, CO and O₃ in Copacabana, Brazil during the Reveillon, which is the largest pyrotechnic event in the world.

METHODS

Copacabana is a very residential zone, so its main emission source of gases and particles pollutants into the atmosphere is the vehicle, especially light vehicles (cars) and heavy vehicles (buses). However, it is also strongly influenced by marine aerosols, due to it is in the coast of the Atlantic Ocean (Massone et al, 2015, Ventura et al, 2017). Figure 1 shows an aerial view of the air quality monitoring station and its coverage radius.

The meteorological and air pollutant data were collected from the air quality monitoring performed by the Copacabana automatic station, located in the south zone of Rio de Janeiro city (22°57' 53.9" S, 43°10' 49.75" W), operated by the Rio de Janeiro Municipal Environment Secretariat (SMAC), which has a coverage radius of 2km (SMAC, 2012). SO₂ was monitored by the Ecotech PTY Serinus 50 analyzer with fluorescence detection, PM₁₀ was monitored by the Ecotech Spirant BAM analyzer, which uses the beta attenuation method, and CO was monitored by the Ecotech Serinus 30 analyzer with infrared detector (Soares et al., 2018; SMAC, 2012). All parameters were monitored hourly.



Figure 1. Aerial view of coverage radius of the air quality monitoring station of Copacabana
Font: Soares et al., 2018

The study period was January 1st (New year), which was compared with average hourly in December (usual values), as well as December 31 (New Year's eve) from 2015 to 2018. Atmospheric pollutants were compared to National Air Quality Standards (NAAQS) established by Brazilian Environmental Council - CONAMA Resolution No. 491, November 19, 2018 (CONAMA, 2018).

FINDINGS AND ARGUMENT

The hourly average of PM₁₀ for the month of December was shown in Fig. 2 of the monitoring

station from Copacabana, besides the hourly averages of 12/31 and 01/01.



Figure 2. Hourly average PM₁₀ concentrations of December, 12/31 and 01/01 for 2015-2018

The lowest measured concentrations of PM₁₀ were in the hourly averages of December 31, this period associated to the absence of buses and vehicles in the vicinity of Reveillon de Copacabana, with the purpose of improving the circulation of people in the place. However, it is possible to verify that there are some higher concentrations prior to the burning of fires. The levels in the month of December were basically constant without values very high or low of concentration of PM₁₀. The hourly averages of PM₁₀ of 01/01 exceeded the limit of air quality, according to CONAMA Resolution n° 491/2018, for all years in the times between 00:30 LT and 03:30 LT. It was observed that the highest measured value of PM₁₀ was on 2018/01/01, with concentration approximately 2.5 times above the NAAQS. On this day 25 tons of fireworks were burned, which was more than when compared to the years 2015-2019.

Several studies have been conducted to characterize the impacts of firecracker burning on air quality in China during Spring Festival, which occurs during Chinese New Year, which also use intensive firework displays with 1500 tons of fireworks (Li et al., 2017) indicated significant increases in PM₁₀ levels (Wang et al., 2007; Chang et al., 2011; Huang et al., 2012; Song et al., 2017), similar that occurred in Copacabana's Reveillon.

Pandey et al. (2016) analyzed concentration data during Diwali festival's night, which celebrates lights and crackers in October/November every year, for five criteria pollutants (PM₁₀, PM_{2.5}, SO₂, NO₂, and CO) in Delhi, India. This study shows that the burning of firecrackers, sparkles etc. in huge amounts has a substantial impact on increase in the concentration of criteria air pollutants especially PM₁₀ and PM_{2.5}. PM₁₀ concentration during nighttime of Diwali was reported to be ~8 times higher than the 24-h values prescribed by Indian Ambient Air Quality Standards (100 µg m⁻³). Thakur et al. (2010) also studied air pollution during Diwali festival's night and verified pollutant concentrations found were several times (7.16

times higher for PM_{10} compared to a typical winter day value. While, Copacabana's Reveillon was reported to be ~2.5 times higher than NAAQS ($120 \mu g m^{-3}$) and 4.3 time higher than a typical day in December. Therefore, both researches concluded that extensive use of firecrackers during festival leads to substantial increase in air pollutants.

Fig. 3-5 shows the average concentrations of SO_2 , CO and O_3 for the month of December, 12/31 and 01/01 for 2015-2018 years measured by the automatic monitoring station of Copacabana.



Figure 3. Hourly average SO_2 concentrations of in December, 12/31 and 01/01 for 2015-2018

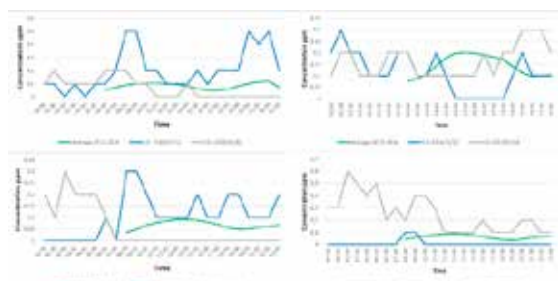


Figure 4. Hourly average CO concentrations of in December, 12/31 and 01/01 for 2015-2018



Figure 5. Hourly average O_3 concentrations of in December, 12/31 and 01/01 for 2015-2018

SO_2 hourly concentrations were very below the NAAQS ($125 \mu g m^{-3}$), don't exceeding $21 \mu g m^{-3}$.

The same way, CO hourly concentrations was 15 time below the NAAQS (9 ppm). Due to it, it was not plotted the NAAQS in Figure 3 and Figure 4, in order to evaluate the behavior of these pollutants in the atmosphere. Both Figures show that SO_2 and CO didn't varied significantly along the time for any year studied during the fire burning. Therefore, this type of event has little effect for this pollutant in air quality. However, Thankur et al. (2010) verified SO_2 concentration higher 1.73 than typical winter day value during Diwali festival's night.

For O_3 , the results show that there was not exceeded the NAAQS ($140 \mu g m^{-3}$). High O_3 concentrations observed over the day (08:30 LT-19:30 LT) of all periods analyzed. High temperatures, low clouds formation and high solar radiation incidence are the main reasons for the results obtained. These are common phenomena in this period of the year that naturally helps O_3 formation in the atmosphere, especially in subtropical climate regions, like the Rio de Janeiro city (Silva et al. 2018). The lowest O_3 concentrations were observed during the early morning due to weak sunlight as well as the consumption processes prevailing over the forming processes (Martins et al. 2015).

CONCLUSIONS

Fireworks display during festive celebrations can cause acute short term air pollution. Although fireworks activities usually take a relatively short time, the high concentrations of gaseous and particulate pollutants can have huge impacts on air quality.

The concentrations of gaseous and particles were lower than those observed in large firework events in cities of China and India. Since these countries suffer with high air quality degradation. However, the fireworks pollution was sufficiently intense to trigger warnings of low visibility and hazy conditions, as well as exceeding the 24-h local air quality standard for PM_{10} during the celebration day. High loads of firecrackers burned during a relatively shorter time span in a mega-city where the situation of ambient air quality has already been alarming almost through-out the year increase the environment degradation. Therefore, it is extremely important reduce other anthropogenic emission sources in this celebration day, to minimize the impact on ecological and human health. Such as applied by Rio de Janeiro Government when interrupt the vehicle circulation around the event and increase the metro offer to dislocation of citizens.

ACKNOWLEDGE

The authors are grateful to the Environment Institute of Rio de Janeiro State (INEA) and Municipal Secretary of Conservation and Environment of Rio de Janeiro (SECONSERMA) for providing the data.

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STUDY OF CIRRUS CLOUDS PHYSICAL PROPERTIES USING THE LIDAR-DUSTER SYSTEM AND RADIOSOUNDING DATA AT NATAL/RN- BRAZIL

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Abstract: Cirrus clouds are classified as the highest clouds in the atmosphere occurring generally from 7 to 18 km, depending on the global region of appearance, and have necessarily ice crystals in their composition. They still have an uncertain influence role in climate, therefore are seen as important atmospheric elements to be studied. Lidar systems (*Light Detecting and Ranging*) have shown efficiency in the collection of cirrus characteristics which can help in its better parameterization in climatic and atmospheric models. In this work a collection of physical characteristics of cirrus was carried out, for January and February of 2017 and 2018, at Natal's atmosphere using Lidar DUSTER's data (5.84 S 35.20 W), a partnership UFRN/IPEN-SP. Morphological patterns of that clouds have been observed according to its heights as well as variations. Clouds with thinner depths and tenuous are observed at the top regions of troposphere, around 16.0 km. Otherwise, clouds with bigger vertical extensions are found around 12.0 km. The height of occurrence of cirrus in Natal, for the considered period vary from a minimum height of 7.0 km to a maximum of 16.0 km. Cirrus clouds most frequently occurred at a medium height of 12.0 km, considering both years. Those clouds had a considerable representativeness over the city atmosphere corresponding to 67% of total Lidar measured days. Besides the Lidar system was also used data from radiosounding technique. The behavior of the meteorological variables such as relative humidity was analyzed for the regions in which were found cirrus by the Lidar DUSTER. Within the region limits was verified a significant increase of relative humidity values. This behavior is not observed in lower regions where there is not any clouds presence as well in a day without cirrus appearance. In addition, future analyzes of the potential equivalent temperature profile will be studied in order to verify the effect of the cirrus clouds occurring in the temperature and humidity profile in a combined manner. Also, is expected to evaluate the possible impacts of cold air intrusion of the stratosphere in layers of cirrus clouds. In conclusion, Lidar DUSTER data demonstrates to be efficient in the identification of cirrus clouds over Natal's atmosphere contributing to a better comprehension of its behavior and role in the region of study.

Keywords: Cirrus clouds, Lidar-DUSTER, Radiosounding.

INTRODUCTION

Cirrus clouds are those found at the highest regions of the troposphere. They have a fibrous visual appearance and their height can vary generally between 7 and 18 km, depending on the region of the globe (SEINFELD; PANDIS, 2016). They have ice crystals in their composition and can be found at temperatures well below the freezing point necessary for homogeneous nucleation of water which is -41 ° C (LYNCH et al., 2002). It is known that clouds, in general, have an important influence on the terrestrial radiative balance. According to Chen, Chiang and Nee (2002), cirrus-like high clouds have both the ability to absorb long-wave radiation returning from the earth's surface and to reflect short-wave radiation from the sun. Therefore, a

better understanding of the interference factors responsible for the balance between the warming and cooling of the atmosphere caused by these clouds is necessary. Characterization studies of the optical and physical properties of cirrus clouds are important in order to facilitate the understanding of their degree of influence on the climatic aspects on Earth. The Lidar remote sensing system allows the collection of information from the atmospheric vertical structure with high spatial and temporal resolution (WEITKAMP, 2005) and, therefore, is seen as an important tool in the studies of these clouds. The Lidar system, named DUSTER, installed in a container in Natal at the Federal University of Rio Grande do Norte contributes as a tool of extreme importance for the study of these clouds for the region. At the same time, relative humidity data

obtained from radiosoundings released by the *Centro de Lançamentos Barreira do Inferno* were essential to allow the comparison with lidar data, reinforcing the validity of the Lidar product to study cirrus and vice versa. Thus, for the first time, a survey and discussion of the physical properties of cirrus clouds over Natal's atmosphere is carried out. This study intends to be the first step to further researches which may include not only macrophysical aspects but microphysical and optical properties of these clouds which are important parameters to enhance climatic models for the region.

METHODS

The Lidar DUSTER

The Lidar DUSTER system was installed in the city of Natal in January 2016 and began to be officially operated in the month of February of the same year. The DUSTER installation is done via a collaboration between the Center for Lasers and Applications (CLA) of the Nuclear and Energy Research Institute (IPEN) and the Federal University of Rio Grande do Norte (UFRN). The laboratory is located in a container at the Federal University of Rio Grande do Norte - Campus Natal Central, in the Department of Atmospheric and Climatic Sciences (5.84 S 35.20 W). Such a container allows the opening of a window in the ceiling through which the laser beam from Lidar is directed to the atmosphere for data collection of atmospheric profiles. The Laboratory can be seen at Figure 1 below:



Figure 1 – DUSTER Laboratory. Department of Atmospheric and Climatic Sciences of UFRN, Campus Natal - Central (5.84 S 35.20 W). Source: The author's collection.

Figure 2 presents the DUSTER Lidar system in operation. One can observe the main components of the DUSTER system which includes: the transmitter part consisting of the laser source(1), the beam expander *BMX* (2) - a device used to decrease the divergence of the laser - and a small mirror (3) that directs the laser into the atmosphere, all on the same axis of direction; the receiving part, consisting of a Cassegranian type telescope (4); the detector part (5), located just below the telescope, consisting of a box of sensors which select the

wavelengths and polarization state of interest of the collected light; the data acquisition system, *Licel* (6) and the control box (7). The data logging, storing, and processing part is performed by the operator on a computer with specific softwares (located near the system but not shown in the picture).

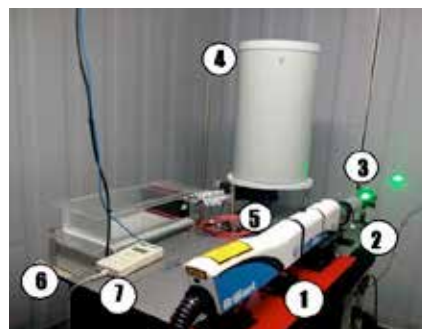


Figure 2 – Lidar DUSTER system in operation and its main components. Source: The author's collection.

Data Analysis

The data collected by the DUSTER system is so-called raw data. These data represent measures of the total backscatter signals from the interaction of the radiation emitted by the laser pulse with the atmospheric constituents, mainly molecules and particles. A pre-processing and processing data is done to get the final products as showed in the flow chart of Figure 3 below:

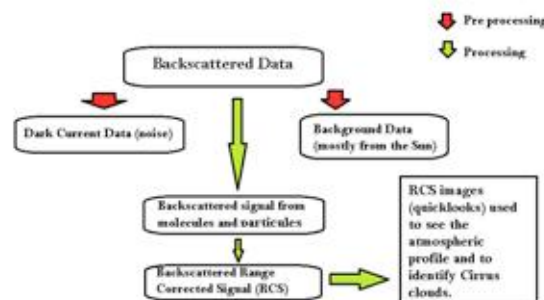


Figure 3 - Flow chart of the main data processing steps. Source: Author.

The dark current and background signals are removed in a pre-processing step so that only the signal of the backscatter of the particles and molecules remains in the vertical profile of the data (SILVA RIQUELME, 2015) which is corrected by the square of the distance to obtain the final products - the so called Range Corrected Signal (RCS) graphs. These steps are done using the Lidar Range Corrected Signal algorithm - LIRACOS, developed by IPEN's Laser Environmental Applications Laboratory and adapted by the UFRN research group once this methodology can be used for the different contexts in which applies, and in this case for Natal's data to obtain false-color graphics of the corrected signal for further interpretation and identification of cirrus clouds. The interpretation of the graphs is

based on the analysis of the backscatter signal intensities represented by different colors on an arbitrarily defined scale. The final result/product is evidenced in the image plotted, in which is possible to identify the regions of greater and lesser intensity of the signal according to the respective colors defined. Thus, the final image will represent the temporal distribution of the atmosphere, retrieved by the vertical intensity profile of the total backscattered signal. The RCS images provides the so-called curtain plots of the atmosphere, which is possible to identify the Atmospheric boundary layer and also clouds of the Cirrus type.

The measurement period considered for this study comprises data from two measurement campaigns carried out in Natal named MOlitoring campaign LOng-range Transportation Over Natal I and II (MOLOTOV I and MOLOTOV II). The months of January and February of 2017 and 2018 were used from the respective campaigns. The data analysis was divided as follows:

1) Block I:

Corresponding to MOLOTOV I and II for afternoon period (from 14 and 18 hours, local time, varying within the range): Survey of the physical characteristics of the clouds with the definition of minimum, maximum and average heights, frequency of occurrence and morphology analysis comparing the same period for both campaigns.

2) Block II:

Only MOLOTOV I data was used for its morning period (from 09h to 11h30, local time). The purpose was to compare DUSTER data with Radiosounding data which is released at the nearest to Lidar measurements (09h local time) similar to what was done by Gouveia, Barbosa and Barja (2014). This allows the investigation of correlation between cirrus physical characterization with vertical profiles of relative humidity collected by the radiosondes.

FINDINGS AND ARGUMENT

In a total 77 days were processed for both blocks from which 52 days presented cloud of the Cirrus type. This corresponds to approximately 68% of the days, a significant value over the data. From these 52 days, 35 corresponds to Block I and 17 to Block II which are analysed as follows.

Block I: Survey of physical characteristics of cirrus clouds in Natal

Figures 4 and 5 are quicklooks also named RCS graphs, obtained from the DUSTER's processed data which shows the minimum and maximum heights (emphasized by the red lines) identified for cirrus for the total period of data (MOLOTOV I + MOLOTOV

II). This was carried out for the total data to account for physical properties of cirrus on the vertical profile. These two figures were chosen from all graphics to exemplify the final product from which is possible to see the cirrus signal in the vertical profile as a cyan colour in both graphs.

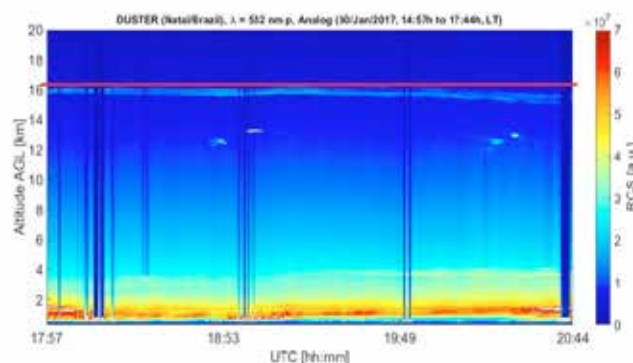


Figure 4 - RCS graphic showing the maximum height of cirrus over Natal on 30 January 2017, around 16.0 km (red line at the top of the cloud). MOLOTOV I. Source: Author.

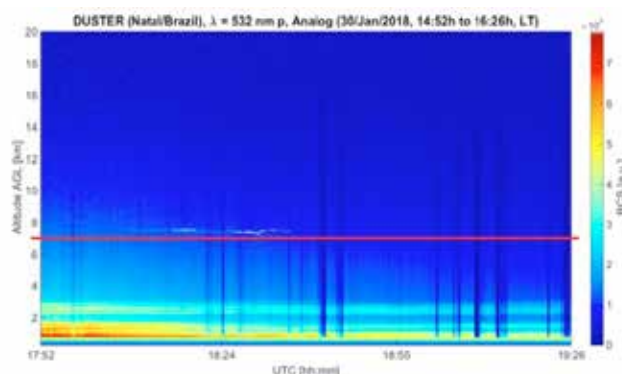


Figure 5 - RCS graphic showing the minimum height of cirrus over Natal on 30 January 2018, around 7.0 km (red line at the bottom of the cloud). MOLOTOV II. Source: Author.

In terms of morphology, it was possible to observe a similar morphological behaviour of the cirrus according to the time they were observed in the MOLOTOV I campaign. When they are observed in higher heights, at the top of the troposphere, they have finer, thin and dispersed thicknesses, with less intense backscatter signal; whereas when observed at medium heights they generally present large extensions, thicknesses and high density, returning a much more intense backscatter signal. An example of these two main morphology patterns can be seen in Figures 6 and 7 as follows.

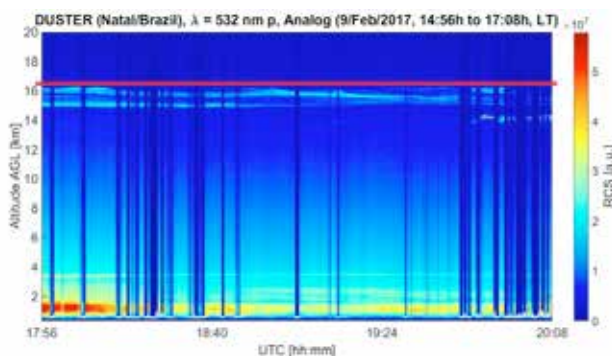


Figure 6 - RCS graphic showing a typical cirrus cloud shape at higher altitude over Natal on 09 February 2017, maximum height around 16.0 km (red line at the top of the cloud). MOLOTOV I. Source: Author.

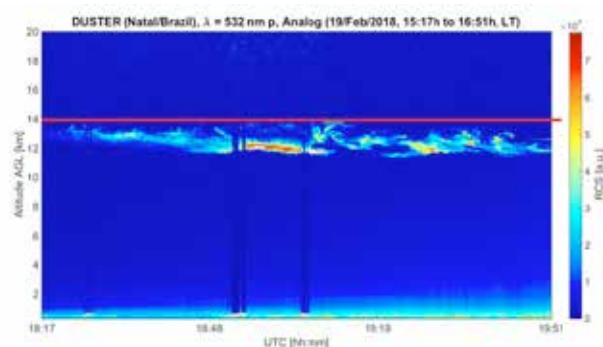


Figure 9 - RCS graphic showing a morphological variation of cirrus over Natal on 19 February 2018, the maximum height is around 16.0 km (red line at the top of the cloud). MOLOTOV II. Source: Author.

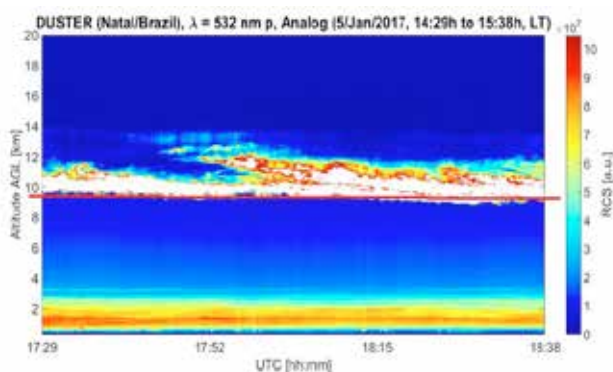


Figure 7 - RCS graphic showing a typical cirrus cloud shape at medium altitude over Natal on 05 January 2017, minimum height around 10.0 km (red line at the bottom of the cloud). MOLOTOV I. Source: Author.

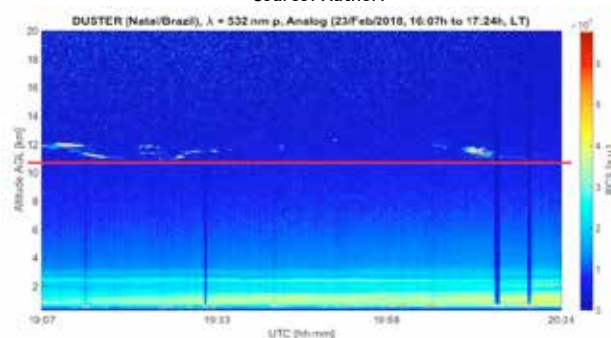


Figure 10 - RCS graphic showing a morphological variation of cirrus over Natal on 23 February 2018, minimum height around 11.0 km around (red line at the bottom of the cloud). MOLOTOV II. Source: Author.

In general, it is possible to say that, during the MOLOTOV I campaign in its afternoon period, there was a considerable presence of cirrus clouds over the city's atmosphere. They covered more than half of the data collected for the two months, representing 74% of the entire campaign, corresponding to 23 days out of 31. MOLOTOV II presented a wider variation of morphology. Examples of this varied morphology can be seen at Figure 8, 9 and 10.

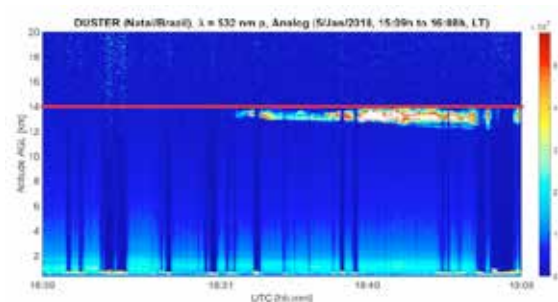


Figure 8 - RCS graphic showing morphological variation of cirrus over Natal on 05 January 2018, the maximum height is around 14.0 km (red line at the top of the cloud). MOLOTOV II. Source: Author.

The second campaign presented a smaller number of cirrus occurrences than its previous which corresponded to 57% of the total number of days, accounting for 12 days out of 21. Despite this, the presence of cirrus is still considerable once it corresponds to more than half of the total measurements.

Below at Figure 11 is the graph of frequency of cirrus average heights for total period of data.

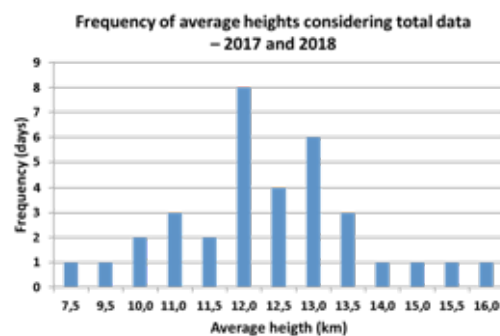


Figure 11 - Frequency chart of average cirrus occurrences in Natal for the total of the two campaigns corresponding to Block I. Source: Author.

As can be seen in Figure 11, the more frequent average height of occurrence of cirrus within the period of the two campaigns is around 12.0 km. Thus, it can be said that for the afternoon of January and February at Natal's atmosphere will be more likely to observe cirrus at an average height of approximately 12.0 km.

The chart 1 shows the summary of results, the main findings and physical parameters obtained related to Cirrus occurrence over Natal's Atmosphere for the First Block of data.

Chart 1 - Summary of results

DESCRIPTION	AFTERNOON		
	MOLOTOV I (2017)	MOLOTOV II (2018)	TOTAL
LIDAR MEASUREMENTS DAYS	31	21	52
MEASURED DAYS WITH CIRRUS	23	12	35
% DAYS WITH CIRRUS	74%	57%	67%
MINIMUM HEIGHT OF CIRRUS OCCURRENCE	8,0 km	7,0 km	7,0 km
MAXIMUM HEIGHT OF CIRRUS OCCURRENCE	16,0 km	14,0 km	16,0 km
AVERAGE HEIGHTS OF CIRRUS OCCURRENCE	12,6 km	11,6 km	12,3 km
MORE FREQUENT AVERAGE HEIGHT	13,0 km	12,0 km	12,0 km

Source: Author.

Cirrus demonstrated to have a considerable percentage of appearance over the data corresponding to 67%. Its minimum height, considering its bottom, was 8.0 km for MOLOTOV I and 7.0 km for MOLOTOV II and its maximum height, considering its top, occurred at 16.0 km and 14.0 km respectively. The average height of occurrence were similar for both campaigns as well as its more frequent average height basically around 12km.

Block II: Association of DUSTER data with radiosounding data

To compare the height of cirrus with the meteorological variable of relative humidity corresponding to these heights, the days with more expressive presence of cirrus in the two months of the campaign were selected. Data from January 2017 (morning), counted the total of 17 days of measurements. Of these, the days with presence of cirrus totaled 9 which corresponds to approximately 53% of the measures. For the month of February 2017, only 8 days were measured, due to atmospheric conditions that made it impossible to collect data, with cloudy sky and rainy days. From this total measured, all the quicklooks showed presence of cirrus, counting 100% of the data with presence of the same ones.

One day of each month was selected to investigate these characteristics. In addition, for the month of

January a day was also selected in which no presence of cirrus was observed in the quicklook to investigate any differences in the vertical profile corresponding to the relative humidity for this day compared to the profiles of days with cirrus. In the figures 12 and 13 below it is possible to see one day with cirrus presence and one day without from lidar RCS graphs and also the respective radiosondes vertical profiles of relative humidity for each day.

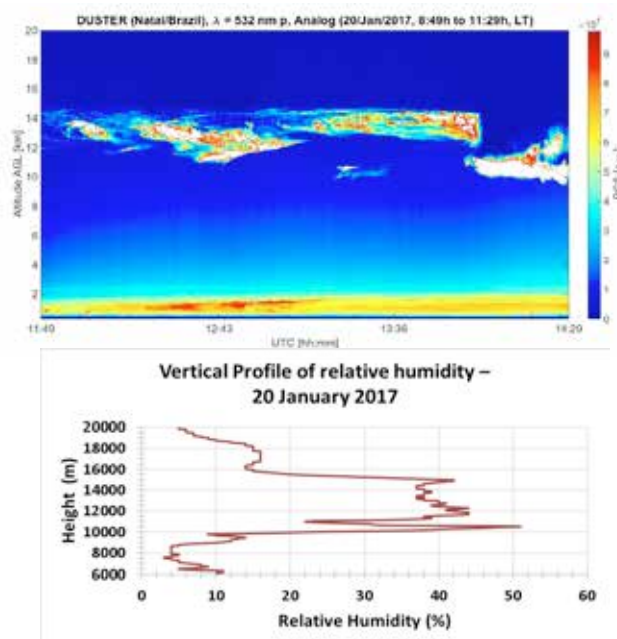


Figure 12 - Quicklook and relative humidity vertical profiles, respectively, for a day with Cirrus presence from around 10.0 to 15.0 km. Day: 20 January 2017. Source: Author.

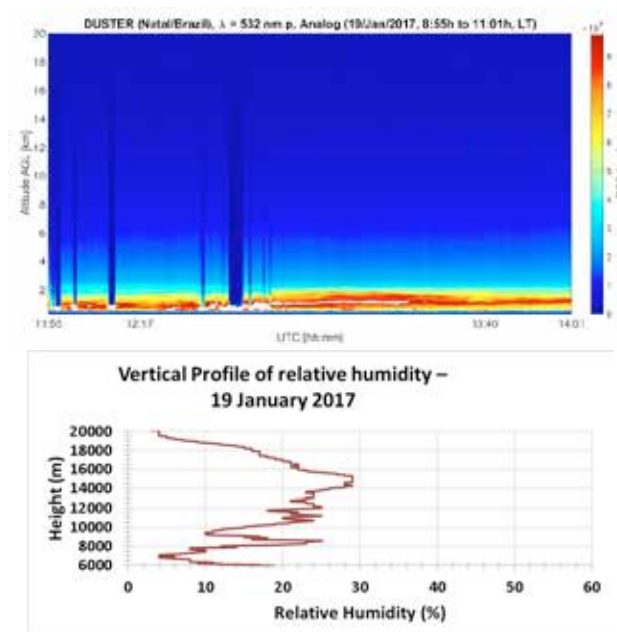


Figure 13 - Quicklook and relative humidity vertical profiles, respectively, for a day without Cirrus presence in the

atmosphere vertical profile. Day: 19 January 2017. Source:
Author.

Figure 12 shows the quicklook for January 20, 2017. On this day, it is clearly observed cirrus clouds signal between the altitudes of 10.0 km and 15.0 km on Lidar profile. This signal varies from less intense to more intense colors, from cyan through red to white, showing regions where there is less and more signal intensity and consequently density of cirrus. The graph of Figure 12 shows the relative humidity variable (collected with the radiosonde) and how it varies with altitude on the same day. The x-axis corresponds to the values of relative humidity (in percentage). In the range of the region of interest, where the presence of cirrus was visualized on the RCS image, is observed that relative humidity was around less than 15% (slightly below 10000 m). As the altitude increases in the vertical profile of the graph, this value suffers a great variation reaching a maximum of 50%. In the delimited region, from 1000 m to 15000 m, a higher relative humidity value is verified, compared to the lower and higher regions, indicating a variation in the presence of water vapor in this region and thus cloud presence. This is something expected when there are clouds in general and also cirrus clouds, since the presence of water vapor is a prerequisite for the formation of ice crystals characteristic of this type of cloud.

On the other hand, in Figure 13, the RCS image for January 19, 2017, demonstrates a profile in which no signal is verified that could possibly corresponds to the appearance of cirrus that day over the city's atmosphere. Thus, a quicklook is observed in which the blue colour, close to zero intensity, remains for the entire range varying between 7.0 and 18.0 km where some cirrus signal would be expected. When the relative humidity chart is observed for this day, it can be seen that its values do not exceed 30% remaining below it along the vertical profile. These values indicate a lower presence of water vapor in the atmosphere in this day, not sufficient to form cirrus, in the regions where those clouds could appear confirming that there is no cloud presence in the region as visualized by the Lidar.

CONCLUSIONS

Cirrus clouds are still the subject of few studies, mainly in Brazil. However, due to its growing importance related to the investigation of its role in climate change studies, this perspective has changed. The Lidar equipment provides the opportunity to study these clouds and obtain information about their main characteristics, such as their physical properties. In Natal, for the first time, through this study, it was possible to survey and discuss these characteristics. More specifically the study of physical characteristics of cirrus clouds

corresponding to their minimum, maximum and average occurrence heights, coverage and thicknesses. It was possible to survey their representativeness in two campaign periods, corresponding to the years 2017 and 2018; their frequency of occurrence according to average height of appearance; and their morphological patterns and their variations. For a first study, the results obtained are of great relevance once now there are data of great temporal and spatial resolution about cirrus clouds for the atmosphere of Natal. At the same time, it was possible to combine the data obtained by Lidar with the radiosonde data. This is an important analysis since two sources of data are used to giving consistency and reliability to the information about the target of interest. In future studies, to reinforce this analysis it can be considered more days and also the inclusion of other relevant meteorological variables for comparison. Future analyzes of the potential equivalent temperature profile will be studied in order to verify the effect of the cirrus clouds occurring in the temperature and humidity profile in a combined manner and also is expected to evaluate the possible impacts of cold air intrusion of the stratosphere in layers of cirrus clouds. It is important to maintain the operation of the Lidar continuously to obtain more seasonal data to verify the behaviour of the physical characteristics of these clouds throughout the year, for example. It is known, however, that this operation will always depend on the weather conditions of the city, something that limits the data collection.

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WET DEPOSITION FLUX IN SUBTROPICAL AREAS: CASE STUDY OF FLORIANÓPOLIS

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Abstract: Wet deposition of air pollutants is a concern for ecosystems. Understanding the wet deposition fluxes and dominating factors of this process is a challenge due to lack of information. In this study, the chemical composition of the rainwater of Florianópolis-SC was evaluated, using two sampling locations along the city. The sampling period was between 10/10/2017 and 08/03 of 2018, representing the end of spring and early summer. The concentrations of chloride, sulphate, nitrate and ammonium ions were determined through the analytical technique Capillary Zone Electrophoresis (CZE). Throughout the results, it was also observed the influence of the number of dried days previously to the sampling event on the variability of the chemical composition of wet deposition. A strong marine influence on chloride fluxes ($1.23 \text{ g.m}^{-2}.\text{year}^{-1}$) was observed. The nitrate and sulfate fluxes presented values of $0.12 \text{ g.m}^{-2}.\text{year}^{-1}$ and $0.29 \text{ g.m}^{-2}.\text{year}^{-1}$, respectively, lower than those found in the literature. This study provides key quantitative information of wet deposition fluxes in coastal areas.

Keywords: Air Pollution, Wet deposition, Acid rain, Precipitation chemistry.

INTRODUCTION

Wet deposition is considered the most important atmospheric cleaning process. This mechanism removes pollutants from the atmosphere through precipitation, transferring air contaminants to another reservoir (such as soil, water bodies and plants), and working as source of nutrients and pollutants for ecosystems (Lacaux et al., 2009). The emissions growth due to burning fossil fuels and biomass would drive to significant impact on atmospheric chemistry and also on wet deposition fluxes (Conradie et al., 2016). It would rise the wet deposition fluxes of nitrate, chloride, ammonia and sulphate, for instance. The oxidation of these chemicals causes several deleterious consequences to the environment, such as decline of forests and crop productivity, increasing lake and soil acidification, and loss of biodiversity (Vet et al., 2014).

Although the main air pollutants are regularly monitored in a few Brazilian cities, there is no monitoring of wet deposition fluxes and its transfer to another reservoirs (Rocha et al., 2002). There are only few studies on the literature about rainwater chemistry in Brazil, especially in subtropical and urbanized areas. It is a relevant question in states like Santa Catarina (SC) in Brazil, where industrial, agroindustrial, urban and preserved environments coexist. Moreover, there is no air quality monitoring network in SC.

In the present study, we investigate the wet deposition fluxes of NO_3^- , Cl^- , NH_3 and SO_4^{2-} in Florianópolis - Santa Catarina. Florianópolis is the most important city in Santa Catarina, with large fleet and population.

METHODS

Capital of Santa Catarina state, Florianópolis has a population of 485,838 inhabitants and a vehicle fleet of 346,736 automobiles (IBGE, 2018). Wet deposition samples were collected using a rainwater sampler with diameter of 21.6 cm. These samplers can handle a maximum rain volume of 20 liters. Wet deposition samplers were installed on the campus of the Federal University of Santa Catarina (UFSC) and in the Municipal Park of Lagoa do Peri, displaced 14 km from each other. Figure 1 shows the locations of each sampling point in Florianópolis. In this study, Capillary Zone Electrophoresis (CZE) were used as analytical technique in the chemical characterization and quantitation of NO_3^- , Cl^- , NH_3 and SO_4^{2-} .

To exclude the influence of storm size on sample dilution, the volume-weighted average (VWM) (1) was used to calculate the monthly and annual wet deposition fluxes (2). For each solute of rainwater, the measured concentrations in the sample were combined to create a VWM concentration for each collection date (Huang et al., 2012):

$$VWM_a (\mu\text{g.m}^{-3}) = \frac{\sum_{i=1}^n C_{ai} \cdot V_i}{\sum V_i} \quad (1)$$

$$Flux_a (\mu\text{g.m}^{-2}.\text{year}^{-1}) = \frac{VWM_a \cdot \sum V_i}{A \cdot t} \quad (2)$$

where C_{ai} is the concentration of species a in sample i , n is the number of samples, V_i is the volume of precipitation solution for sample i , A is the area of sampler and t is the time of sampling camping. The rainwater concentrations measured

during sampling campaign (from October 2017 to March 2018) were extrapolated to the whole year.

A total of 50 samples were collected. Python was applied for data manipulation and analysis.

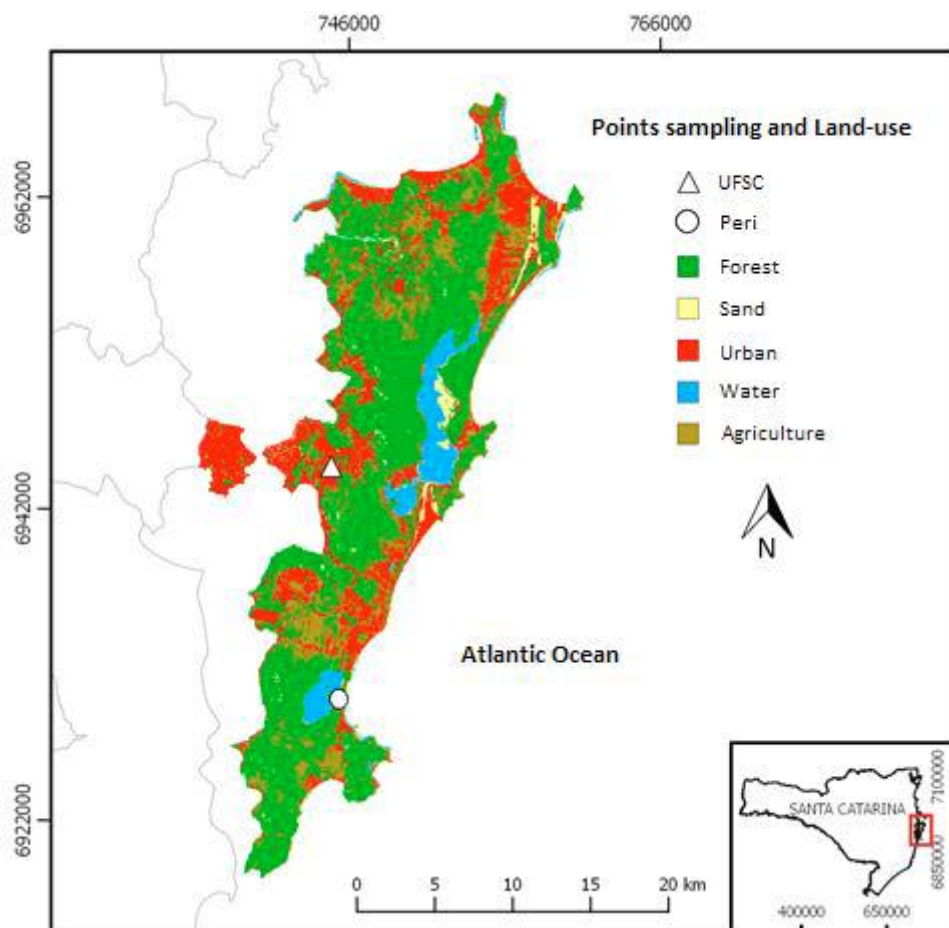


Figure 1. Location map of sampling points (Santos et al., 2019)

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Figure 2 presents the frequency, dispersion and correlation tests of wet deposition fluxes at two sampling sites in Florianópolis. Gray circles represents the samples collect at Peri, while black circles represents UFSC. It is possible to observe the a linear correlation among SO_4^{2-} , Cl^- , NO_3^- and NH_3^+ . The Spearman test showed a strong correlation between Cl^- and SO_4^{2-} in Florianópolis. The city is located in coastal zone, where is observed a strong sea salt influence and, consequently, high concentration of its associate ions (i.e. Cl^- and SO_4^{2-}). Another interesting correlation was

between SO_4^{2-} and NO_3^- , which could be responsible for the acidification of rainwater. The nitrate is emitted mainly by vehicules and its the correlation with sulfate may indicate a possible anthropogenic origin of both ions found in wet deposition. However, sulfate could be also found in marine spray. Therefore, the exact origin of theses ions remains unknown.

NH_3 has an alkaline character and could mainly be associated with natural sources or vehicular emissions. Further analysis would be required to better understand the relationship between ions and its origin.

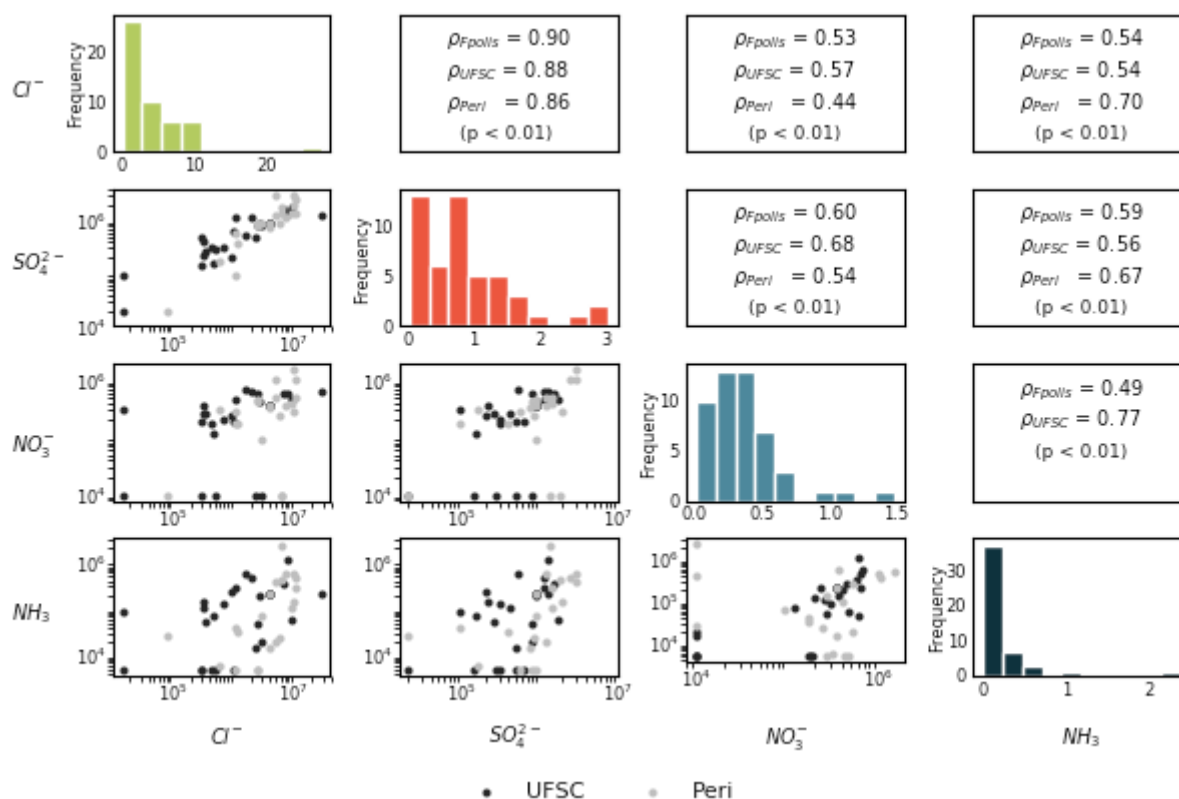


Figure 2. paired analysis of ions at collection points

Table 1 shows the comparison of wet deposition fluxes of some sampling sites around the world. It can be seen that the wet deposition fluxes in Florianópolis is lower than the other sampling sites on Table 1. When compared to São Paulo/BR sampling site, the sulfate and nitrate levels in

Florianópolis were much lower. São Paulo is a megacity with intense industrial and urban activity. When compared to Asian, African and North American areas, the capital of Santa Catarina still has a lower flux of pollutants.

Table 1. Annual wet deposition fluxes of Cl^- , SO_4^{2-} , NO_3^- and NH_3 at various sites. Unit: $\text{g.m}^{-2}.\text{yr}^{-1}$

Sites	Category	Cl^-	SO_4^{2-}	NO_3^-	NH_3	References
Delhi, India (1994)	Miscellaneous	----	----	0.052	0.27	Kulshrestha et al. (1996)
São Paulo, Brazil (1997-1998)	Urban	0.16	2.5	2.2	0.78	Rocha et al. (2002)
São Paulo, Brazil (2003-2007)	Urban	0.15	0.50	1.17	0.44	Coelho et al. (2011)
USA (1985/2012)	Miscellaneous	----	----	0.15	0.20	Du et al. (2014)
China (1995-2007)	Urban	----	----	0.89	1.42	Du and Liu (2014)
South Africa (2009-2014)	Urban	0.47	2.36	1.51	0.38	Conradie et al. (2016)
Florianópolis, Brazil (2017-2018)	Urban/Coast	1.23	0.29	0.12	0.059	Present Study

Figure 3 shows the monthly wet deposition fluxes in Florianópolis. In this same figure the daily precipitation is also presented. The higher flux of NO_3^- occurred in november ($0.072 \text{ g.m}^{-2}.\text{month}^{-1}$). High concentrations of chloride were found, due to sea salt spray and marine influence. The annual flux of Cl^- was $1.23 \text{ g.m}^{-2}.\text{year}^{-1}$. A study with similar geographic location was performed by Davies et al (2018) in the coastal zone in Australia,

where high concentration of Cl^- in wet deposition flux was also found.

The annual ammonium flux in Florianópolis was $0.059 \text{ g.m}^{-2}.\text{year}^{-1}$, representing a tenth of flux of São Paulo (Coelho et al., 2011). The maximum flux of NH_3 occurred in march, with value of $0.024 \text{ g.m}^{-2}.\text{month}^{-1}$. Annual sulphate fluxes was $0.29 \text{ g.m}^{-2}.\text{year}^{-1}$, with maximum value in november.

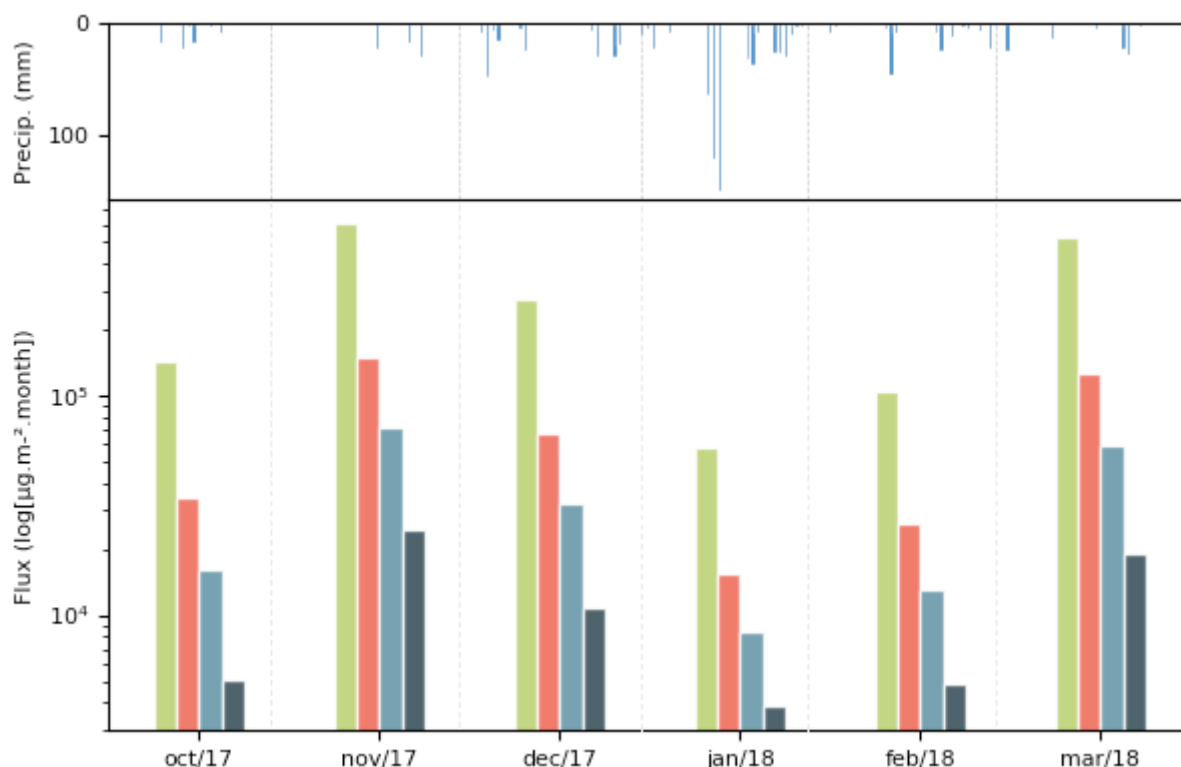


Figure 3. Comparison between fluxes over the months.

From Figure 3, it is possible to identify the influence of dried days on the chemical composition of wet deposition. November/2017 and March/2018 presented the higher concentration of pollutants in wet deposition. These months presented lower precipitations, respectively 135.33 mm and 128.17 mm, and higher frequency of dried days before sampling event. These factors would lead to higher concentration of ions in wet deposition (Coelho et al., 2011).

The climate in Florianópolis is subtropical, with humid season from January to March. In January/2018 was observed 539.27 mm of precipitation and a reduced number of dried days. In this month, the samples were collected in events after intense precipitation, with the atmosphere unload of air pollutants. Therefore, the results show that wet deposition fluxes is higher when the total montly precipitation is lower and the frequency of dried days is higher.

CONCLUSIONS

The estimation of wet deposition fluxes has high significance due to the impact of pollutants on the ecosystem. This study provides important information of wet deposition of air pollutants in the coastal zone. Cl^- was the most abundant ion in the collected samples, due to the proximity

between sampling site and the ocean. The anions Cl^- and SO_4^{2-} showed a high correlation, mainly due to sea salt/marine influence. Annual deposition fluxes of chloride found in Florianópolis are like those observed in a costal environment in Australia. The annual fluxes of sulphate and nitrate deposition were lower than those found in other urbanized regions of the world. Ammonia annual wet deposition fluxes found in Florianópolis were lower than those found in the literature.

During the sampling camping, in the months of march and november were found the highest deposition fluxes of the analysed ions. The results showed that the wet deposition of air pollutants is higher when the monthly precipitation is lower and the occurrence of dried days is higher before the sampling event.

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DETERMINATION OF AIR POLLUTION MAIN SOURCES IN A MEDIUM-SIZED CITY IN SÃO PAULO

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Abstract: Just as important as knowing the air quality of a region is knowing the main sources that contribute to the levels of its pollution. The chemical compounds present in the measured particulate matter indicate the sources that are responsible for the concentration of particles. The identification of the sources is important in future decisions to reduce their concentrations and its health impacts. Most of the studies is focused in big metropolitan areas, but the medium-size cities concentration important fraction of population in Brazil. This study aims to evaluate the active polluting sources and air quality in Valinhos city (São Paulo), and the relation of the surface concentrations of PM_{10} , $PM_{2.5}$, O_3 and NO_x with meteorological conditions. The receptor model chosen for the source estimates of ambient particulate matter was Positive Matrix Factorization (PMF), where 4 sources were identified to $PM_{2.5}$. Valinhos is a medium-sized city with 128,000 people approximately, which is located in the Campinas Metropolitan Region (CMR), the second largest Metropolitan Region of the state, and nearby to São Paulo Metropolitan Region (SPMR) and may be impacted by transport of pollution from these sites. The sample site is located in an area with native vegetation cover and away from the center of the city. During the sampled period (from 05/12 to 07/12) PM_{10} , $PM_{2.5}$ and NO_x concentrations were below the air quality standard established by the São Paulo Decree whereas the O_3 overrun the standard in one day only. In this study it was concluded that the $PM_{2.5}$ main sources were vehicular, biomass burning, soil resuspension and industrial. In addition, based on the parameters measured and in the analyzed period, it can be stated that the air quality in Valinhos can be considered good.

Keywords: air quality, chemical compounds, receptor model.

INTRODUCTION

Air pollution in urban environments comes from numerous sources. In large cities, vehicular emissions generally respond for a higher percentage of contribution when compared to others (industrial, biomass burning and waste, crustal and particle resuspension), and this is due to the number of vehicles in circulation.

In a study carried out in six Brazilian capitals, Andrade et al. (2012) found that the predominance of emissions by vehicular source in three of them (São Paulo, Rio de Janeiro and Recife). However, Belo Horizonte presented as main source the crustal elements due to mining activities that predominate in this region and throughout the state.

Identifying and understanding each source's contribution to local pollution helps in the development of strategies for controlling air pollution. This type of analysis is necessary for both small and medium-sized cities and megacities, either to support policy-making to prevent air from becoming polluted or to improve air quality.

As part of a comprehensive study that aims to analyze the air quality at many middle size cities in Southeast of Brazil, the objective of this work is to evaluate the main pollutant sources and air quality

in the city of Valinhos (SP) from concentrations of particulate matter (PM_{10} and $PM_{2.5}$), nitrogen oxides (NO_x) and ozone (O_3) and how neighboring cities may be influencing their concentrations.

METHODS

Sampling was performed from May to July 2018 (05/12 to 07/12) in the city of Valinhos, a medium sized city located in the state of São Paulo. The sampling site was set at Abraão de Moraes Observatory (OAM) of the Institute of Astronomy, Geophysics and Atmospheric Sciences (IAG) of the University of São Paulo (USP) (Figure 1). The observatory is far from the city in an area of 450,000 m² with native vegetation cover (OBSERVATÓRIO, 2018).

The analyzed pollutants were particulate matter (PM_{10} and $PM_{2.5}$), ozone (O_3) and nitrogen oxides (NO_x). The equipment was installed approximately 10 meters above the ground, in the observatory dome. The NO_x and O_3 monitors were installed (Thermo Fischer Scientific) with continuous measurements (hourly) and the particulate sampler (Tupiniquim) (Hetem, 2014) with automatic filter

replacement (Polycarbonate - 47 mm diameter) every 48 hours.

The concentrations of the pollutants were organized in order to analyze the air quality of the region. The meteorological data were obtained from the Environmental Company of São Paulo State (CETESB) and National Center for Natural Disaster Monitoring and Alerts (CEMADEN) database and related to the concentration data. To determine the different pollutant emission sources, the multivariate analysis of Positive Matrix Factorization (PMF) was applied.

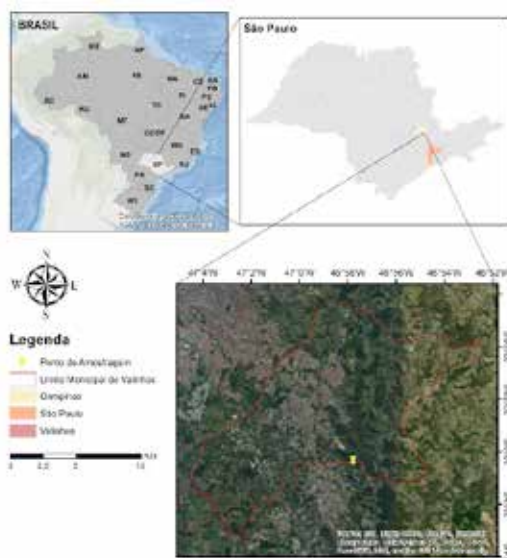


Figure 1. Location of study area.

FINDINGS AND ARGUMENT

The sampling period was relatively dry, with few occurrences of precipitation (Figure 4). The temperature and relative humidity averages were around 20 °C and 64%, respectively, which was already expected (drier winters and wetter summers) (Alvares et al., 2014).

Figure 2 presents the moving average concentrations (8h) of O₃ for the city of Valinhos during the entire sampling period. According to State Decree n° 59113 of 2013, which establishes a limit of 140 µg m⁻³ for the 8-hour moving average, ozone standard was not exceeded. The periods with the highest concentrations were between 05/22 and 05/24, at the beginning of sampling, and at the end of sampling between 06/30 and 07/09.

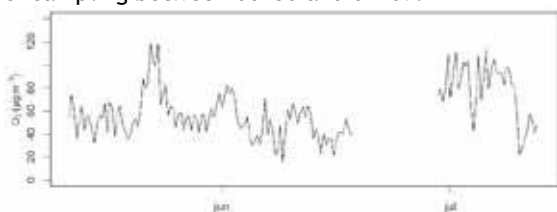


Figure 2. 8-h moving average O₃ concentration.

In Figure 3 is presented the daily profile of O₃ concentration for the city of Valinhos. It can be noticed a prolonged peak (11 am to 9 pm), with maximum around 4 pm. The average concentration throughout the evening-night (period that there is no solar radiation) remained close to 40 µg m⁻³.

In a comparative study of O₃ daily profiles, Martins et al. (2016) found similar profiles in stations with distinct characteristics (population and economic activity). The city of Londrina (PR) was the station that presented a more similar behavior to the city of Valinhos, with a longer and less accentuated peak. However, the mean concentration of the period in Valinhos was higher than the concentrations obtained in Martins et al. (2016), with an average value of 60 µg m⁻³.

In general, sampling in cities less urbanized or located in spaces with greater vegetation (parks, reserves, etc.) has presented concentrations of O₃ greater/equal to more urbanized cities. This is because in less polluted places there is a lower consumption during the day of O₃ produced, whereas in more polluted places there will be more consumption (Banan et al., 2013; Martins et al., 2015).

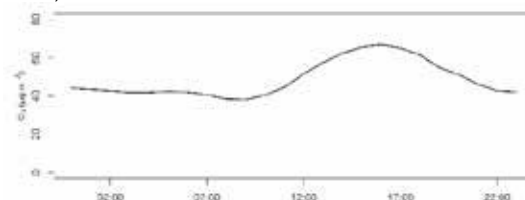


Figure 3. Hourly average O₃ concentration.

Particulate matter measurements showed failures, as shown in the series below (Figure 4), however it was possible to observe that particulate concentrations (PM₁₀ and PM_{2.5}) were low.

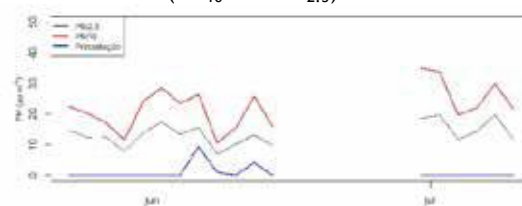


Figure 4. 48-h average PM concentration and precipitation.

Figure 5 shows the wind-rose for O₃ pollution. It can be seen that the predominant direction of the wind is southeast, but with relatively lower concentrations. In less occurrence, it was observed winds of northeast and northwest with slightly higher concentrations. Southeast and northwest winds may have influenced the concentrations of SPMR and CMR, respectively.

With the help of the Hysplit program, the trajectories of the wind were traced for the periods in which the PM concentrations were higher (beginning of June and July). The analyzed days presented predominance of north and northwest

winds, as well as observed for O₃ concentrations (Figure 5).

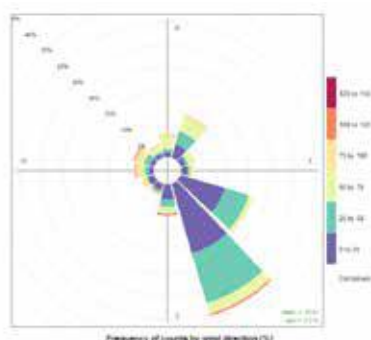


Figure 5. Wind rose for O₃ concentrations.

In Figure 6 is presented the concentration of chemical compounds of the measured particulate matter. The application of PMF showed the possible related sources. Factor 1 was considered as vehicular emission (BC, S, V, Zn, Pb and Br), factor 2 was considered as vehicular and biomass burning source (BC, P, S and K), factor 3 as vehicular and industrial (P, S and V) and factor 4 as resuspended soil (Al, Si, Cl, K, Ca, Ti, Fe).

Although the four factors presented similar contributions (approximately 25% each factor), vehicular emission was the most significant source because their tracers elements were presented in three of the four factors found.

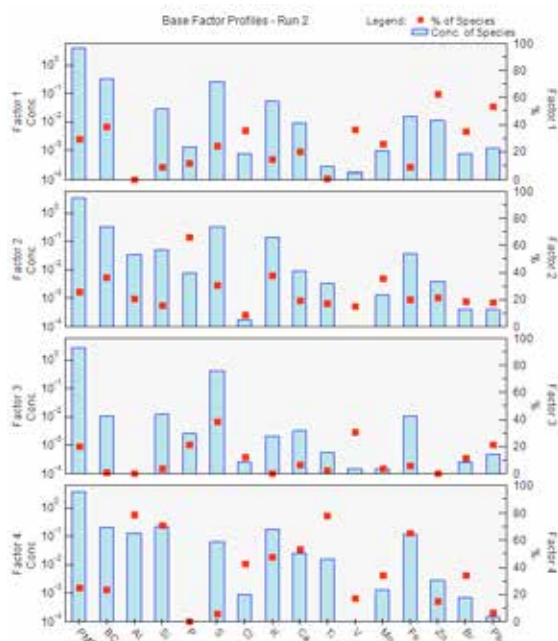


Figure 6. PMF factors identified in the PM_{2.5}.

CONCLUSIONS

Air pollution has no barriers and, can impact small and medium-sized cities that can have high

concentrations of specific pollutant. Pollution generated in large cities often affects neighboring cities.

Despite the short study period and the fact that NO_x concentrations were not accurately measured, the results were considered satisfactory. The study revealed particulate matter and O₃ concentrations, below the limits established by State Decree nº 59113 of 2013, even in a period of low precipitation. The concentrations measured that are below the standard, characterize Valinhos' air quality as good. With the support of Hysplit trajectory analysis and the use of meteorological data, direction and wind speed, it was possible to verify the wind predominance and corroborated the hypothesis that the pollution of cities like São Paulo and Campinas can influence the concentrations of Valinhos.

Finally, Valinhos presents as main sources of particulate matter concentration, vehicular, industrial, biomass burning and soil resuspension, being the vehicular source the more important.

The next step of this study is perform more measurements at Valinhos city of more pollutants (NO_x, CO, SO₂, HC, O₃ and PM₁₀ and PM_{2.5}) and for a longer period.

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PRELIMINARY STUDY OF THE DAILY PROFILE OF CARBON DIOXIDE IN THE METROPOLITAN AREA OF SÃO PAULO

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Abstract: São Paulo has the largest fleet of vehicles in Brazil, that burn biofuels: ethanol, gasohol and biodiesel. All these factors contribute to making this city an unique example for studying the greenhouse gases, such as Carbon Dioxide and Methane, behavior. MASP is integrating a network with the measurements of GHG in urban areas, altogether with Los Angeles and Paris. The objective of this study is to analyze the carbon dioxide concentrations in the MASP, in order to understand the daily behavior of the plume from and to São Paulo. The measurements were carried out through an wavelength-scanned cavity ring-down spectroscopy instruments (Picarro Inc.) Two equipment were located in distinct points of the MASP, one of them is installed in the Institute of Astronomy, Geophysics and Atmospheric Sciences in the University of São Paulo (IAG) and the second one is situated 25 km away, in the northwest region at an altitude of 1135 m in relation to sea level in the Jaraguá Peak (the highest point of the city). Statistical analysis to determine the average values, maximum and minimum of the time series were performed through the R software. The values obtained were compared to other cities of the megacity project (www.megacities.jpl.nasa.gov) that are similar to the demographic density of the city of São Paulo, Los Angeles and Paris. On average, São Paulo registered values above those registered in LA and below the averages obtained in Paris. The maximum values registered in MASP occurred in the month of May, in the southern autumn.

Keywords: GreenHouse Gases, Methane, carbon dioxide, megacities.

INTRODUCTION

The existence of a balance among the environment, the economy and the world's population density is a challenge, due to the direct impacts of growing urbanization on the climate (UN-HABITAT, 2011). Knowing the impact that cities cause on climate change would facilitate the creation of measures that would minimize the damage to the population that is in these large urban centers, in addition to enabling ideas to mitigate greenhouse gases (UN-HABITAT, 2011).

Several authors have already addressed the importance of the contribution of megacities to GHG emissions, such as carbon dioxide (CO₂), methane (CH₄), among others (Verbeeck *et al.*, 2011; Duren and Miller, 2012; Turnbull *et al.*, 2015; Kristal R Verhulst *et al.*, 2017). According to the International Energy Agency, more than 70% of CO₂ emissions from the burning of fossil fuels and much of the anthropogenic emissions of CH₄, are from the urban areas around the globe (International Energy Agency, 2008). This factor was the motivation for creation the megacity project (www.megacities.jpl.nasa.gov), which aims to analyze the behavior of these pollutants in cities, which due to their large number of inhabitants, don't have a homogeneity in emissions (Kristal R. Verhulst *et al.*, 2017). Currently, cities that maintain a monitoring of greenhouse gas emissions integrating the

megacity project are: Los Angeles (<https://megacities.jpl.nasa.gov/portal/>), see also in, Kristal R. Verhulst *et al.*, 2017; Viatte *et al.*, 2017), Paris (CO₂-Megaparis: <http://co2-megaparis.lscce.ipsl.fr/>), see also in, (Breón *et al.*, 2015; Xueref-Remy *et al.*, 2016) and São Paulo is just starting.

The metropolitan area of São Paulo (MASP), with a territorial area of 1521 km² is housing of approximately 12 million people, with a population density of 7398 hab/km², and is impacted by air pollution sources, mainly the vehicular emission by the fleet of 8 million vehicles (IBGE, 2017). Under the influence of a hot and temperate climate the city has a precipitation regime with high value from September to March, but even in the months referring to the minimum of precipitation (austral winter), mean precipitation values reach 60 mm. São Paulo has the largest fleet of vehicles in Brazil, that burn biofuels: ethanol, gasohol and biodiesel. All these factors contribute to making this city an unique example for studying the greenhouse gases, such as Carbon Dioxide and Methane, behavior. MASP is the biggest metropolitan area in the South Hemisphere and was precursor in the study of the atmospheric pollutants. Now is also measuring the GHG in urban areas. The objective of this study is to analyze the carbon dioxide concentrations in the MASP, in order to understand the daily behavior of the plume from and to São Paulo.

METHODS

The measurements were carried out through an wavelength-scanned cavity ring-down spectroscopy instruments (Picarro Inc.) The main advantage of this equipment is its high temporal resolution in the data collection, since a mean of the pollutant is registered every 3 seconds, which allows to perceive subtle variations in the measurements throughout the days. Two equipments were located in distinct points of the MASP, one of them is installed in the Institute of Astronomy, Geophysics and Atmospheric Science in the University of São Paulo (IAG) and the second one is situated 25 km away, in the northwest region at an altitude of 1135 m in relation to sea level in the Jaragua Peak (the highest point of the city). Statistical analysis to determine the average values, maximum and minimum of the time series were performed through the R software. values obtained were compared to other cities of the megacity project that are similar to the demographic density of the city of São Paulo, Los Angeles and Paris.

FINDINGS AND ARGUMENT

The period of 2016 was chosen in order to compare with the results published by the authors (Xueref-Remy *et al.*, 2016; Kristal R. Verhulst *et al.*, 2017). The hourly variation of CO₂ and CH₄ at both sites is shown in Figure 1, where the first two time series refer to methane and carbon dioxide concentrations located in the IAG, and the last two series indicate concentrations of pollutants in the site located in the Jaraguá Peak, respectively.

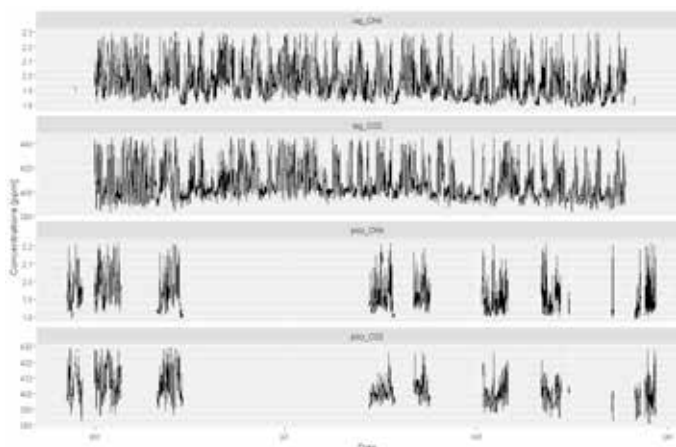


Figure 1. Hourly variations of GHG concentration for the IAG and Jaraguá Peak sites

It was possible to observe in this figure that the concentrations of CO₂ and CH₄ in the IAG, registered values a little higher when compared with the concentrations obtained in the Jaraguá Peak. This factor was expected due to the location of the respective collection points, since the IAG

site is located closer to the central region of the MASP, while the Jaraguá Peak is less impacted by the vehicular emission and with a different profile of the boundary layer daily variation. During the morning the Jaraguá Peak is above the boundary layer at some days, mainly in the winter season.

In Table 1 it is presented the basic statistics for the data, maximum and minimum values of each pollutant for each station. Looking at the literature, the values mentioned for maximum concentrations in Paris was approximately 430 ppm. While for LA maximum values ranged from 621 ppm for regions with heavy vehicular traffic and 427 ppm for more remote locations. Thus, it was observed that the comparison of CO₂ concentrations of the Metropolitan Region of São Paulo with LA, indicated that the maximum values were lower in the regions with higher vehicle flow (IAG) and higher when compared to more distant regions (Peak of Jaraguá). However, the maximum values of carbon dioxide were higher than those found in Paris. However, all the minimum values reported in the literature, 388 ppm (LA) and approximately 390 ppm for the city of Paris, were higher than the minimum values registered in the MASP even in places of intense traffic of vehicle, as well as for the more distant region.

Table1. Maximum and minimum concentrations (in ppm) recorded in both sites

	CO ₂ (ppm)		CH ₄ (ppm)	
	IAG	Jaragua Peak	IAG	Jaragua Peak
Max.	445.33	428.92	2.30	2.22
Min.	382.94	380.90	1.78	1.79
Mean	405.78	402.03	1.94	1.92
Standard deviation	12.79	8.99	0.11	0.09

Figure 2 shows the variation of the CO₂ concentration for the IAG site (in salmon) and the Jaraguá Peak (in green) along the days of the week, in addition to hourly, monthly and weekly variations.

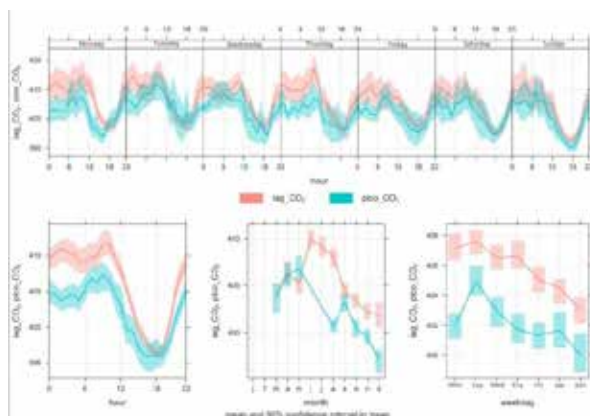


Figure 2.Changes in CO₂ concentrations: Hours, Weekly and Monthly in PPM

Important factors such as seasonality were observed when the comparison occurred for the monthly averages, where the drier months (austral winter) showed a greater difference in the concentrations between the two sites. Another important factor observed is the variability of the concentrations along the day, where it was observed that in the Jaraguá Peak exists a variability almost opposite to the concentrations obtained in the IAG, this fact can be connected with the increase of the planetary boundary layer and the arrival of the plume emitted from the center of the MASP. Finally, it was noted that Tuesday was the day with the highest CO₂ emissions while Sunday recorded the lowest concentrations, which was expected due to the decrease in vehicular traffic on weekends.

CONCLUSIONS

For this initial work, it was possible to highlight the importance of the measurements related to Greenhouse Gases in large population centers, such as the Metropolitan Region of São Paulo. There is much to be done with the data recorded in the São Paulo stations, understand the contributions of the weather to the concentrations, as well as to determine the biogenic and anthropogenic contributions of these gases to the study site.

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Relationship between PM_{2.5} concentration and meteorological parameters in the East Zone of São Paulo Capital

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Abstract: The Metropolitan Area of São Paulo (MASP) is one of the largest areas in the world, with more than 21 million inhabitants in an approximate area of 7 thousand km². With a big population density, as occurs with the biggest cities in the world, they face serious problems, such as atmospheric pollution, caused by the excess of vehicles. Currently, MASP has a fleet of approximately 9 million motor vehicles. Several studies show that vehicles are the main emitters of different pollutants in the MASP, generating diverse impacts on the environment and human health. Among the various pollutants emitted by vehicles are Black Carbon (BC) and fine particulate matter (PM_{2.5}). The BC can be considered one of the main elements that contribute directly to the increase of the greenhouse effect, as its physical and chemical properties alter the radiative forcing of the atmosphere. PM_{2.5} is one of the main pollutants linked to the increase of cardiorespiratory diseases, and problems caused to the environment, such as the decrease of visibility and direct and indirect effects in the atmospheric radiative forcing. The objective of this work is to quantify the concentrations of PM_{2.5} and BC in samples collected at the School of Arts, Sciences and Humanities, East campus of the University of São Paulo (EACH-USP) and correlate to meteorological parameters. During one-year period PM_{2.5} samples were collected over a 24-h period, each 72 hours, using a Partisol Model 2025i. BC concentrations were monitored using a Multi Angle Absorption Photometer MAAP-5012. The annual average of fine particulate matter and BC were 17.63±11.42 µg/m³ and 2.61 ± 2.55 µg/m³, respectively. During this period, the São Paulo State 24h standard for PM_{2.5} (60 µg/m³), was not exceeded. The results obtained in the samples were correlated with meteorological parameters (wind speed and direction, temperature and relative humidity). The results showed a direct influence of the meteorology in the seasonality of the concentrations. In the period of low temperatures and humidity, winter, it was observed an increase in the concentration of both pollutants, PM_{2.5} and BC. However, during periods with a high percentage of humidity, temperature and wind speed, the concentrations decreased.

Keywords: Black Carbon, Particulate Matter, Vehicle emissions, Metropolitan Area of São Paulo.

INTRODUCTION

Air pollution is defined by the excess of substances present in the air at levels that can affect human life and the environment (SEINFELD and PANDIS, 2006, CONAMA, 1990). Large urban centers, such as São Paulo, present serious problems related to air pollution, due mainly to excess of vehicles. Currently the Metropolitan Area of São Paulo (MASP) has around 9 million fleet vehicles (DETRAN, 2018; CETESB, 2018). Several studies show that vehicles are the main sources of different pollutants in the MASP, generating diverse impacts on the environment and human health (ANDRADE et al., 2010 and 2017; BRAGA et al., 2001; MIRANDA et al., 2017).

The inhalable fine particulate matter (PM_{2.5}) is considered the pollutant most frequently related to health damage and cardiorespiratory diseases, because of the small size it can reach deep into the respiratory tract (BRAGA et al., 2001). The aerosols can also alter cloud properties, decrease visibility, and contribute to climate effects such as heat islands and thermal inversions. Aerosols can affect the terrestrial radiative balance by the scattering or absorption of light, depending on its physicochemical characteristics, can increase or

decrease the albedo (PANICKER et al., 2010; FINLAYSON-PITTS and PITTS, 2000; BARROS and LOMBARDO, 2016). Organic compounds found in the PM_{2.5}, such as black carbon (BC), is a type of compound derived from the incomplete fuels combustion, emitted mainly by diesel-powered heavy duty vehicles, can absorb solar radiation and trap radiation infrared emitted by the Earth, contributing to the atmosphere warming up (BAIRD, 2011; MIRANDA et al., 2017).

In this work PM_{2.5} and BC concentrations were quantified at the School of Arts, Sciences and Humanities, East campus of the University of São Paulo (EACH-USP) and correlated to meteorological parameters to identify these influence on the pollutants behaviour.

METHODS

The samples of PM_{2.5} and BC were collected at the EACH-USP, during one-year period (April 2016 - April 2017). The PM_{2.5} samples were collected over a 24-h period (24:00 to 24:00), each 72 hours, onto 47-mm Teflon membrane filters with the sampler Partisol Model 2025i (Thermo Scientific) operating at a flow rate of 16.7 l min⁻¹. BC concentrations were monitored using a Multi Angle Absorption

Photometer MAAP-5012 (Thermo Scientific). The meteorological parameters were provided by REDEMET (Aeronautic Meteorological Network, collected at São Paulo International Airport, close to EACH (www.redemet.aer.mil.br).

FINDINGS AND ARGUMENT

$PM_{2.5}$ concentration was obtained through the gravimetry analysis. The annual average of $PM_{2.5}$ and BC were $17.63 \pm 11.42 \mu\text{g}/\text{m}^3$ and $2.61 \pm 2.55 \mu\text{g}/\text{m}^3$, respectively. During this period, the São Paulo State 24h standard for $PM_{2.5}$ ($60 \mu\text{g}/\text{m}^3$), was not exceeded. Figure 1 shows a significant anticorrelation between the meteorological parameter, relative humidity (RH) (pink) and the concentration of $PM_{2.5}$ (gray bars). In the example highlighted in red, in July, the RH reaches its lowest point in the period ($\sim 75\%$), and the $PM_{2.5}$ concentration reaches its highest average to the period ($\sim 32 \mu\text{g}/\text{m}^3$). The correlation of the seasonality and pollutants concentration is demonstrated and corroborated in SÁNCHEZ-CCOYLLO and ANDRADE (2002).

Figure 2a shows the wind rose. The direction of the aerosol concentration is observed predominantly from East (E) to West (W), followed by direction Southeast (SE), South (S), North (N) and Northeast (NE), respectively. In figure 2b, the pollution rose in the EACH's map area. The Ayrton Senna road and Guarulhos Airport are highlighted in yellow.

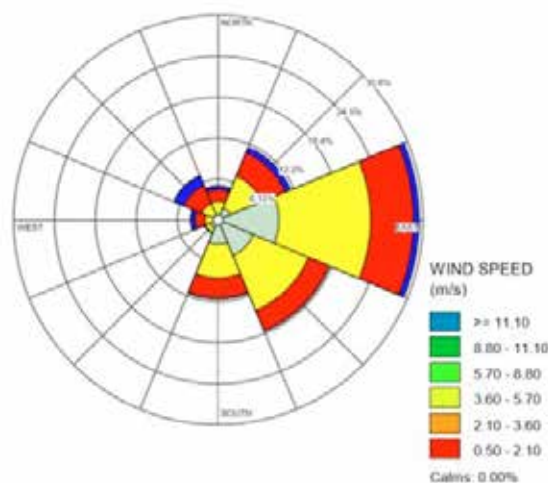


Figure 2a. Wind Rose to the period total sampled (April 2016 and April 2017).



Figure 2b. Pollution Rose at EACH-USP for all the studied period. Map of USP Eastern Campus (EACH), including location of the Guarulhos airport and Ayrton Senna Highway (yellow).

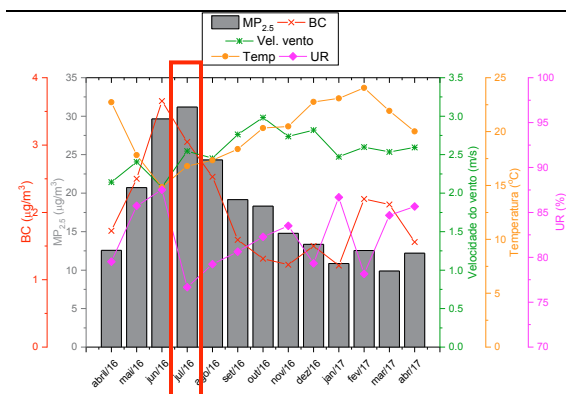


Figure 1. Concentration of BC and $PM_{2.5}$ (left); Meteorological parameters (wind speed, temperature, and relative humidity) (right).

The variation of pollutants concentrations also were correlated weekly with the amount of vehicles that passed by the highways, such as light duty vehicles (LDVs) and heavy duty vehicles (HDVs). When the number of HDV decreases, on the weekends, the concentration of BC also decreases (see Figure 3), corroborating with some researches that demonstrate these influences, because HDV are the main source of BC (ANDRADE et al, 2010; MIRANDA, 2017).

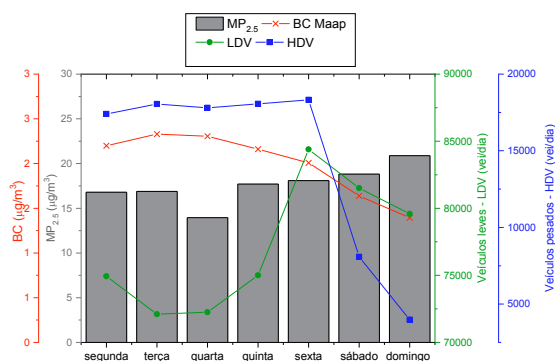


Figure 3. Average weekly concentration of the BC and PM_{2.5} (left) and, quantity of vehicles (LDV and HDV) that travelled the highway in both directions (right).

CONCLUSIONS

The results showed a direct influence of the meteorology in the seasonality of the pollutants concentrations in the east zone of the MASP. In the period of low temperatures and humidity, it was observed an increase in the concentration of both pollutants, PM_{2.5} and BC. However, during periods with a high humidity, temperature and wind speed, it was observed that the concentrations decreased. Vehicles can also influence the BC concentrations, when the number of HDVs decreases, BC concentrations also decreases. More analysis are being performed in order to identify the main sources of the pollutants in the area.

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Session 08
**Atmospheric Boundary Layer:
Observing and Modeling**

LARGE-EDDY SIMULATION OF MICROSCALE POLLUTANT DISPERSION IN URBAN AREAS

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Abstract: The objective of this work was to simulate the microscale pollutant dispersion by means of large-eddy simulation (LES) based on the Smagorinsky-Lilly subgrid scale model. The simulations were performed using the commercial code ANSYS Fluent for three different geometries: two staggered arrays with uniform (UBSA) and random height buildings (RBSA) and an aligned array with random height buildings (RBAA). For the considered cases, an area source with constant concentration was placed on the ground level in a neutrally stratified boundary layer. It was found that the dispersion pattern is significantly more complex for arrangements with different building heights. However, the dispersion field presents some similarities among the considered arrays such as a high concentration zone in the wake region and a more diluted zone in front of the buildings. It was concluded that the average concentration is higher in the region below the canopy layer for the UBSA configuration when compared to the arrays with random height buildings. It was also shown that the average concentration is quite similar between RBSA and RBAA arrays in the region above the area source, however the staggered array presents a steeper concentration gradient after the source producing, consequently, lower concentrations. These facts are probably due to the presence of taller buildings throughout the domain, which act enhancing both lateral and vertical pollutant transfer.

Keywords: Urban areas, Random height buildings, Pollutant dispersion, Large-eddy simulation

INTRODUCTION

Air pollution in urban areas is a current issue and every day becomes more relevant due to short and long-term effects on population health, mainly affecting people who live in high-density populated cities (YUAN; NG; NORFORD, 2014).

Rapid urbanization and the evident impact associated with the increasing atmospheric pollution encouraged several researchers around the world to study airflow and dispersion patterns in urban environments. These patterns are affected not only by micro and macro-scale meteorological phenomena but also by the presence of buildings and other urban elements.

Urban configurations are commonly represented by a single or a group of buildings. Nevertheless, some authors consider slightly more complex urban configurations in their studies, seeking to assess the influence of different building heights in the airflow and pollutant dispersion (BOPPANA; XIE; CASTRO, 2010; CHENG; CASTRO, 2002; PHILIPS; ROSSI; IACCARINO, 2013).

The aim of this work is to increase the understanding on the effects of different building heights and arrangements on the scalar mass transfer within urban environments using large eddy simulation (LES).

METHODS

Figure 1 presents the simulated cases. The first one is a staggered array with uniform height buildings - UBSA, the second is a staggered array with random height buildings - RBSA, and the last one is an aligned array with random height buildings - RBAA. The computational domain is of size $L_x \times L_y \times L_z = 24H_m \times 16H_m \times 10H_m$ for RBSA and RBAA configurations and $L_x \times L_y \times L_z = 24H_m \times 16H_m \times 6H_m$ for UBSA (H_m is the average building height equal to 10 mm).

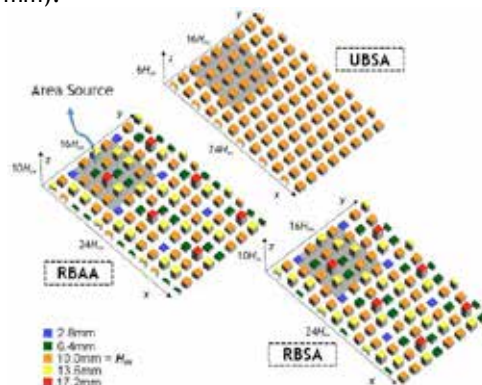


Figure 1. Plan view of simulated urban configurations. The colors at the top of each building indicate the heights of buildings in millimeters.

Large-eddy simulation was used to simulate incompressible flow with $\rho = 1.225 \text{ kgm}^{-3}$ and $\mu = 8.71 \times 10^{-6} \text{ kgm}^{-1}\text{s}^{-1}$. The Smagorinsky-Lilly model, which has a near-wall damping function, with $CS = 0.1$ was used to handle Subgrid scales, with the SGS turbulent Schmidt number taken as $Sc_t = 0.9$.

All the simulations were run for at least $200T_c$ (eddy turnover time) before statistics were computed, which was sufficient to assure the development of the flow. Then, the statistics were collected and averaged for a duration of $200 T_c$ at each time-step resulting in converged results. The validation of the flow and dispersion fields are presented in Goulart *et al.* (2019).

FINDINGS AND ARGUMENT

Figure 2 shows the contours of normalised concentration ($c^* = c/c_0$, where c_0 is the constant concentration imposed at the area source) in the vertical x - y plane for all configurations.

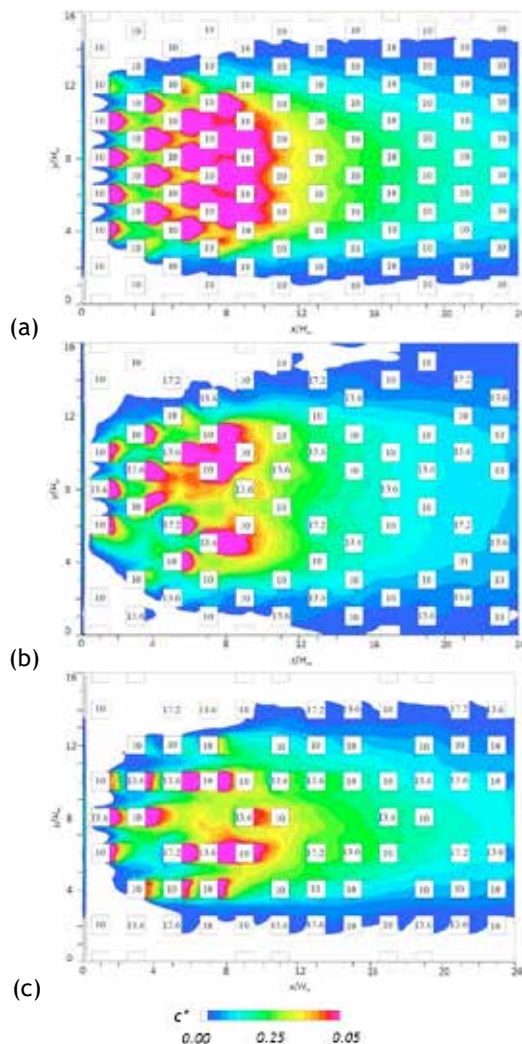


Figure 2. Contours of normalised concentration at $z/H_m = 1$ for (a) UBSA, (b) RBSA and (c) RBAA.

It can be seen in Figure 2(b) that the randomness in the height of the buildings is responsible for the irregularity on dispersion field for RBSA configuration above the area source (until $x/H_m = 10$). On the other hand, a regular dispersion pattern is observed for the uniform array, consisting of high concentration zones behind the buildings and low concentration zones in front of them as can be seen in Figure 2(a). Figure 2(c) demonstrates that the concentration field in RBAA configuration at $z/H_m = 1.00$ are similar to the dispersion pattern presented for RBSA array. Observing the concentration distributions for the plans located at $z/H_m = 1.00$, it is possible to note that tall buildings act just like chimneys, transporting pollutants vertically to upper levels, due to strong updrafts behind them. Moreover, the lateral dispersion for RBSA is higher than from UBSA after the distance of $8.0H_m$ downwind the area source, while the latter presents almost constant spanwise dispersion with distance, as for RBAA. The aligned array promotes a lower amount of pollutant within the channels, however great recirculation due the skimming flow pattern promotes high concentration zones, especially in the gap between two tall buildings.

Figure 3(a) demonstrates a regular concentration pattern above the area source in the UBSA configuration, where the high concentration zone reaches the rooftop level behind the buildings and is minimized in front and in the lateral sides. On the other hand, the random height arrays demonstrate an irregular pattern, with high concentration zones reaching greater vertical distances from the ground, supporting that the stronger upward motions behind tall buildings are responsible for removing the pollutant from within the canopy (Figures 3(b) and 3(c)).

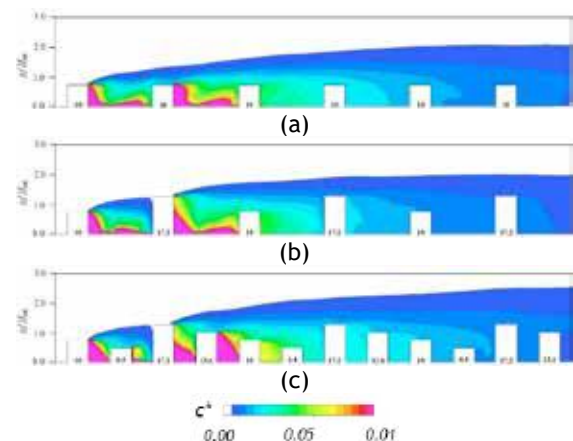


Figure 3. Contours of normalised concentration in the x - z plane at $y/H_m = 6$ for (a) UBSA, (b) RBSA and (c) RBAA.

The patterns found on concentration contours are of great relevance to identify the influence of different morphologies on the dispersion field.

However, quantitative analysis becomes relevant in order to investigate how such morphologies affect the accumulation of pollutant within the urban canopies. Therefore, spatially-averaged scalar concentration was locally-averaged (over volumes that are representative of different rows, as shown in Figure 4) throughout the domain. Each volume comprises $L_x \times L_y \times L_z = 2H_m \times 8H_m \times 1H_m$. It is important to note that the area source is below the volumes from the row 1 to the row 4.

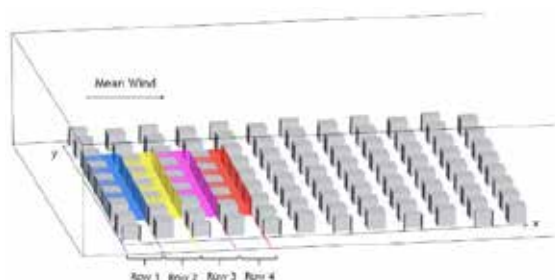


Figure 4. Representation of specific volumes for UBSA configuration. Colours indicate the volumes.

Figure 5 demonstrates that the volume-averaged is higher in the region within the canopy for UBSA configuration, when compared to arrays with random height buildings. In addition, volume-averaged remains higher throughout the domain but the difference for RBSA and RBAA is more remarkable in the region above the area source, where the pollution is more trapped next to the ground.

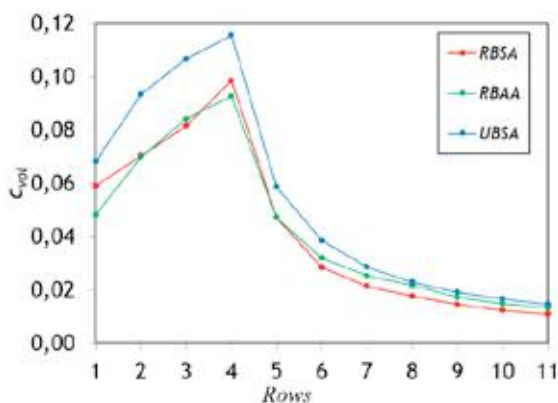


Figure 5. Normalised volume-averaged concentration for specific rows.

Both random height building configurations have slightly lower concentration above the area source, while the concentration becomes slightly higher in the region after the source for the RBAA configuration. In addition, the RBSA array promotes slightly higher concentration above the area source, while further away from the source the concentration decreases presenting lower concentration compared to the other

configurations. These facts support the indication of stronger vertical and lateral dispersion due to the presence tall buildings.

CONCLUSIONS

The results obtained in the present study show that the height variability of the buildings is an important parameter to study the dispersion phenomena in urban areas. Besides the building height variability, local geometrical features proved to be relevant to determine the dispersion behaviour such as the presence of a taller building upwind the approaching flow.

In general, the UBSA configuration promotes high concentration within the canopy compared to random building arrays. The volume-averaged concentration above the area source is approximately 25% and 30% higher than RBSA and RBAA configuration, respectively. Between the random building cases, the staggered array presents higher mean concentration below (5%) the average height after the source, demonstration that the aligned array transports more efficiently the pollutant away from it.

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ANALYSIS OF THE ATMOSPHERIC FLOW AT ALCÂNTARA LAUNCH CENTER (CLA) BY NUMERICAL SIMULATIONS

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Abstract: The objective of this study was to simulate the atmospheric flow in the Alcântara Launch Center (CLA) using Computational Fluid Dynamics (CFD) techniques, inserting elements that represent the structure and topography of the site. For this, the computational domain considered the presence of the cliff of 40 meters, with three different inclinations (45, 70 and 90°). The input velocity profile was prepared according to the power law, with an exponent of 0.11, freestream velocity of 20 m/s and Reynolds number of 4.3×10^5 , considering a neutral atmosphere. Two wind directions were considered, 90 and 135°. The numerical model used was the Reynolds Stress Model (RSM), based on the Reynolds-Averaged Navier-Stokes (RANS) equations. The solutions of the equations were obtained by ANSYS FLUENT 19 software, which uses the finite volume method. In order to validate the simulations, the mean velocity profiles in the TMI wake are being compared with wind tunnel results. The results represent well the wind tunnel experiments. Recirculation and separation zones were identified around the cliff and buildings (TMI and exit tower). The higher velocities and vorticities were obtained in the separation regions. It was concluded that the cliff inclination and incident wind direction influence the flow dynamics in the Launch Pad Area (SPL). This is a study in progress and the next step will be the analysis of pollutants dispersion emitted by launching rockets, such as HCl, due to the combustion of solid propellant.

Keywords: Fluid flow around an obstacle, Computational Fluid Dynamics (CFD), atmospheric turbulence, rocket launch.

INTRODUCTION

The Alcântara Launch Center (CLA) is the main Brazil's gateway to space, located in the north part of northeast Brazil. The Launch Pad Area (SPL) is positioned 150 meters from the coastline, on an irregular cliff. Therefore, some important points for the atmospheric flow passing over the SPL are observed: abrupt change of roughness (smooth surface of the ocean to the rough surface of the continent) and topographic variation caused by the cliff. Furthermore, the launching platform has some buildings nearby necessary for rocket integration as the Mobile Integration Tower (TMI) with an exit tower coupled (Figure 1). The space vehicle is prepared and assembled inside the TMI, which is then displaced by approximately 55 meters to start the rocket launching process. In this situation the vehicle is subject to the wind and atmospheric turbulence action coming from the ocean.

It is well known that the flow around obstacles is dominated by shear-generated mechanical turbulence. In this way, the presence of buildings modifies the flow pattern, causing the formation of characteristic regions as the separation and recirculation areas and the turbulence wake behind the obstacle (ARYA, 1999). Thus, the understanding of the flow pattern around the launch pad buildings and how the flow changes due the geography of the region are important to

establishing the conditions in which the CLA is exposed and providing the necessary basis for the development of rockets as well as the procedures during the launches. Another important issue is associated with the pollutants dispersion emitted by the launches, such as HCl, and to the wind loads on the rockets.



Figure 1. Launch Pad Area (SPL).
Reference: AEB (2019)

In this context, experimental essays in wind tunnel (WT) and numerical simulations are important tools and they have been used in order to understand better the atmospheric flow in the CLA region.

Roballo, Fisch and Girardi (2009) were pioneers in these analyzes. The authors conducted wind tunnel tests considering the presence of the cliff, represented by a step with two different inclinations: 70° and 90° . In addition, some tests were performed with the presence of surface elements that represented the surface roughness of the region. The best results, when compared with field measurements, were obtained for the 90° cliff and without the presence of roughness elements. It was observed typical flow characteristics after the step: detachment, forming recirculation zone and reattachment.

Pires et al. (2010) and Pires et al. (2011) analysed the atmospheric flow in a coastal cliff of different configurations through WT experiments and 2D numerical simulations, respectively. Pires et al. (2010) also considered the presence of a rectangular building representing the TMI. The results showed a modification near the surface of the atmospheric flow when reaching the coastal cliff and the formation of the recirculation region. The vorticity generated downwind of the coastal cliff has a strong turbulence. The presence of the TMI results in a downwind turbulence similar to the generated by coastal cliff. For coastal cliffs of the same height and different inclination angles, the intensity of the maximum vorticity remains the same, but with increasing angles, the inner boundary layer (IBL) heights suffer a small decrease.

Souza, Fisch and Goulart (2015) conducted 3D numerical simulations using the Computational Fluid Dynamics (CFD) technique with the presence of the (90° inclination) and of the TMI. The results showed vortex structures next to cliff and upstream and downstream of the TMI. A reduction of the flow velocity was also observed as it passed through the cliff.

Faria, Avelar and Fisch (2019) performed WT tests using a scaled model of the SPL with different cliff inclinations and incident wind intensity and direction. The vortexes pattern behind the TMI or exit tower structures is strongly influenced by the wind incidence angles. These vortexes may induce vibrations or load excess on these buildings structures if they remain there for a long time.

Few investigations of the atmospheric flow in the CLA were performed by computational methods. Furthermore, the complementation the information already acquired by WT experiments is important to promote new analyses. Thus, the objective of this study was to simulate the atmospheric flow in the CLA region using CFD techniques, inserting elements that represent the structure and topography of the site.

METHODS

The test cases are based on an experiment recently conducted by Faria, Avelar and Fisch (2019) in a boundary-layer wind tunnel. In their experiment, a free-stream flow with velocity of $U_\infty = 20\text{m/s}$, Reynolds number of 4.3×10^5 and 0.05 to 0.10 turbulence intensity.

Three obstacles (representing the TMI, exhaust tower and engine room) and a step (representing the cliff) were considered in geometry, 1:120 scale. The TMI with $270 \times 85\text{ mm}$ dimensions. The tower of escape, the engine room and the cliff with 210, 35 and 330 mm of height, respectively. The domain should be sufficiently far from the obstacle to avoid any influence on the results. Thus, the height, width and length downwind the TMI were of $10h_{\text{cliff}}$, $10h_{\text{TMI}}$ e $10h_{\text{TMI}}$, respectively. See Figure 2.

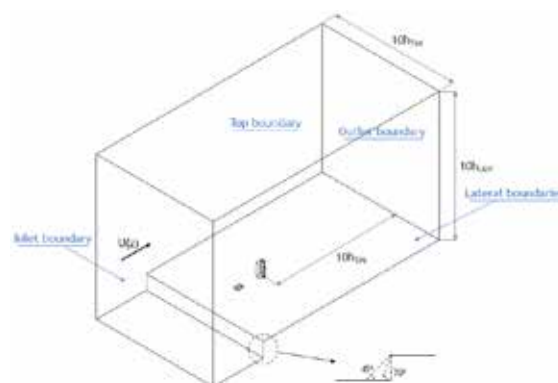


Figure 2. Computational domain.

Three cliff inclinations β (45° , 70° and 90°) and two incident wind directions α (90° and 135°) were considered. The wind direction variation was obtained from the geometry rotation in the computational domain.

Reynolds Averaged Navier-Stokes simulation was used to simulate incompressible flow with $\rho = 1.225\text{ kg m}^{-3}$ and $\mu = 1.7894 \times 10^{-5}\text{ kg m}^{-1}\text{ s}^{-1}$. The turbulence model used to solve the conservations equations was the second-order Reynolds Stress Model (RSM) model - ω -baseline, which obtained a better performance for this case when compared to κ - ω SST first order model. This model considers the anisotropy of turbulent viscosity and closes the system calculating a transport equation for each Reynolds stress tensor component.

The incident turbulent velocity profile is approximated using a power law at the inlet boundary according the wind tunnel experiments:

$$\begin{cases} \text{if } (z < 1170 \text{ mm}), & \frac{U(z)}{U(z_{ref})} = \left(\frac{z}{z_{ref}}\right)^\gamma, \\ \text{if } (z > 1170 \text{ mm}), & U(z) = U_\infty \end{cases}$$

in which $U(z)$ is the mean velocity at height z , $U(z_{ref})$ is the mean velocity at reference height z_{ref} (10 meters according World Meteorological Organization) and γ is 0.11, determined according to Hsu, Meindl and Gilhousen (1994), who performed measurements on the sea surface considering stability near neutral.

At the outlet boundary, a zero gauge pressure boundary condition is adopted. Symmetry boundary conditions are applied to the lateral boundaries. At the top a free slip condition is applied. No-slip boundary condition is applied to all solid surfaces.

The numerical simulations were performed using the commercial software Fluent Ansys version 19, which employs the finite volume method to discretize the conservation equations. The algorithm SIMPLE, proposed by Patankar (1980), was used for pressure-velocity coupling. A second order scheme was chosen to spacial discretization of momentum, specific dissipation energy rate and Reynolds stresses variables.

The meshes used in the cases have:

- Case 1 (β 90° and α 90°): 6.954.630 elements and 7.165.897 nodes;
- Case 2 (β 45° and α 90°): 7.758.559 elements and 7.965.414 nodes;
- Case 3 (β 70° and α 90°): 7.866.900 elements and 8.079.659 nodes;
- Case 4 (β 90° and α 135°): 12.267.718 elements and 12.873.664 nodes.

In order to validate the atmospheric flow field, the numerical results were compared with the wind tunnel data obtained by Faria, Avelar and Fisch (2019). The performance indices according Chang e Hanna (2004) was used to evaluate the approximation between the results in a region of the TMI wake.

FINDINGS AND ARGUMENT

The influence of the cliff inclination on the flow in the SPL was analyzed. For these cases, it was considered a 90° wind direction (east). The Figure 3 presents the streamlines in the central XZ plane (horizontal) and the Figure 4 the streamlines in the XY plane (vertical) in $z/h_{TMI} = 0.6$.

From Figure 3, it can be observed that for all studied cliff inclinations, there is a flow separation downstream from the cliff. In the upper part of the separation there is an velocity acceleration and in the lower part there is the formation of a

recirculation region, with low velocity in the opposite direction to the flow. As evidenced by Pires et al. (2011), the higher the cliff inclination, the greater the upstream recirculation region, the greater the height of the flow separation zone and, consequently, the farthest is the flow reattachment point.

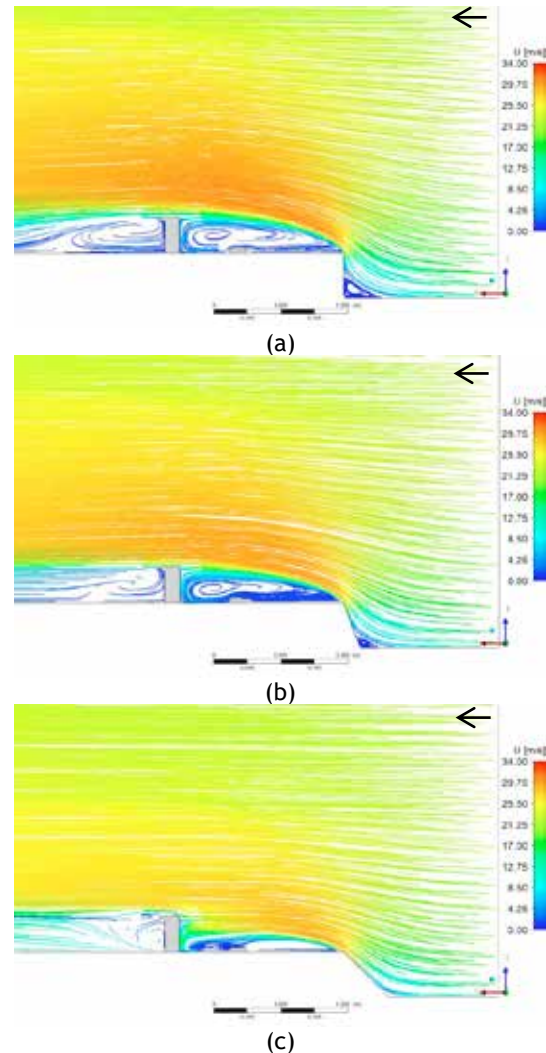


Figure 3. Streamlines in the central XZ plane for 90° wind direction and cliff inclination of: a) 90°; b) 70° and c) 45°. The arrow indicates the wind direction.

Figure 3a shows that the flow detached in the cliff has not yet reached the reattachment point when it reaching the TMI and, therefore, the presence of this building further delays its reattachment. Two recirculation regions are formed, upstream and downstream of the TMI and the exit tower, with low velocity values. This can also be seen in Figure 4a, the formation of low-velocity recirculation zones around the TMI.

The same occurs for the cliff with a inclination of 70° (Figure 3b). The presence of TMI retards the flow reattachment. But, it causes a new separation in the flow. Figure 4b shows a large recirculation downstream of the TMI, especially behind the exit tower.

In Figure 3c it is possible to see that the flow better follows the geometry of the cliff, creating a very small recirculation zone upstream. The flow is separated in the cliff and it is reattached when arrives at the TMI. Part of the flow in the TMI is then reattached and part is separated again. Downstream of the TMI it is observed a perturbed flow region at low velocities (Figure 4c). For this case the highest velocities in the horizontal plane are observed (Figure 4c).

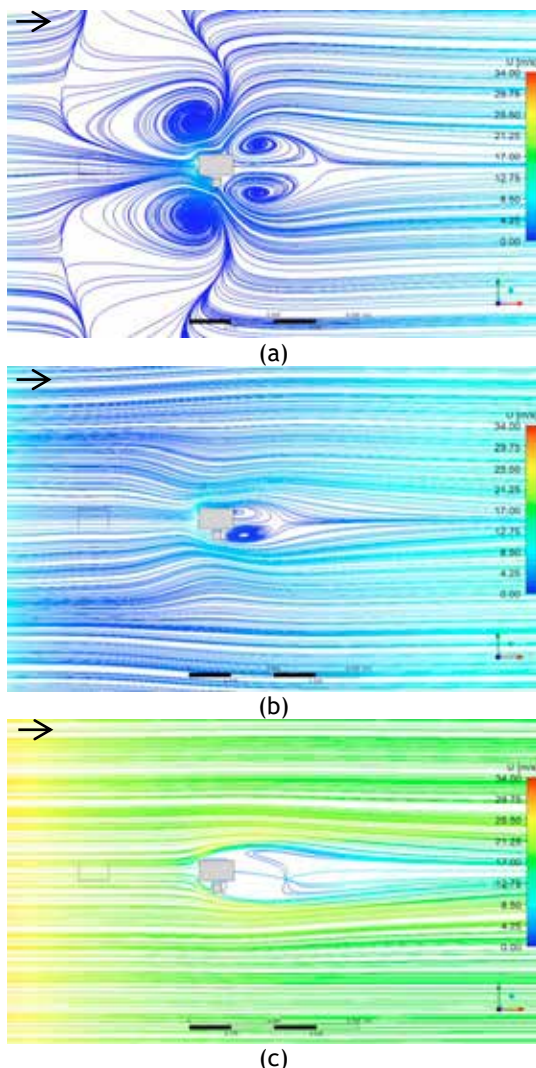


Figure 4. Streamlines in the XY plane ($z/h_{TMI} = 0.6$) for 90° wind direction and cliff inclination of: a) 90° ; b) 70° and c) 45° . The arrow indicates the wind direction.

Saeedi, LePoudre and Wang (2014) analysed the turbulent wake behind a parallelepiped with high aspect ratio and Reynolds number in order of 10^5 in developing boundary layer through direct numerical simulation. The authors verified that, due of the relatively high Reynolds number and the high aspect ratio of the parallelepiped tested, the wake is widely spread behind the cylinder and exhibits complex and energetic vortex motions. This was also observed in this study.

For the case of inclination cliff of 90° and wind direction of 135° (for which the geometry was rotated), a flow disturbance is observed when passing through the cliff, but the recirculation zone was created just downstream of the TMI, with the formation of large low-velocity vortex (Figures 5a and 5b).

The influence of the wind direction on the atmospheric flow in SPL was analyzed. The results are in Figures 3a and 4a and Figure 5.

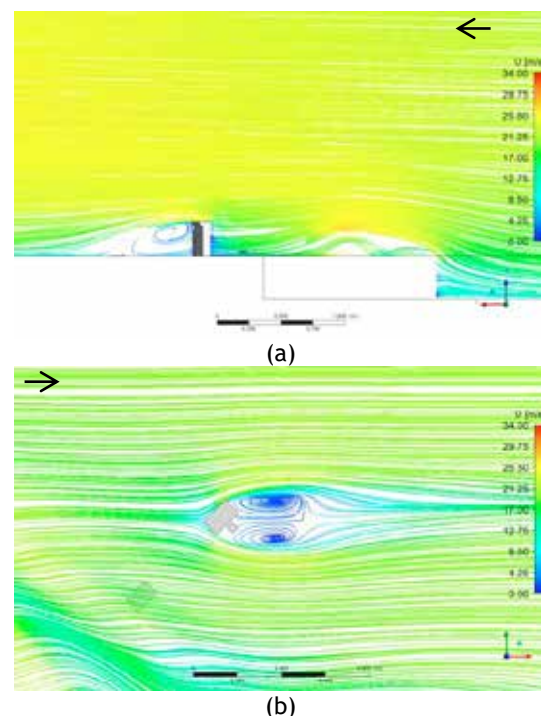


Figure 5. Results for 135° wind direction and cliff inclination of 90° : a) streamlines in the central XZ plane; b) streamlines in the XY plane ($z/h_{TMI} = 0.6$). The arrow indicates the wind direction.

Observing the both cases with cliff inclination of 90° and wind direction of 90° (Figures 3a and 4a) and 135° (Figures 5a and 5b), it appears that the highest velocities in the horizontal plane are for the case of wind direction of 135° and the TMI has a greater influence on the flow in this case (Figure 5b). On the other hand, in the vertical plane, there

is a greater velocity acceleration up to the TMI for the case of wind direction of 90° (Figure 3a), but this acceleration is due to the presence of the cliff and the TMI has little influence.

Luo et al. (2011) studied models of cuboid obstacles to characterize the three-dimensional responses of airflow behind obstacles to variations in the incident flow in wind tunnel tests. As well in the present study, the flow patterns behind obstacles were complicated by changes in the incidence angles. The flows separated both horizontally and vertically, creating reverse flow zones downwind of the obstacles. The horizontal plane is characterized by two asymmetrical, opposing reverse vortices just at flow incidence angle 90° (also occurs for incidence angle 135° for this study). In both studies, the vertical plane presents a single vortex at all angles.

The characteristics presented here are consistent with the wind tunnel results of Faria, Avelar and Fisch (2019).

As expected, the higher vorticities (close to 1000 s⁻¹) were found at flow separation points in the cliff and the TMI. An example is shown in Figure 6. Just for the case of cliff inclination and wind direction of 90° was observed a low vorticity above TMI compared to the other cases. This was also observed by Faria, Avelar and Fisch (2019).

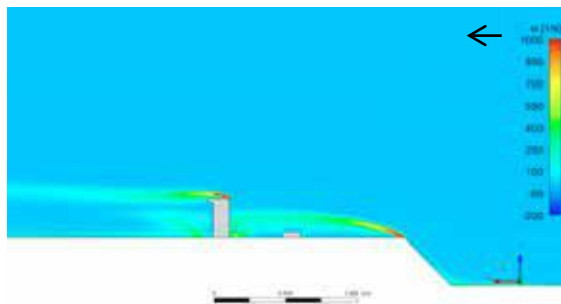


Figure 6. Vorticity XZ plane for inclination cliff of 45° and wind direction of 90°. The arrow indicates the wind direction.

Comparing the case of inclination cliff and wind direction of 90° with the wind tunnel experiments of Faria, Avelar and Fisch (2019), has the simulation validation. Figure 7 shows the variation of velocity with the height in the TMI wake. It is observed that the results of wind tunnel and numerical simulation showed the same tendency, with lower velocities in the lower heights and higher velocities above the TMI. The simulation resulted in higher velocities above 350 mm.

Table 1 presents the results of the performance indices analyzed. These indices were calculated according to Chang and Hanna (2004). NMSE

(normalised mean square error) is a measure of dispersion and reflects systematic and random errors and meets the criterion considered satisfactory. r (correlation coefficient) is a little below than expected. FB (fractional bias) reflects the tendency of overestimation or underestimation of the values and also meets the criterion considered satisfactory.

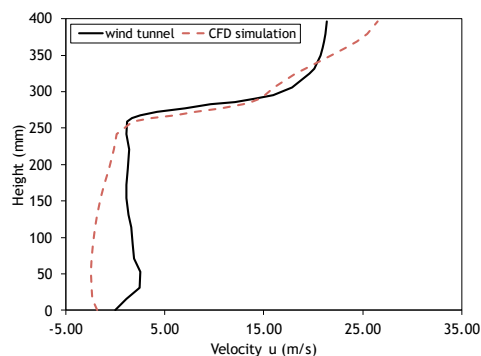


Figure 7. Comparison between the wind tunnel results and the numerical simulation in the TMI wake and for 90° wind direction and cliff inclination.

Table 1. Comparison indices of simulation and wind tunnel results. Optimal values and criterion from Chang and Hanna (2004).

Index	Value	Optimal value	Criterion
NMSE	0.06	0	$\sqrt{NMSE} \leq 2$
r	0.78	1	-
FB	0.04	0	$-0.3 \leq FB \leq 0.3$

CONCLUSIONS

The numerical simulations results have the same tendency of the wind tunnel measured. The best results were obtained in the region just above TMI.

Recirculation regions were observed in the horizontal and vertical planes. It was observed that the greater the cliff inclination, the larger the upstream recirculation zone and the greater the height of the recirculation zone formed to its downstream by the flow. The presence of the TMI generates a new separation and influences more its dynamics the smaller the cliff inclination. For the wind direction of 135° the impact of the TMI in the flow was also greater.

It is concluded, therefore, that the presence of the cliff at different inclinations and of the buildings, mainly the TMI and the exit tower, change the flow dynamics in the CLA region, generating typical flow regions like separation and recirculation. In addition, the wind direction has an important role in the flow, causing changes in the characteristics of these formed regions.

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WIND SPEED SCALE BEHAVIOR ON THE COAST OF BRAZIL AND THE SOUTH ATLANTIC OCEAN

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Abstract:

The accumulation of climatic data has been a constant practice in the last-minute worlds, especially in Brazil, observing the records of intensification on coastal and oceanic species through the National Marine Buoy Program of Brazil (PNBOIA). The same was implemented through two sub-programs of international meetings with the World Meteorological Organization (WMO), with the objective of consolidating, consolidating and assuming a South-Atlantic mission. These data compose a set of time modules that represent the variables that are spaced as they do not go back with heterogeneous records depending on the chronology of operation of each collection Buoy. This study this text this site is a rare the velocigráfico and the event of this article is to catalog and the speed the guidance of the scale of the vintage and the velocity of 2016-2017 climatológicos in the sea. The consolidation of the concepts is used as a literature analysis model, as well as the mathematical instruments of analysis of fluctuation in the written analyzes of these variables, following the method of Flotation Analysis Detected (AFD). Finally, with the record that there are laws of governance as climatological magnitudes analyzed in the sea, the Brazilian coast and the Atlantic, nevertheless, the existence of the phenomenon of the crossover in off-shore scenarios as well as other particular and related things is not verified.

Keywords: Off-Shore. Complexity. DFA. PNBOIA.

GENERAL GUIDELINES

The world energy crisis has been a recurrent scenario since the end of the last century and with this new demands of alternative sources of energy are consolidated as a focus of research around the world (Brazil, 2019). In order to prospect for new energy sources, it is common practice to search for and observe natural behavioral behaviors of all kinds, such as the movement of waters of a river, the behavior of temperature variations in a specific environment, the analysis of variations in energy in chemical reactions *etc.*, generating a vast source of data that, in the cases of climatological variables, accumulate in numerical and temporal series with automatic collections that grow databases worldwide (Koçak, 2009) and (Orun; Koçak, 2009), this research considers the bases with information about the speed of the wind at sea.

INTRODUCTION

It is observed that much of the accumulated data is of record origin of the sea and the ocean is an important source of mass and energy flows for the atmospheric circulation that, in turn, is the main forcing of the superficial oceanic circulation, and thus a strong indexing between the ocean and the atmosphere. The dynamics of this relationship are not yet well known, but there are strong indications that they come from mesoscale

meanders. In addition, the South Atlantic Ocean, which bathes the entire Brazilian coast, is considered to be one of the most energetic regions of the oceans due to intense gradients (temperature, salinity, nutrients, *etc.*).

METHODS

In this sense it is possible to record the existence of several studies on the wind behavior, especially with its velocity, and other environmental magnitudes with the correlation with the same, in the continent and in the sea, in regions near the coast and in the high seas, as shown in the work of, where they analyze the temporal correlations of variations in sea surface temperature (SST) around seasonal mean values in the Atlantic and Pacific oceans with classical methods and Ferreira and Alves (2003), who analyze the variations of sea surface temperature in the tropical Pacific and Atlantic oceans, recording data with the El Niño-Southern Oscillation (ENSO) phenomenon and the temperature variability modes of the southern Atlantic, however without the record of any persistence analysis or associated power laws, as early as 2008 examined several methods for detecting long-range correlations, especially DFA, with their derivations in two methods, the CMA and Modified Detected Flotation Analysis (MDFA) and found that for a given time series analyzed

with the DFA method presents a slightly better performance than the others, thus indicating the DFA as more objective of the methods for the detection of long-range rules, although they do not record wind speed power laws.

The analysis using the DFA method favors the perception of the trendless fluctuations that was introduced by Peng *et al.* (1994), where, at the time, a gene sequence analysis was used and, since then, it has been used as a technique to quantify correlations in non-stationary time series in several applications (Ivanov *et al.* al., 2004), Table 1.

Table 1

Valores de α	Caracterização da Série	Descrição Comportamental	Implicações e Desdobramentos
$0 < \alpha < 0.5$	Comportamento subdifusivo .	Valores grandes (quentes) tendem a serem seguidos por valores pequenos (quentes) e desta forma tem-se as séries temporais anti-correlacionadas .	Valores altos são normalmente seguidos por valores baixos e vice-versa.
$\alpha \approx 0.5$	Comporta-se com memória e apresenta um passo aleatório, caracterizando-se como uma série não correlacionada.	Apresenta valor zero para a função de autocorrelação, o que por vezes é denominado de série temporais brancas.	Sinal sem nenhuma correlação, isto significa que não se pode relacionar o comportamento passado com o comportamento de série no futuro, porque não há memória no processo.
$0.5 < \alpha < 1$	Indica que a série original apresenta condição de longo alcance.	Valores grandes (quentes) tendem a serem seguidos por valores grandes (quentes), ou seja, tem-se a existência de séries temporais correlacionadas de longo alcance, indicando-se uma série persistente.	Valores altos (baixos) são normalmente seguidos por valores altos (baixos).
$\alpha \geq 1$	A dinâmica do sistema é caracterizada por ser não estacionária e a mesma dada de ser na forma de lei de potência do tipo de inverso da frequência em potência.	Regime transiente ou condições transientes.	Para $\alpha < 0.2$, trata-se de um comportamento subdifusivo. Para $\alpha = 0.2$ tem-se um comportamento difusivo. Para $\alpha > 0.2$ tem-se um sinal superdifusivo. Para outros valores de α tem-se outros comportamentos de superdifusividade.

FINDINGS AND ARGUMENT

Still in 2017 verified the complexity of the wind direction dynamics in Fernando de Noronha Island, but did not analyze the velocity and its behavior, verifying the existence of persistence for the direction as well as the lacunarity in hourly data of direction of the wind in the period 2003-2010, that is, they measured the distribution of gaps in the data set in daily time series of wind direction with the results demonstrating the persistence in the direction dynamics.

Finally, it is verified that Santos *et al.* (2018), analyze the time series of wind speeds in different regions of the state of Bahia and the Archipelago of Abrolhos, Brazil, through the use of the DFA technique and ratify the existence of long-range correlations and associated power laws onshore, evidencing correlations with the power laws in two regions of distinct scales (subdiffusive and persistent).

It is a classical method that was initially applied to the analysis of Deoxyribonucleic Acid (DNA) and its evolution (Peng *et al.*, 1994), and then to analyzes of time series behaviors in several, in analyzes of the dynamics of human heart beats (Ivanov In this work, we present the results of a series of surveys of the seismic series, in river flow and discharge, in series studies, in the

economic area for analysis of time series of financial data as well as stock prices. in the transitions of (Zebende *et al.*, 2004), in the analysis of amplitude fluctuation of X-ray signals from binary systems astrophysical systems (Moret *et al.*, 2014), in the transmission of protein energy (Figueiredo *et al.*, 2010), in the records of behavior of time series of sunspot amplitudes (Moret, 2014), in the and in the climate analysis.

Table 2

Localidade da Boia			Figura	Valores de expoente de escala $F(n)/n$			
Litoral	Long.	Lat.		α_1	α_2	α_3	α_4
Fortaleza	-38,431	-3,209	1	0,90	0,01	---	---
Itajaí	-47,389	-28,517	2	1,28	0,02	---	---
Niterói	-43,144	-22,894	3	0,81	0,01	---	---
Porto Seguro	-37,949	-15,993	4	0,68	0,01	---	---
Rio Grande do Sul	-49,842	-31,563	5	0,77	0,01	---	---

Table 3

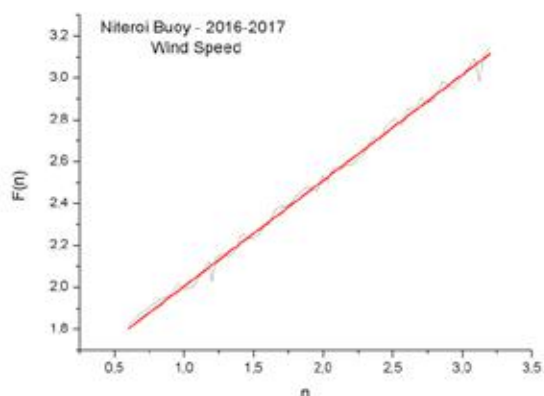
Nomenclatura	Long.	Lat.	Figura	Valores de expoente de escala $F(n)/n$			
				α_1	α_2	α_3	α_4
West Africa	-7.888	-6.003	6	1,42	0,01	---	---
South Atlantic Bury 0	-10,573	-18.947	7	1,30	0,01	---	---
South Atlantic Bury 1	-11,106	-14.994	8	1,33	0,01	---	---
South Atlantic Bury 2	-12,204	-20,004	9	1,33	0,01	---	---
South Atlantic Bury 3	-12,200	-18,504	10	1,38	0,01	---	---
South Atlantic Bury 4	-10,186	-7.945	11	1,06	0,02	---	---
South Atlantic Bury 5	-10,506	-0.015	12	1,31	0,01	---	---
South Atlantic Bury 6	-10,797	-13.328	13	1,37	0,01	---	---
South Atlantic Bury 7	-10,842	-7.945	14	1,33	0,01	---	---
South Atlantic Bury 8	-10,685	-20.465	15	0,77	0,01	---	---
South Atlantic Bury 9	-12,100	-11.476	16	1,02	0,01	---	---
South Atlantic Bury 10	-10,701	-0.003	17	1,02	0,01	---	---
South Atlantic Bury 14	-10,006	-0.012	18	1,28	0,01	---	---
Costa da África	-0.943	-0.013	19	1,32	0,01	---	---
South of Africa	-10,641	-4.693	20	0,88	0,01	0,70	0,04

The measured and collected data were subjected to selection in a common time interval in order to maintain continuity and integrity so that the discontinuous flotation analysis was consolidated in part of them, ie, the time series trend was removed in different scales, analyzing intrinsic fluctuations of the data, so that it became possible to record the existence of a correlation between the series and the power law, indicating a predictable behavior of the same for each float, for wind speed, with a calculated margin of error and in the normalized time interval of two years, 2016 and 2017, in a sequenced way and with the records of the tendencies of the local

climatological cycles and registering the associated trends, adjustments and errors in Table 2 and Table 3.

The Brazilian coast, especially in the vicinity of the continent and in the limits of the continental shelf of Brazil as well as all the South Atlantic Ocean, are part of a vast oceanic region that has a great deficiency of data. In this sense, and in accordance with the International Convention for the Safety of Life at Sea, which Brazil is a faithful signatory, it has the responsibility of generating and disseminating climatic and meteorological products (Brazil, 2017b).

Figure 3



The detection of this phenomenon in the analyzed variables, ie temperature and wind speed, can indicate the existence of a correlation between them as well as the fact that they are governed concomitantly by global phenomena in a long time scale and local fluctuations on small time scales, such as high pressure zones, equatorial regions, and low pressure areas of the tropics, generating constancy, for example, of the wind speed, which is the trade winds and their constancy of velocities, indicating a higher wind potential (Pegorelli *et al.*, 2018).

CONCLUSIONS

Considering that the analysis of the wind speed in the Brazilian coast and in the South Atlantic can be concluded that: contributed to a better understanding of the climatological cycles at sea; there was no existence of the crossover phenomenon for the velocity of the wind at sea (perhaps other variables); these analyzes also indicate that these records should prove useful for the validation of global climate models; as a proposal for future work, in order to further deepen the knowledge about the processes involved, it is suggested to increase the number of buoys under analysis in order to verify other synoptic conditions and, consequently, different dynamic and thermodynamic configurations and to approach a space scale time, with an emphasis on the microscale of the atmospheric boundary layer

through alignment and simulations with numerical models (WRF).

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Solution of the advection-diffusion equation with eddy diffusivity dependent on source distance in a vertically inhomogeneous PBL

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Abstract: The present study aims to solve the steady-state two-dimensional advection-diffusion equation with vertical eddy diffusivity dependent on the source distance in a vertically inhomogeneous planetary boundary layer. The Eulerian models with eddy diffusivity depending on the source distance capture the memory effect present in the adjacencies of the source, making the analytical models more reliable. For this, the GILTT (Generalized Integral Laplace Transform Technique) analytical method was applied in the resolution of the advection-diffusion equation. For the purposes of comparison and validation of the presented model, we used the experimental data from Copenhagen and Prairie Grass, comparing the results obtained by the solution with the coefficient $K_z(x,z)$ with those obtained with the coefficient $K_z(z)$. The obtained values suggest that the inclusion of the memory effect improves the description of the process of turbulent transport of contaminants in the atmosphere, only to sources close to the ground and under extremely unstable conditions

Keywords: GILTT; Pollutant Dispersion, Memory Effect, Advection-Diffusion Equation, Eulerian Models.

INTRODUCTION

The process of dispersion of pollutants in the Planetary Limit (PLP) is, often, modeled by the diffusion-advection equation, which justifies the great interest of the community in the study of analytical solutions of this equation. In this sense there's a significant scientific advance in relation to obtaining solutions analytic/semi-analytic equation of the diffusion- advection, using different methodologies, as described in the works of (Rounds, 1955);(Yeh and Huang, 1975); (Moreira et al., 2005, 2009,2014); (Sharan and Modani, 2006); (Essa et al., 2007);(Tirabassi et al., 2008); (Pimentel et al., 2014).

Another important factor in the transport of pollutants can be found in the choice of the turbulent parameterization, after all, it describes the behavior of turbulence and nature around the source from the point of view physicist. In his statistical theory of diffusion, Taylor (1922) showed that turbulent diffusion is in regions that are close to and distant from a source. In regions adjacent to the source, fluid particles keep the memory of your turbulent environment. For long travel times, this memory is lost, and the particles only follow the properties of turbulence. The diffusion coefficients that depend on the distance from the source allow you to capture the memory effect that is present in areas close to source high and low, turning analytical models more as described in the Sharan et al. (1996), Degrazia et al. (2001) and Moreira et al. (2014).

That one may investigate how the coefficient of diffusion will influence the sensitivity of the proposed model, the diffusion-advection equation was solved analytically, applying the GILTT (Generalized Integral Laplace Transformation Technique). For more information on the GILTT method, consult (Wortmann et al. 2005); (Moreira et al., 2005); (Weymar, 2016); (Buske Daniela et al., 2017).

In this context, the proposed model was parameterized with the diffusion coefficients vertical $K_z(x,z)$, proposed in the work of Mooney and Wilson (1993) and Moreira et al. (2002). The first one is applied to high moderate weather conditions convective, and the second, for low and strongly convective conditions, both data by the following:

$$K_z(x,z) = f(z).g(x) \quad (1)$$

where $g(z)$ the functional form of the coefficient on the diffusion depends only on the spatial z variable, and $f(x)$ is the correction of $g(z)$ points near the source.

To evaluate the performance of the model studied, the data generated by the solutions were with experimental data from Copenhagen and Prairie Grass.

The GILTT methodology

The following are the main steps of the GILTT methodology applied to the diffusion- two-dimensional advection with diffusion coefficient that depend on the distance from the source, stationary, based on theory K, for a system of Cartesian coordinates whose source is in CLP, given by the following

$$U(z) \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left(K_z(x, z) \frac{\partial C}{\partial z} \right) \quad (2)$$

with the following boundary conditions

$$-K_z(x, z) \frac{\partial C}{\partial z} = 0 \text{ em } z = 0 \text{ e } z = h \quad (3)$$

and the condition of source

$$C(0, z) = \frac{Q}{U(z)} \delta(z - H_s) \quad (4)$$

where H_s it represents the height of the source, δ is the Dirac delta and h is PLC height.

To apply the GILTT technique it is necessary that the initial conditions or contour conditions are homogeneous, and that the problem is of finite in this context, GILTT will be applied to variable z .

The first step is to find the equation that represents the auxiliary problem of Sturm-Liouville. For this, Eq. (1) is substituted in Eq. (2), obtaining:

$$\frac{U(z)}{f(x)} \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left[g(z) \frac{\partial C}{\partial z} \right] \quad (5)$$

In order to obtain the auxiliary equation, the substitution of the variable suggested in the Crank, (1968), given by

$$dX = f(x)dx \quad (6)$$

Thus, Eq. (5) can be rewritten as

$$u(z) \frac{\partial C}{\partial X} = \frac{\partial}{\partial z} \left[g(z) \frac{\partial C}{\partial z} \right] \quad (7)$$

Using the chain rule to the diffusive term of Eq. (7) (Wortmann et al., 2005), and applying the necessary simplifications, we obtain the equation auxiliary problem:

$$\phi(z)'' + \lambda^2 \phi(z) = 0 \quad (8)$$

and their respective boundary conditions

$$\phi'(z) = 0, \text{ em } z = 0, h \quad (9)$$

This problem has the traditional solution given by:

$$\phi_n(z) = \cos\left(\frac{n\pi z}{h}\right) \text{ com } n = 1, 2, 3, \dots \quad (10)$$

The next step is to expand the variable $C(X, z)$ in a series of how

$$c(X, z) = \sum_{n=0}^{\infty} A_n(X) \phi_n(z) \quad (11)$$

where $A_n(x)$, $n = 0, 1, 2, \dots$, are the unknown coefficients of the series. To determine them, replace Eq. (11) in Eq. (7), thus:

$$\sum_{n=0}^{\infty} \left(\int_0^h U(z) \phi_m(z) \phi_n(z) dz \right) \frac{dA_n(X)}{dX} = \sum_{n=0}^{\infty} \left[\int_0^h \phi_m(z) \left\{ -g(z) \lambda^2 \phi_n(z) + \frac{dg(z)}{dz} \frac{d\phi_n}{dz} \right\} dz \right] A_n(X) \quad (12)$$

For convenience, Eq. (12) will be rewritten in matrix form, resulting in:

$$A'(X) + F \cdot A(X) = 0 \quad (16)$$

subject to the initial condition

$$Q\phi_m(h_s) = A_m(0) \cdot \frac{h}{2} \quad (17)$$

where $A(X)$ represents a vector, and matrix F is defined as $F = B^{-1}E$,

The Equation (16) is then solved by applying the Laplace transform and the diagonalization (Segatto and Vilhena, 1999), providing the transformed solution:

$$\overline{A(s)} = W(sI + D)^{-1} W^{-1} \cdot A(0) \quad (18)$$

where D represents the diagonal matrix of eigenvalues, W the matrix of the auto functions of F , W^{-1} its inverse and I represent the identity matrix.

The elements of the matrix $(sI + D)$ have the form $\{s + d_i\}$, where d_i are the eigenvalues of matrix F or the elements of the diagonal matrix D . $(sI + D)$ is a diagonal matrix of algebra matrix, we have that its inverse is given by multiplicative inverse of the elements of the diagonal the main elements, so the elements of the matrix $(sI + D)^{-1}$ take the form

$\frac{1}{s + d_i}$, whose transform is Laplace and e^{Xd_i} . Of

Equation (6), one has to $X = \int_0^x f(x^*) dx^*$, meaning

the diagonal matrix $L^{-1} \left\{ (sI + D)^{-1} \right\}$, will have the

elements $e^{d_i \int_0^x f(x^*) dx^*}$. Thus, the final solution of Eq. (18) is given by

$$A(X) = X.L^{-1} \left\{ (sI + D)^{-1} \right\} X^{-1} A(0) \quad (19)$$

For more details, see Wortmann et al. (2005) and Moreira et al. (2005).

Thus, the solution of the problem expressed by Eq. (2) is finally obtained and given by:

$$c(X, z) = \sum_{n=0}^{\infty} A_n(X) \phi_n(z) \quad (20)$$

at where $\phi_n(z)$ represents the eigenvalues obtained from equation (10) (Sturm-Liouville) and the vector $A_n(x)$ the result of the solution of problem transformed (19). It should be noted that solution provided by (20) does not have any approximation, except for the truncation error committed to the expansion of the series.

Parametrization of Turbulence Atmospheric

The parameterization of turbulence is the key factor dispersion models. The reliability of each model depends on how the parameters turbulent are calculated and is related to the understanding of CLP behavior in its current state (Mangia et al., 2002). Therefore, the atmospheric conditions are a major factor relevant in the parameterization process of the coefficient, since they describe environment. In this way, expressions used to represent the parameterization of the diffusion coefficients are considered in accordance with the conditions of the atmosphere.

In this context, the model proposed in this paper was parameterized with two types of coefficients of vertical diffusion, the first one dependent on variable z , and the second, dependent on the spatial variables x and z . It is intended, therefore, to investigate the influence that longitudinal distance source has in the process of diffusing the poisoning.

As for the vertical diffusion coefficient dependent on the spatial variable z , the formulations proposed by Degrazia et al. (1997) and Troen & Mahrt (1986), both applied to atmospheric conditions.

The diffusion coefficient proposed by Degrazia, Velho & Carvalho (1997) was deduced based on the

statistical theory of Taylor and the spectrum of turbulent energy. It shall apply PLC and valid for long diffusion times obtained through the expression

$$K_z(z) = 0,22(\omega_* h) \left[\frac{z}{h} \left(1 - \frac{z}{h} \right) \right]^{1/3} \left[1 - \exp\left(-\frac{4z}{h} \right) - 0,0003 \exp\left(\frac{8z}{h} \right) \right] \quad (21)$$

where h represents the height of the convective layer, ω_* is the convective velocity and z represents the height above ground.

The diffusion coefficient proposed by Troen & Mahrt (1986), proposes an expression where turbulent diffusivities have a profile shape prescribed by z/h and parameters from similarity arguments. Is applicable to all unstable PLC and calculated through of the expression:

$$K_z(z) = k \omega_* z \left(1 - \frac{z}{h} \right) \quad (22)$$

where $k \cong 0,4$ represents the constant of Von Kármán and h is the top of the CLP.

For the dependent vertical diffusion coefficient of the spatial variables x and y , the formulations proposed by Mooney and Wilson (1993) and Moreira et al. (2002).

The first is valid for points located near the source, whose wind direction coincides with that of the axis x , and to a moderately convective. Thus, it is used k is a form modified, the wording of which is given by the product of two independent diffusion coefficients, being the first in terms of altitude and second of the longitudinal distance of the source, given by the following:

$$K_z(x, z) = K_z(z) \left[1 - \exp\left(-\frac{x}{L_1} \right) \right] \quad (23)$$

where $K_z(z)$ represents the functional expression of turbulent diffusivity depending only on the vertical variable z , $L_1 = U(H_s) \tau(H_s)$ is the scale along the wind through which the coefficient of diffusion reaches its asymptotic value and τ is the scale of time Lagrangian time at the source, given for $\tau(z) = K_z(z) / \sigma_w^2$, where σ_w represents the deviation of vertical velocity.

In the present study, Eq. (21) and (22) to the $K_z(z)$ da Eq. (23).

The turbulent diffusion coefficient proposed by Moreira et al. (2002), is only valid for a source at ground level under conditions strongly convective. The similarity theory of Yaglom (1972) was used to estimate these quantities, expressed by:

$$K_z(x, z) = \mu h \omega_* \left(\frac{x \omega_*}{\mu h} \right)^2 \left[\left(-\frac{L}{z} + 3 \right) \right] \quad (24)$$

where μ is a constant whose optimal value found is 2.0 and L is the length of Obukhov.

Profile of the wind

The equations adopted by the model to simulate the behavior of the average winds are those predicted by the theory of similarity (Panofsky and Dutton, 1984):

$$u = \frac{u_*}{k_*} \left[\ln \frac{z}{z_0} - \psi_m \left(\frac{z}{L} \right) \right] \quad (25)$$

Where u_* is the scalar velocity relative to mechanical turbulence, k is von Karmanis the roughness length and ψ_m the stability function expressed in the relations of Businger:

$$\psi_m \left(\frac{z}{L} \right) = -4,7 \frac{z}{L} \quad \text{para} \quad \frac{1}{L} \geq 0 \quad (26)$$

and

$$\Psi_m \left(\frac{z}{L} \right) = \ln \left(\frac{1+x^2}{2} \right) + \ln \left(\frac{1+x^2}{2} \right)^2 - 2 \arctan x + \frac{\pi}{2} \quad \text{para} \quad \frac{1}{L} < 0 \quad (27)$$

$$\text{where } x = \left(1 - 15 \frac{z}{L} \right)^{1/4}$$

The second wind speed profile was described by a power law (Panofsky and Dutton, 1988) expressed by:

$$\frac{u_2}{u_1} = \left(\frac{z_2}{z_1} \right)^n \quad (28)$$

in which u_1 and u_2 are the average speeds of the wind at points z_1 and z_2 measured in the direction of vertical z from the ground, and represents a number associated with the turbulence, roughness and difference between points taken as a reference.

Results

To evaluate the accuracy of the model, the results obtained were compared with the data experiments from Copenhagen and Prairie Grass.

The Copenhagen experiment, described by Gryning and Lyck (1984), was carried out north of in the municipality of Gladsaxe under conditions neutral and unstable atmospheres. The experiment consisted of the release without buoyancy of a tracer chemical, Sulfur Hexafluoride (SF_6), tower of 115 m. The samples were collected level ($z = 2\text{m}$) by 60 collectors in positions located on three concentric arcs the source and perpendicular to the direction of the average radial distances of 2, 4 and 6 km. It is worth noting that the region in which the experiment was performed was predominantly residential, of roughness of 0,6 m.

The Prairie Grass experiment was O'Neill, Nebraska, under atmospheric conditions stable and unstable during the summer of 1956 (BARAD, 1958). It consists of a set of standards of observations (68 experiments) widely used in the validation of dispersal. During the experimental trial, the sulfur dioxide (SO_2) was released from a source point at a height of 0,46 m the experiments of 65 to 68) of the soil. Measurements concentrations were carried out at a height of 1,5 m along concentric arcs located in intervals of 50, 100, 200, 400 and 800 m. By itself deal with a virtually flat terrain, the length of surface roughness is 0.6 cm. About half of the 68 experiments, refers to thermal stratification (diurnal) and the remainder was obtained in conditions (night), in the presence of temperature inversions.

The data generated in this section were obtained from the data of the different experiments (Copenhagen and Prairie Grass) together with the turbulent parameterizations and wind profiles discussed in the previous sections.

Figure 1 shows the numerical convergence of solution parameterized with a coefficient of diffusion dependent on the distance from the source, Eq. (23), and the logarithmic wind profile, Eq. (25), and the micrometeorological data from the experiment 9 of Copenhagen. From this analysis, it is noted that for $N > 80$, the Concentrations reach a numerical stability, that is, it suffers little variation, which shows that the method converges for values of $N = 80$.

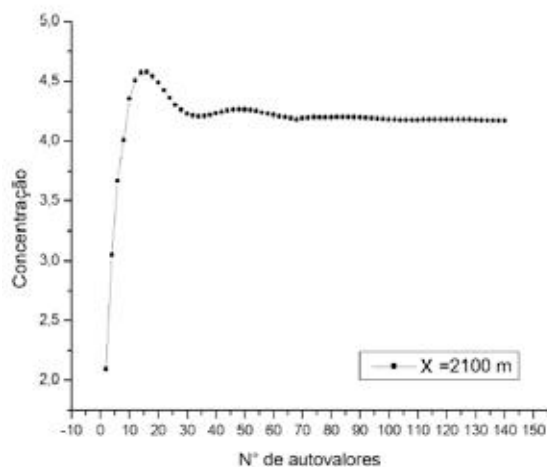


Figure 1. Numerical convergence of concentration of pollutants for experiment 9 from Copenhagen to $x = 2100\text{m}$.
Reference: Soledade et al. (2019)

To verify the contribution of the memory effect, the model was parameterized for sources relatively high, subject to conditions moderately unstable atmospheres, taking the micrometeorological data of the experiment Copenhagen.

In this context, the model was parameterized with the coefficient $K_z(x, z)$ proposed by Mooney & Wilson (1993), Eq. (23), and compared with the solution parameterized with the coefficients $K_z(z)$ proposed by Degrazia et al. (1997), Eq. (21), and Troen & Mahrt (1986), Eq. (22). It was also adopted different wind profiles (power and logarithmic), in order to verify which of them provided the best accuracy in results.

The data obtained were statistically treated (Hanna, 1989), tabulated and organized in the Table 1. In cases I and II, the solution was parameterized with the vertical diffusion coefficient $K_z(x, z)$, given by Eq. (23), taking equation $K_z(z)$ Eq. (21) and (22), respectively. In cases III and IV, the model was parameterized with the diffusion coefficient vertical $K_z(z)$, given by Eq. (21) and Eq. (22), respectively. The logarithmic wind profile was adopted for all cases (I, II, III and IV).

Table 1. Statistical model indices applied the micrometeorological conditions of the experiment in Copenhagen.

	Coeficiente	Nmse	Cor	Fa2	Fb	Fs
I	$K_z(x, z)$	0,06	0,88 8	1,00 0	0,00 6	0,21 7
II	$K_z(x, z)$	0,06	0,89 1	1,00 0	0,00 9	0,18 2
III	$K_z(z)$	0,08	0,90 7	1,00 0	0,11 2	0,28 6

IV	$K_z(z)$	0,09	0,90 1	1,00 0	0,14 0	0,25 8

Reference: Soledade et al.; (2019)

indicate good agreement between the data and the GILTT method. For an analysis satisfactory statistical indice, the results parameters are close to zero for the Nmse, Fb and Fs and close to one for the Color and Fa2 indicators (Hanna, 1989).

Confronting the statistical indices of cases I and II with cases III and IV, it is observed that the values obtained in case I and II are relatively better than those provided in III and IV, with the statistical correlation index, whose value was slightly below 90%, but acceptable. At the However, it is not possible to ascertain the longitudinal distance of the source in the diffusion, since the indices are relatively next.

Figures 2 and 3 show the scatter plots derived from Eq. (20), parameterized with the diffusion coefficients given by Equations (22) and (23), respectively, for the wind profile logarithmic, using the data micrometeorological experiments of the Copenhagen.

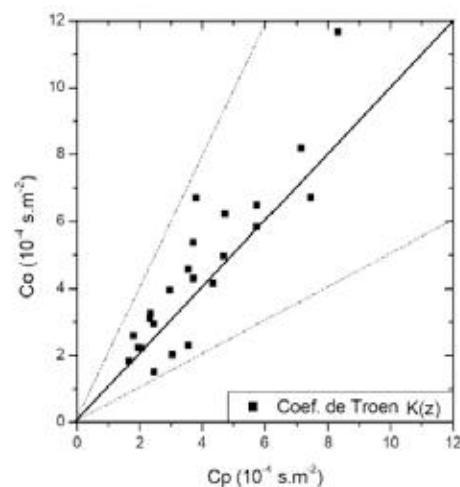


Figure 2. Data scatter plot of observed concentrations (c o) in the experiment compared to the concentration data predicted maximal (c p) in case IV.
Reference: Soledade et al. (2019)

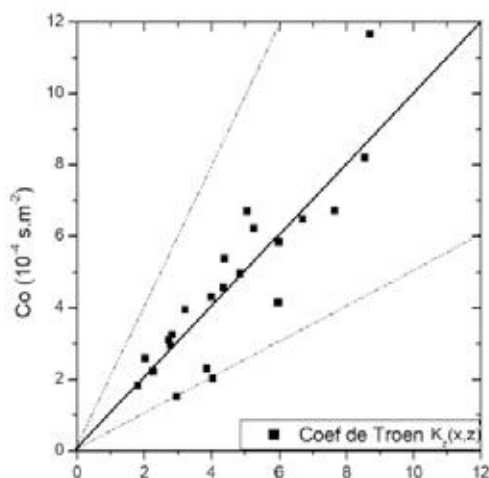


Figure 3. Data scatter plot of observed concentrations (c o) in the experiment compared to the concentration data (p p) in case II.
Reference: Soledade et al. (2019)

The analysis of dispersion plots suggests a greater agreement between the values observed and predicted for case II (Figure 3) when compared to Case IV (Figure 2), since there is a greater concentration of points on the 1st bisector of the spreading chart. However, this analysis is not corroborated when comparing the statistical indices.

In the second part of the research, we investigated the effect of memory for the light sources, waving to intensely convective atmospheric conditions, taking the micrometeorological data from the Prairie Grass experiment. In this scenario, the solution was parameterized with the coefficient $K_z(x,z)$ proposed by Moreira et al. (2002), Eq. (24), and compared with the models parameterized with the vertical diffusion coefficient $K_z(x,z)$, given by Eq. (23), taking for $K_z(z)$ a Eq. (21) and vertical diffusion coefficient $K_z(z)$ given by Eq. (21).

The statistical indices obtained in Table 2 indicate good agreement between the data and the GILTT method only for the case I. Analyzing the statistical indices (Hanna, 1989) we note that this model simulates satisfactorily the observed concentrations, in relative to the values of Fb and Fs close to zero and relatively close to 1.

Confronting the statistical indices of Table 2, it is observed that all indices obtained in case I are better than cases II and III, thus revealing, importance of a good parameterization of the solution, given that the diffusion coefficient proposed by Moreira et al. (2002) describes better the conditions of strong convection present in the the Prairie Grass experiment, while the coefficient proposed by Mooney & amp; Wilson (1993) (cases II)

was formulated into an atmosphere moderately convective.

Table 2. Statistical model indices applied the micrometeorological conditions of the Prairie Grass experiment.

	Coeficiente	Nms e	Cor	Fa2	Fb	Fs
I	$K_z(x,z)$	0,52	0,81 4	0,83	0,16 5	0,00 6
II	$K_z(x,z)$	0.84	0.72 7	0.62 0	0.32 0	0.26 9
III	$K_z(z)$	0,90	0,78	0,63	0,42	0,48

Reference: Soledade (2019)

The results also highlight the insertion of the variable x into the diffusion coefficient vertical. It is of fundamental importance in capturing the memory effect, a fact that can be verified by comparing the statistical indices of cases I and II with case III.

Figures 4 and 5 show the dispersion plots derived from Eq. (20), parameterized with the diffusion coefficients given by Equations (21) and (24), respectively, for the logarithmic wind profile, using the micrometeorological data of the experiment of Prairie Grass.

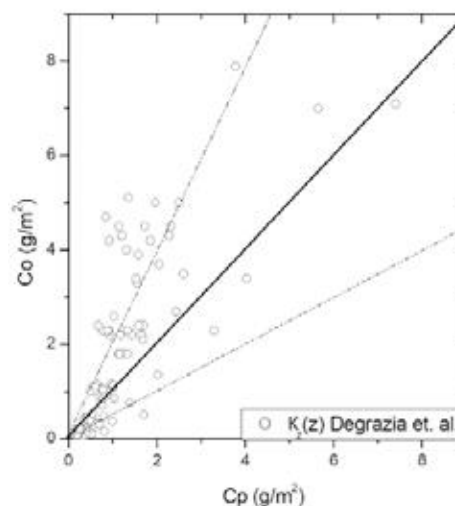


Figure 4. Data scatter plot of observed concentrations (c o) in the experiment compared to the concentration data predicted maxims (c p) in case III.
Reference: Soledade et al. (2019)

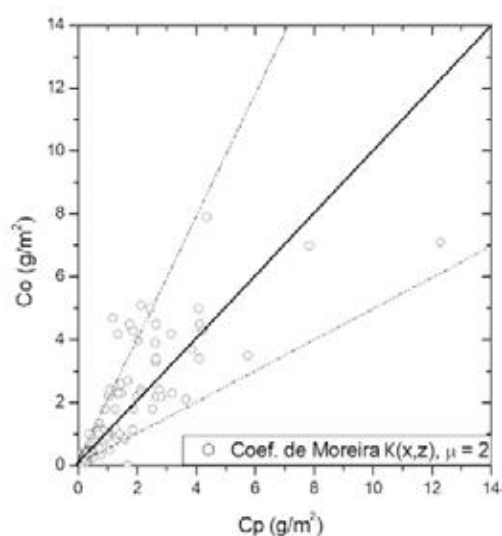


Figure 5. Data scatter plot of observed concentrations (c o) in the experiment compared to the concentration data predicted maxima (c p) in case I.

Reference: Soledade et al. (2019)

The analysis of the scatter plots corroborates with the results obtained by the indices statistics. Comparing Figures 4 and 5, it was observed that in case I (Figure 5) there is a greater number of points within a factor of two that in case III (Figure 4), which shows the influence of the memory effect on the solution.

CONCLUSIONS

For the Copenhagen experiment (source relatively high and atmospheric conditions moderately convective), the concentrations provided by the parameterized model with the coefficient $K_z(x, z)$ indicated good results. Its analysis is validated by statistical indices provided in Table 1 (Case I and II). Despite the good performance, it was not possible to influence of the memory effect, confront the parameterized models with the coefficient $K_z(x, z)$ (cases I and II) with that parameterized with the coefficient $K_z(z)$ (cases III and IV), it can be seen that their statistical indices are very close.

With respect to the Prairie Grass experiment, possible to verify the influence of the memory. The concentration values obtained for the models parameterized with the coefficient $K_z(x, z)$ proposed for low sources, under conditions strongly convective (MOREIRA et al. al., 2002), presented the best results when compared to the model parameterized with coefficient $K_z(z)$, as evidenced by the indices Table 2. Therefore, they obtained with the coefficients of distance-dependent diffusion of the source are better than the results achieved with the coefficient $K_z(z)$, which suggests

that the inclusion of memory effect, as predicted by the theory of Taylor, improves the description of the turbulent transport of a passive pollutant abandoned from a low point source and are continued.

Thus, the analysis of the results reveals that the methodology of solution of the diffusion- advection suggested in this paper, together with parameterizations that describe the physics of non-homogeneous turbulence and dependent on the distance from the source, good accuracy for the concentrations obtained in the experiments from Copenhagen and Prairie Grass, but the memory effect was only verified for low sources under atmospheric conditions strongly convective.

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A new direction in the modeling of air pollution considering anomalous dispersion

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Abstract: The transport of pollutants under the combined effects of advection and diffusion is described by the advection-diffusion equation, with which many physical processes can be modeled. Atmospheric pollution caused by natural or anthropic effects is an example systematically modeled by traditional differential equations (whole order). There is, however, a gap in the analytical solutions of fractional-order (non-integer order) differential equations in the literature in relation to the dispersion of atmospheric pollutants, where the use of fractional calculation in turbulent diffusion modeling is justified by non-differential behavior in the problem and by the presence of anomalous diffusion. In this study, the authors propose an analytical solution of the three-dimensional advection-diffusion equation of the fractional order, in the Caputo sense, applied to the dispersion of atmospheric pollutants; the solution is obtained by applying the generalized integral transformation technique (GITT), solving the problem transformed by the Laplace decomposition method (LDM), considering lateral and vertical turbulent diffusion dependent on the longitudinal distance of the source, as well as a fractional parameter. The fractional solution has adequate generalization capacity, considering the fractional integer parameter, since it deals with a known solution. In addition, the methodology adopted is simple, easy to implement and has fast convergence. Numerical simulations are presented and their performances are compared with experimental data collected in the field. The best results are obtained with the use of fractional derivatives.

Keywords: Laplace decomposition method; GITT; Advection-Diffusion Equation; Fractional Derivatives; Dispersion of Pollutants.

INTRODUCTION

Due to the increasing and constant industrialization and urbanization, the major centers urban areas are experiencing the harmful impacts degradation of air quality the life of the population and the environment. As a consequence of this, the scientific community investigates means aimed at understanding emission of pollutants into the atmosphere and your control. Thus, dispersion as a practical and rapid alternative which allow the study of the dispersion of way to control.

The effectiveness of Eulerian dispersion models (Theory K) is directly related to a suitable parameterization of the diffusion coefficient, for being responsible for the description of the behavior of the diffusion of pollutants in the atmosphere.

Several researchers have been contributing with studies focused on the physical modeling of the planetary boundary layer (CLP) through development of new parameterizations for the diffusion coefficient. Given the vast literature, the works of Hanna (1982), Panofsky and Dutton (1988), Pleim and Chang (1992), Degrazia et al. (2000), Moreira and Tirabassi (2004) and Pleim (2007).

Currently, there is an important terms of mathematical modeling with the use of of the fractional derivative. The history of this calculation

is as old as that of full-length differential and integral calculus, seen being of the time of Newton and Leibniz, the two constructors of the differential and integral calculus of entire order. The term arbitrary order calculation it is more appropriate, however, to call it fractional calculation, perhaps in reference to the correspondence between Leibniz and L'Hôpital in 1665, about what would be the derivative of the non-integer order (Oldham and Spanier, 1974). However, despite many contributions of that time, only in the century, that is, in the 1970s almost three years centuries later, the theme was once again debated in the first international conference on fractions and their applications to science (Ross 1974). From this event, several articles discussed the mathematical and physical aspects of this important theme, which is known with the generalization of integral and differential calculus (Debnath and Bhatta, 2007). Against this background, despite the great numerical solutions of equations, there is a strong interest in analytical solutions of equations differential, where the fractional calculation, especially fractional differential equations, has been used to describe many natural phenomena (Zaslavsky, 1994; Meerschaert and Tadjeran, 2004; Gorenflo and Mainardi, 2009; Schumer et al. 2009). However, fractional derivatives recently obtained practical applications (Debnath, 2003; Moreira and

Moret, 2018; Santos, 2019). Thus, the fractional calculation has become a very useful tool for studying anomalous dispersion and other transport processes, initially with greater attention to the environment (Benson et al., 2013; Deseri et al. Zingales, 2015). In the atmospheric environment, traditional differential equations do not solve the problem of turbulent diffusion because the usual derivatives are not well defined in non-differentiable behavior introduced by turbulence. Consequently, it is expected that the classical equations do not explain completely the anomalous dispersion of pollutants, because in this case the system parameters generally grow faster than obtained by the classical models, with the memory, which is generally considered only in the diffusion coefficient depending on the distance of the source.

In atmospheric problems, the transport of a pollutant under the combined effects of advection and diffusion is described by the advection-diffusion equation, where many physical processes can be modeled by this equation using the known theory Fickian. Air pollution caused by natural or anthropogenic effects is an example, which has been systematically modeled by traditional whole-order differential equations using analytical solutions (Moreira et al., 2005a, b, 2009, 2014; Sharan and Modani, 2006; Essa et al., 2007; Perez-Guerrero et al., 2012; Pimentel et al. 2014). However, analytical solutions have been recently proposed for the diffusion- 2D fractional advection (Goulart et al., 2017; Moreira and Moret, 2018; Acioli et al., 2018; Xavier et al., 2018; Moreira and Santos, 2019). In that sense, given that the errors inherent in the mathematical models are due to the modeling of physical phenomena and numerical errors, it is verified that the analytical solutions, somehow, eliminate the numerical error of the solution of the equation, except for rounding. deactivation error. As Consequently, it becomes possible to make a more realistic error modeling due to physical phenomena. This the mathematical model we propose in this study does not solve the advection-diffusion equation traditionally expressed but modifies the mathematical structure of this equation to represent a more realistic picture of developments in concentration of dispersed pollutants in the atmosphere. Therefore, we introduce operators fractions in the equation that governs of pollutants in the planetary boundary layer (CLP). Focusing our attention in this direction, in this work we have reported on an analytical solution

in series for the diffusion-advection equation three-dimensional (3D), in order to simulate the dispersion of pollutants into the atmosphere. The new this work is based on the analytical solution of this equation combining the Decomposition Method of Laplace (LDM) (Adomian, 1994; Jafari and Gejji, 2006) and the generalized integral transformation

technique (GITT) (Cotta, 1993; Costa et al., 2006), considering the effect of memory on the diffusion turbulent and fractional derivative. The LDM approach is based on the Laplace transform technique, resulting in a numerical algorithm to solve differential equations linear. The method is very well adapted to physical problems, since it does not require unnecessary linearization, disturbance and other restrictive methods and assumptions that may change the problem to be solved, sometimes seriously. O GITT is a well-known hybrid method that solved a wide range of direct and investments, mainly in the area of heat and fluid mechanics (Cotta, 1993; Cotta and Mikhailov, 1997; Cheroto et al., 1999; Cotta et al. 2003). The main steps of this method include construction of the Sturm-Liouville auxiliary problem associated with the original problem, the determination integral processing technique in one series, based on the self-function of the problem of Sturm-Liouville resolved, the replacement of this expansion into the original problem and moments. This procedure leads to a set of ordinary differential equations, classically resolved by numerical methods. Combining the methods, we obtained a new technique for analytical solutions that can be used to linear and non-linear problems. To achieve this goal, we outline the work of the following form: we report the derivation of the solution for the three-dimensional diffusion-diffusion equation stable stationary; the numerical results given by the new method are announced, as well as comparison with experimental data; finally, we present the conclusions.

METHODS

The integer-order advection-diffusion equation is widely used to model the dispersion of atmospheric pollutants; however, the non-integer order is the generalisation of the traditional equation. However, it has remained a great challenge that no analytical solution has existed to the traditional equation in its general form and with the physical parameters all dependent on spatial and temporal variables. In addition, fractional derivatives increase the complexity of obtaining an analytical solution if all the derivatives are of non-integer order. Thus, to obtain an analytical solution, simplifying assumptions are usually made.

Let us consider a Cartesian coordinate system with the x axis aligned with the mean wind speed u in the longitudinal direction, the y axis aligned with the mean wind speed v in the transverse direction, and the z axis aligned with the mean wind speed w in the vertical direction. Let us also make the following simplifying assumptions: i) steady-state conditions exist; ii) the wind speeds v and w in the transverse and vertical directions, respectively, are zero; iii) the advective term in the x direction is much greater than the diffusive term in the same direction; iv) no chemical reaction occurs; v) in the

study case, the wind speed u in the longitudinal direction is constant and the diffusive terms are dependent only on x ; and vi) a fractional derivative exists only for the longitudinal advective term. Based on these assumptions, the three-dimensional (3-D) equation with a fractional derivative of the advective term can be written as follows:

$$U \frac{c \partial^\alpha c(x,z)}{\partial x^\alpha} = K_y(x) \frac{\partial^2 c(x,z)}{\partial y^2} + K_z(x) \frac{\partial^2 c(x,z)}{\partial z^2}, \quad 0 < \alpha \leq 1 \quad (1)$$

to $0 < z < h$ e $x > 0$, where h is the height of the boundary layer (PBL), L_y represents a length in the satisfying a certain condition of contour, c is the concentration of pollutant, C indicates derivative in the Caputo sense, α represents the order of the operator fraction, is the longitudinal velocity of the wind, and K_y are K_z the diffus of lateral vortices and respectively.

In this work, lateral turbulent diffusion and depend only on the longitudinal distance of the source (Goulart et al., 2017):

$$K_y(x) = \left(\frac{\sigma_v}{U}\right)^2 U x^\alpha = \beta x^\alpha \quad (2)$$

$$K_z(x) = \left(\frac{\sigma_w}{U}\right)^2 U x^\alpha = \omega x^\alpha \quad (3)$$

where α it has similar order of the fractional derivative (Goulart et al., 2017; Xavier et al., 2018), β and ω constant, σ_v and σ_w are the standard deviations of lateral and vertical velocities, respectively. For the solution of the equation (1), variable replacement is required in the form below, as proposed by (Moreira et al. 2014; Xavier et al., 2018):

$$X^\alpha = \int_0^x x(dx)^\alpha \quad (4)$$

it is observed that Eq. (1) falls in the case where turbulent diffusion and wind speed are constant. For the solution of Eq. (1) it is necessary determine the boundary conditions. Thus, the usual condition of zero flow of contaminants in the surface and top of the vertical domain is used:

$$K \frac{\partial c}{\partial z} = 0 \text{ em } z = z_0 \text{ e } h = z \quad (5)$$

$$K \frac{\partial c}{\partial z} = 0 \text{ em } z = 0, L_y \quad (6)$$

where h is the height of the planetary boundary layer (PBL). In addition, there is a source with Q emission rate at height of the source, H_s :

$$c(0, y, z) = \frac{Q}{U} \delta(z - H_s) \delta(y - y_0) \text{ em } x = 0 \quad (7)$$

where H_s and y_0 indicate the position of the source; the delta function of Dirac, $\delta(\cdot)$, is approximated by the following expression:

$$\delta(z - H_s) = \frac{1}{h} \left[1 + 2 \sum_{n=1}^{\infty} [\cos(\lambda_n z) \cos(\lambda_n H_s)] \right] \quad (8)$$

being the eigenvalues given by:

$$\lambda_n = \frac{n\pi}{h}, n = 1, 2, 3, \dots \quad (9)$$

Thus, the origin condition can be rewritten as:

$$c(0, y, z) = \frac{Q}{Uh} \left[1 + 2 \sum_{n=1}^{\infty} [\cos(\lambda_n z) \cos(\lambda_n H_s)] \right] x = 0 \quad (10)$$

The first step to obtain the three-dimensional solution of Eq. (1) will be the GITT application in the variable y . The formalism of the GITT (Generalized Integral Transform Technique) method (Cotta, 1993; Cotta and Mikhailov, 1997), is related to the choice of the auxiliary problem, with similarity to the original problem and its respective boundary conditions. Here we determine the Sturm-Liouville auxiliary problem as follows: Thus, the original condition can be rewritten as:

$$\psi_i''(y) + \lambda_i^2 \psi_i(y) = 0; \quad 0 < y < L_y \quad (11)$$

with the boundary conditions,

$$\psi'(y) = 0 \text{ em } y = 0, L_y \quad (12)$$

The solution is $\psi_i(y) = \cos(\lambda_i y)$, where λ_i are the positive roots of the expression $\sin(\lambda_i L_y) = 0$. Thus, $\lambda_0 = 0$ and $\lambda_i = i\pi/L_y$. Are functions $\psi_i(y)$ and λ_i are and are eigenfunctions and eigenvalues, respectively, associated with the Sturm-Liouville problem, satisfying the following orthogonality condition:

$$\frac{1}{\sqrt{N_i}} \frac{1}{\sqrt{N_j}} \int_v \psi_i(x) \psi_j(x) dx = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases} \quad (14)$$

where N_i it is defined as:

$$N_i = \int_v \psi_i^2(x) dx \quad (15)$$

GITT's formalism postulates that it $C_n(x, y, z)$ can be expressed as a series expansion of orthogonal orthogonal functions $\psi_i(y)$ for the y direction, where i is the order of the corresponding eigenvalues λ ,

$$C_n(X, y, z) = \sum_{i=0}^{\infty} \frac{C_i(X, z) \psi_i(y)}{N_i^{1/2}} \quad (16)$$

Substituting Eq. (16) into the EQ. (1) is obtained:

$$U \sum_{i=0}^{\infty} \frac{c \partial^{\alpha} c_i(x, z)}{\partial x^{\alpha}} \frac{\psi_i(y)}{N_i^{1/2}} = \beta \sum_{i=0}^{\infty} c_i(X, z) \frac{\psi_i(y)}{N_i^{1/2}} + \omega \sum_{i=0}^{\infty} \frac{c_i(X, z) \psi_i(y)}{\partial x^2} \frac{1}{N_i^{1/2}} \quad (17)$$

the next step is to apply the operator $\frac{\int_0^{L_y} \psi^2(x) dx}{N_i^{1/2}}$ in

Eq. (17), and watch this $\psi''(y) = -\lambda_i^2 \psi_i(y)$.

the next step is to apply the operator in Eq. (17), and watch this. In addition, by using the property orthonormal, Eq. (17) can be written as:

$$U \frac{\partial^{\alpha} C_i(X, z)}{\partial x^{\alpha}} = \omega \frac{\partial^2 C_i(X, z)}{\partial z^2} - \beta \lambda_i^2 C_i(X, z) \quad (18)$$

where the contour conditions (5) remain unchanged. However, the origin condition is now rewritten as,

$$U \sum_{i=0}^{\infty} \int_0^{L_y} C_i(0, y, z) \frac{\psi_i \psi_j}{N_i^{1/2} N_j^{1/2}} dy = Q \delta(z - H_s) \int_0^{L_y} \frac{\delta(y - y_0)}{N_j^{1/2}} dy \quad (19)$$

so

$$c(0, z) = \frac{Q}{Uh} \left[1 + 2 \sum_{n=1}^{\infty} [\cos(\lambda_n z) \cos(\lambda_n H_s)] \right] \frac{\psi_i(y_0)}{N_i^{1/2}} \quad (20)$$

The next step is to use the Laplace decomposition (CDM) to obtain the solution $C(X, z)$. In this way, applying the Laplace (L) in Eq. (18) for the variable X , we get:

$$L \left[U \frac{\partial^{\alpha} C_i(X, z)}{\partial x^{\alpha}} \right] = L \left[\omega \frac{\partial^2 C_i(X, z)}{\partial z^2} \right] - L [\beta \lambda_i^2 C_i(X, z)] \quad (21)$$

$$= \mathcal{L} \left[\omega \frac{\partial^2 C_i(x, z)}{\partial z^2} \right] - \mathcal{L} [\beta \lambda_i^2 C_i(x, z)] \quad (22)$$

Reorganizing Eq. (22) to obtain $C_i(s, z)$,

$$C_i(s, z) = \frac{1}{s} C_i(0, z) + \frac{1}{U s^{\alpha}} \mathcal{L} \left[\omega \frac{\partial^2 C_i(X, z)}{\partial z^2} \right] - \frac{1}{U s^{\alpha}} \mathcal{L} [\beta \lambda_i^2 C_i(X, z)] \quad (23)$$

To obtain the desired solution $C_i(s, z)$, the Inverse Laplace Transform $\mathcal{L}^{-1}$ in Eq. (23) and using the standard method, where the solution is represented as an infinite series,

$$C_i(X, z) = \sum_{n=0}^{\infty} C_{i(n)}(X, z) \quad (24)$$

results,

$$\sum_{n=0}^{\infty} C_{i(n)}(X, z) = c(0, z) + \mathcal{L}^{-1} \left[\frac{1}{U s^{\alpha}} \mathcal{L} \left\{ K_z \frac{\partial^2 C_i(x, z)}{\partial z^2} \right\} \right] - \mathcal{L}^{-1} \left[\frac{1}{U s^{\alpha}} \mathcal{L} \{ K_y \lambda_i^2 C_i(x, z) \} \right] \quad (25)$$

Combining these first terms, we have:

$$c_{(i)} = \frac{Q}{Uh} \frac{\psi(y_0)}{N_i^{1/2}} \left\{ 1 - \frac{X^{\alpha}}{\Gamma(\alpha+1)} \frac{\beta \lambda_i^2}{U} + \frac{X^{2\alpha}}{\Gamma(2\alpha+1)} \left(\frac{\beta \lambda_i^2}{U} \right)^2 + \dots \right\} + \frac{2Q}{Uh} \frac{\psi(y_0)}{N_i^{1/2}} \sum_{n=1}^{\infty} \cos(\lambda_n z) \cos(\lambda_n H_s) \left\{ 1 - \frac{X^{\alpha}}{\Gamma(\alpha+1)} \left(\frac{\omega \lambda_n^2 + \beta \lambda_i^2}{U} \right) + \frac{X^{2\alpha}}{\Gamma(2\alpha+1)} \left(\frac{\omega \lambda_n^2 + \beta \lambda_i^2}{U} \right)^2 + \dots \right\} \quad (26)$$

at where Γ and the Gamma function. Therefore, the solution is given by:

$$c_i(X, z) = \frac{Q}{Uh} \frac{\psi(y_0)}{N_i^{1/2}} E_{\alpha} \left[-X^{\alpha} \frac{\beta \lambda_i^2}{U} \right] + \frac{2Q}{Uh} \frac{\psi(y_0)}{N_i^{1/2}} \sum_{n=1}^{\infty} \cos(\lambda_n z) \cos(\lambda_n H_s) E_{\alpha} \left[-X^{\alpha} \frac{\omega \lambda_n^2 + \beta \lambda_i^2}{U} \right] \quad (27)$$

results,

$$c_i(X, z) = \frac{Q}{Uh} \frac{\psi(y_0)}{N_i^{1/2}} E_{\alpha} \left[-X^{\alpha} \frac{\beta \lambda_i^2}{U} \right] \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos(\lambda_n z) \cos(\lambda_n H_s) E_{\alpha} \left[-X^{\alpha} \frac{\omega \lambda_n^2 + \beta \lambda_i^2}{U} \right] \right\}$$

(28)

where E_α is the Mittag-Leffler function, which is the generalization of the exponential function, and is intrinsic to the solution of problems with fractional derivatives.

Returning the variable x , we have,

$$c_i(X, z) = \frac{Q}{Uh} \frac{\psi(y_0)}{N_i^{1/2}} E_\alpha \left[- \int_0^x \zeta^\alpha(d\zeta)^\alpha \frac{\beta \lambda_i^2}{U} \right] \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos(\lambda_n z) \cos(\lambda_n H_s) E_\alpha \left[- \int_0^x \zeta^\alpha(d\zeta)^\alpha \frac{\omega \lambda_n^2}{U} \right] \right\} \quad (29)$$

where (Jumarie, 2008),

$$\int_0^x \zeta^\alpha(d\zeta)^\alpha = \frac{\Gamma(\alpha+1)\Gamma(\gamma+1)}{\Gamma(\alpha+\gamma+1)} x^{\alpha+1}, \quad 0 < \alpha < 1 \quad (30)$$

and, if $\gamma = \alpha$,

$$\int_0^x \zeta^\alpha(d\zeta)^\alpha = \frac{\Gamma(\alpha+1)\Gamma(\alpha+1)}{\Gamma(2\alpha+1)} x^{2\alpha}, \quad 0 < \alpha < 1 \quad (35)$$

if, $\alpha = 1$, in the equations (4) e (5), this is $\gamma = 1$ in Eq. (31), results,

$$\int_0^x \zeta^\alpha(d\zeta)^\alpha = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha+2)} x^{\alpha+1}, \quad 0 < \alpha < 1 \quad (32)$$

and, if $\gamma = 0$

$$\int_0^x \zeta^\alpha(d\zeta)^\alpha = x^\alpha, \quad 0 < \alpha < 1 \quad (33)$$

According to the Eq. (16) ($\psi(y_0) = \psi(0) = 1$), we have the final solution

$$c(x, y, z) = \frac{Q}{Uh} \sum_{i=0}^{\infty} \frac{\cos(\lambda_i y)}{N_i^{1/2}} E_\alpha \left[- \frac{\Gamma(\alpha+1)\Gamma(\alpha+1)}{\Gamma(2\alpha+1)} \left(\frac{\sigma_v}{U} \right)^2 x^{2\alpha} \lambda_i^2 \right] \cdot \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos(\lambda_n z) \cos(\lambda_n H_s) \cdot E_\alpha \left[- \frac{\Gamma(\alpha+1)\Gamma(\alpha+1)}{\Gamma(2\alpha+1)} \left(\frac{\sigma_w}{U} \right)^2 x^{2\alpha} \lambda_n^2 \right] \right\} \quad (34)$$

NUMERICAL RESULTS AND DISCUSSIONS

To evaluate the performance of the model obtained in this study, the results of the simulations are compared with the data observed in the the Copenhagen experiment (data set 3D), using to

obtain the concentrations of center line. The dispersion experiments in Copenhagen, described in Gryning and Lyck (1984) and Gryning et al. (1987), and updated in Gryning and Lyck (2002) consisted in the release of the SF₆ tracer (sulfur hexafluoride) north of Copenhagen. The tracer was released without floating a tower with a height of 115 m was collected at the level of the ground. The sampling units were positioned at a distance of 2 to 6 km from the where the pollutant was released. The length of the surface roughness was 0.6 m. The parameters describing the weather conditions and concentrations during the experiments are shown in Table 1. Note that the concentration was normalized by the emission rate (c/Q). Parameter U10 indicates the wind speed measured at 10 m in height and the wind speed U115 measured at 115 m height

Table1: Observed meteorological concentrations laterally $c^y(x,0)/Q(10^{-4}\text{sm}^{-2})$ and the maximum concentrations observed $c(x,0,0)/Q(10^{-7}\text{sm}^{-3})$ during the Experiment of Copenhagen, x is the distance from the source.

Exp.	$U_{10} \text{ (ms}^{-1}\text{)}$	$U_{115} \text{ (ms}^{-1}\text{)}$	$h \text{ (m)}$	$\sigma_y \text{ (m)}$	$\sigma_z \text{ (m)}$	$x \text{ (m)}$	$c^y(x,0)/Q \text{ (10}^{-4}\text{sm}^{-2}\text{)}$	$c(x,0,0)/Q \text{ (10}^{-7}\text{sm}^{-3}\text{)}$
1	2.1	3.4	1980	0.98	0.83	1900	6.28	10.50
						3700	2.31	2.14
2	4.9	10.6	1920	1.39	1.07	2100	5.38	9.85
						4200	2.95	2.83
3	2.4	5.0	1120	0.85	0.88	1900	8.2	16.33
						3700	6.22	7.95
						5400	4.3	3.76
4	2.5	4.6	390	0.47	0.47	4000	11.66	15.71
5	3.1	6.7	820	0.77	0.71	2100	6.72	12.11
						4200	5.84	7.24
						5100	4.97	4.75
6	7.2	13.2	1300	2.26	1.33	2000	3.96	7.44
						4200	2.22	3.37
						5900	1.83	1.74
7	4.1	7.6	1850	1.61	0.87	2000	6.7	9.48
						4100	3.25	2.62
						5300	2.23	1.15
8	4.2	9.4	810	1.35	0.72	1900	4.16	9.76
						3600	2.02	2.64
						5300	1.52	0.98
9	5.1	10.5	2090	1.77	0.98	2100	4.58	8.52
						4200	3.11	2.66
						6000	2.59	1.98

First, it begins with the evaluation of the solution (23) with the Copenhagen data from experiment 1 shown in Table 1. Figure 1 shows the numerical convergence of the solution proposed for concentration at ground level at two distances from source ($x = 1900\text{m}$), considering the wind speed

U115, increasing number of terms in the sum (n) with values other than ($\alpha = 0,95$).

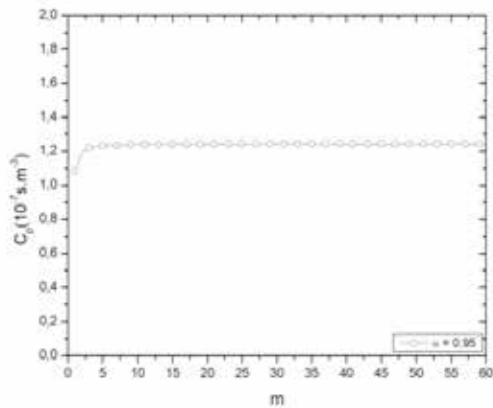


Figure 1: Convergence test of the solution in y applied to the GITT Method.

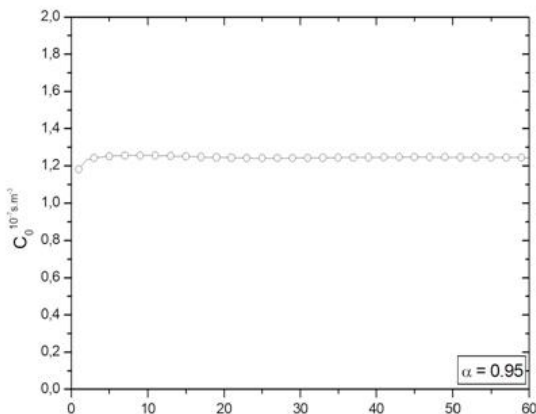


Figure 2: Teste Convergence test of the solution in z applying the Laplace Transform.

The next analysis will be a statistical simulation of the model to verify which α value best results. A Tables 2 shows some performances of the results of the model for the experiment above using the bootstrap resampling software for the statistical evaluation procedure described by Hanna (1989) and defined as follows way:

$$\text{NMSE (normalized mean square error)} = \frac{(\overline{C_o} - \overline{C_p})^2}{\overline{C_p} \overline{C_o}},$$

$$\text{FAT2 = fraction of data (\%, normalized to 1) to } = 0.5 \leq (C_p / C_o) \leq 2,$$

$$\text{COR (correlation coefficient),} = \frac{(\overline{C_o} - \overline{C_o})(\overline{C_p} - \overline{C_p})}{\sigma_o \sigma_p},$$

FB (fraction of bias)

$$= \overline{C_o} - \overline{C_p} / 0.5(\overline{C_o} - \overline{C_p}),$$

$$\text{FS (fractional standard derivations)} = (\sigma_o - \sigma_p) / 0.5(\sigma_o + \sigma_p),$$

where the indexes o and p refer to quantities observed and predicted, respectively, and the bar indicates an average value. The statistical index FB states whether the quantities envisaged underestimate or overestimate those observed. The statistical index NMSE represents the dispersion of the values of the model in relation to the dispersion of data. It is expected that best results have values close to zero for the NMSE, FB and FS indexes, and close to 1 in the COR and FAT2 indices.

At this point, it should be noted that the experiment of Copenhagen provides wind speed data in two different heights: measured at 10m (U_{10}) and measured at a height of 115m (U_{115}).

Therefore, it is possible to analyze the solution with these two heights separately. Table 2 shows the results of the model represented by equation (23), considering different values of wind e measured at 115m high (U_{115}). where the indexes o and p refer to quantities observed and predicted, respectively, and the bar indicates an average value. The statistical index FB states whether the quantities envisaged underestimate or overestimate those observed. The statistical index NMSE represents the dispersion of the values of the model in relation to the dispersion of data. It is expected that best results have values close to zero for the NMSE, FB and FS indexes, and close to 1 in the COR and FAT2 indices.

At this point, it should be noted that the experiment of Copenhagen provides wind speed data in two different heights: measured at 10m (U_{10}) and measured at a height of 115m (U_{115}). Therefore, it is possible to analyze the solution with these two heights separately. Table 2 shows the results of the model represented by equation (23), considering different values of wind e measured at 115m high (U_{115}).

Table 2: Statistical performance indicators models for different values of α with U_{115} .

Modelo de Dispersão	NMSE	COR	FAT2	FB	FS
$\alpha = 1.00$	0.57	0.85	0.69	0.51	0.51
$\alpha = 0.99$	0.41	0.82	0.73	0.39	0.39
$\alpha = 0.98$	0.31	0.80	0.78	0.26	0.26
$\alpha = 0.97$	0.25	0.78	0.87	0.14	0.14
$\alpha = 0.965$	0.24	0.77	0.96	0.78	0.08
$\alpha = 0.962$	0.24	0.76	0.96	0.04	0.45
$\alpha = 0.96$	0.24	0.76	0.91	0.01	0.02
$\alpha = 0.95$	0.27	0.74	0.82	-0.10	-0.93

Table 2 indicates that the best results occurred for $\alpha = 0.962$; $\alpha = 0.965$, with lower NMSE (0.24) and FAT2 of 96% (0.96). The worst result occurs with $\alpha = 1.00$, which represents the integer-order derivative with higher NMSE (0.57) and lower FAT2 (69.0%). Besides the statistical analysis, some graphs are presented in the sequence for a better visualization of results. In the diagnostic evaluation are used plots comparing waste, which are the difference or ratio between concentrations observed and predicted, with the variation in the model parameter. If there is a graph, this may indicate an error in the model. Scatter plots between proportions of the planned integrated and observed cross-wind and the observed concentrations is shown in Figures 3 and 4, considering simulations with wind speed U_{115} .

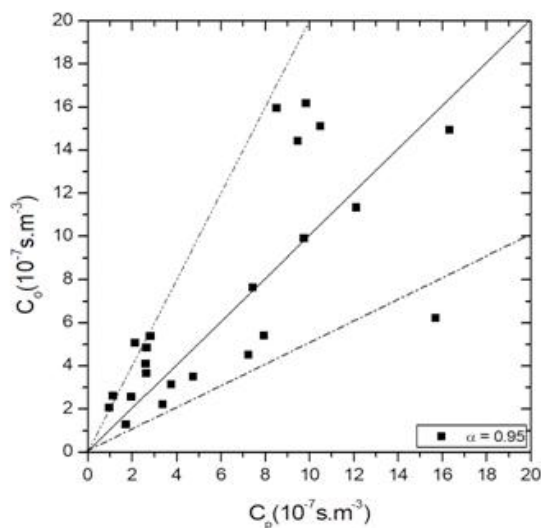


Figure3: Scatter plot of the concentrations observed and predicted by. Considering Eq (28), using the coefficient of diffusion of Eqs. (2, 3) with measured velocity 115m. For the

Copenhagen

experiment.

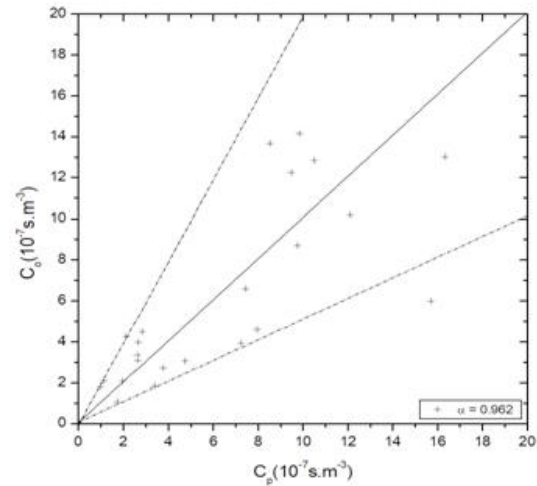


Figure 4: Scatter plot of concentrations observed and predicted by. Considering Eq (28), using the coefficient of diffusion of Eqs. (2, 3) with measured velocity 115m. For the Copenhagen experiment.

CONCLUSIONS

Our study proposes the use of a new methodology to obtain the solution of equation 3D-diffraction advection-diffraction for to simulate the dispersion of pollutants emitted in planetary boundary layer. To obtain this solution, for the first time, the GITT and LDM applied simultaneously, combined with the concept of fractional derivatives. We show that the memory effect, which is usually considered only when the diffusivity of vortices is depending on the distance from the source, now depended both source and derivative distance fractional This is an interesting result because is a practice in dispersion problems in the the effect of memory only in turbulent diffusivity.

In relation to the simulations, the best result, in comparison with the other models, it was parameter $\alpha = 0.95$ and wind speed measured at height, with lower NMSE (0.08) and higher FAT2 (0.96). At the However, this result is similar wind speed at high, with $\alpha = 0.99$ (NMSE = 0.11 and FAT = 0.91). The bad result occurs $\alpha = 1$, with represents the derivative of the whole order $10m$, and wind speed is measured as it has the highest NMSE (0.71) and the lowest FAT2 (0.30). Besides that, with the 3D solution found here, it was possible find a parameterization slightly modified to σ_y e σ_z , which can be used in Gaussian models, because they present very satisfactory when compared to more complex models.

The fact that the physical parameters of the model (turbulent diffusivity and wind speed) does not explicitly depend on the variable z , which is more influenced by the surface of the Earth, meteorological data from the Copenhagen Experiment. Finally, in this work we pave the way

to solve, in the future, the advection-diffusion equation with fractional parameters in the diffusive terms. This is a challenge, but certainly the new models must take into account the fundamental aspects of fractional modeling, since it is the generalization of the calculation as we know it today.

ACKNOWLEDGEMENT

The authors thank the Supercomputing Center for Industrial Innovation (CIMATEC) for providing the computational infrastructure needed to run the models, and the Fundação de Amparo à Pesquisa do Estado da Bahia (FAPESB) for the financial support.

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Session 09

Environmental Odours

H₂S MASS TRANSFER MODELING IN A US EPA FLUX CHAMBER

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Abstract: Flux chambers are widely used to measure emission rates at area sources whose geometry must promote complete mixing of the internal air phase, in order to measure representative emission rates. In this work, the H₂S mass transfer were modeled applying Computational Fluid Dynamics in a US EPA flux chamber, considering two different approaches for the boundary condition at interface gas-liquid: a constant concentration and a flux based on friction velocity. The results showed a complex flow inside the flux chamber with the concentration needing at least six residential times to become stable. Clean air jets can reach the sampling probe, affecting in the concentration values measured. The emission rate modeled with a constant concentration at interface generated better agreement with experimental data.

Keywords: Flux chamber, CFX, mass transfer, H₂S.

INTRODUCTION

The hydrogen sulfide (H₂S) is the most common odorous gas emitted by wastewater treatment plants (WWTP) due to both its high emission rate and its very low detection threshold (Santos et al., 2009). Among the WWTP that have units with quiescent liquid surfaces, which are surfaces with a low degree of perturbation, H₂S emission occurs mainly in tanks and lagoons. A sample collection enclosure system, as portable wind tunnels and dynamic flux chambers, can be used for sampling purposes, in order to determine specific odor emission rates.

The main concern regarding the use of a flux chamber is that when it is placed on a quiescent liquid surface, odorant compounds may accumulate inside the chamber, raising its concentration in the gas phase. Such increase could lead to a suppression of the emission rate of the compound in the fraction of the net surface enclosed by the equipment, resulting in an incorrect measurement of the emission rate at the site, differing from the emission that would occur in the absence of the flux chamber. Therefore, if the air inlet system is not well designed, the chamber atmosphere may not be well mixed, and the measurement results will be biased.

In this context, Computational Fluid Dynamics (CFD) constitutes a tool with great potential to contribute for the analysis of enclosure gas sampling devices to study the influence of configuration and operating conditions on the flow and mass transfer. Therefore, the aim of this work is to assess the performance of the US EPA flux chamber in H₂S mass transfer using CFD modeling.

METHODS

The flux chamber was drawn in 3D configuration, showed in Figure 1, and it was inspired by the standard design described by Kienbusch (1986). The diameter is 40 cm; the height is 26.5 cm with 15 cm as the height of the cylinder body. The exit line probe is 15 cm long and the flux hood contains a pressure release opening.

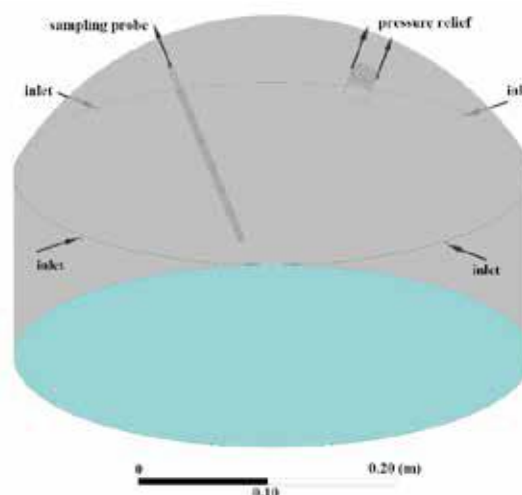


Figure 1 - Schematic drawing of flux chamber.

Ansys CFX 17.2 software was used to solve the governing equations. Equations were solved for isothermal (25 °C) and incompressible flow. The flow was assumed turbulent and the Shear Stress Transport (SST) turbulence model was used. Mass, momentum and turbulence model equations were solved considering steady state conditions. The chemical species equation was solved in transient

condition, with an initial condition of no H_2S inside the chamber. The configuration of Time Steps Adaptive was used to determine the size of the time interval (between 0.001 s and 0.5 s).

Non-slip conditions were considered at flux hood walls and at air-liquid interface. The airflow value used at the inlet holes was $2.47 \times 10^{-5} \text{ kg s}^{-1}$ and at pressure relief, a differential pressure of 0 Pa was used. For solution of chemical species equation, non-flux conditions were imposed at flux hood walls. For interface air-water, two approaches were considered: (i) a constant concentration of $4.813 \times 10^{-5} \text{ kg m}^{-3}$ (Prata Jr. et al., 2016) and (ii) an emission flux based on overall mass transfer coefficient, showed in Equation 1, derived from Mackay and Yeun (1983).

$$K_L = 1.0 \times 10^{-6} + 144 \times 10^{-4} (u^*)^{2.2} Sc_L^{-0.5} \quad (1)$$

where K_L is the overall mass transfer coefficient (m s^{-1}); u^* is the friction velocity (m s^{-1}) and Sc_L is the Schmidt number. Knowing the value of K_L it is possible to estimate the flux at the interface, using Equation 2:

$$E = K_L C_L \quad (2)$$

where E is the emission rate ($\text{kg m}^{-2} \text{s}^{-1}$) and C_L is the concentration of liquid phase, equal to 0.01 kg m^{-3} in this study.

With the concentration values of the diluted species at outlet sampling probe, the emission rate of the flux chamber is calculated using Equation 3 (Eklund, 1992), and then, compared with the experiments values of Prata Jr. et al. (2016).

$$E = 1000^3 \cdot [C] \cdot Q / A \quad (3)$$

where E is the emission rate ($\mu\text{g m}^{-2} \text{s}^{-1}$); $[C]$ is the concentration of the chemical specie at exit line probe (kg m^{-3}); Q is the inlet flow rate ($\text{m}^3 \text{s}^{-1}$) and A is the area of interface (0.126 m^2).

The convergence criterion was set equal to 10^{-6} for mass, momentum, turbulence and chemical species mass equation and an overall imbalance in the domain less than 1%.

A non-uniform non-structured grid was constructed, using Ansys Package Meshing software with grid refinement near walls and exit line probe (prismatic elements constructed by inflation). After grid sensitivity tests, a mesh with 3 million nodes was selected for the simulations.

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Figure 2 shows the streamline pattern. The inlet air jets induce several recirculation regions inside the flux chamber, and they are responsible for sweeps the air-liquid interface, transporting the odorant compounds from the interface to the core of the fluid flow, creating turbulence inside the chamber, which tends to increase mixing and homogenize concentration.

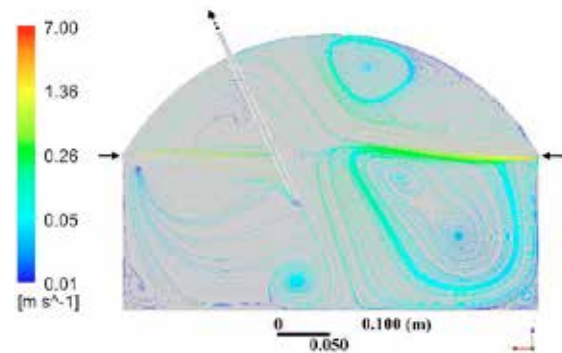


Figure 2 - Streamlines.

The friction velocity is shown in Figure 3 for the interface air/water. The average value found was 0.01 m s^{-1} . Higher values were found in the center of the interface.

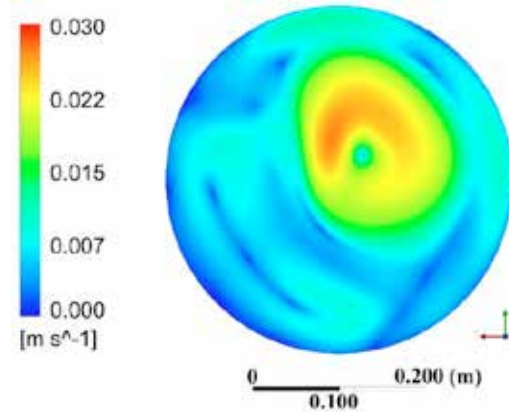


Figure 3 - Friction velocity at interface.

Figure 4 shows the vertical profiles of the H_2S concentration for the two approaches considered for the interface. In general, higher concentration was found close to the interface and flux chamber walls. The approach that considered an emission flux resulted in lower concentrations and consequently, lower emission rate. There are several non-homogeneous spots in regions with low turbulence. Inlet air may reach the sampling probe, what may affect the concentration value measured at the outlet.

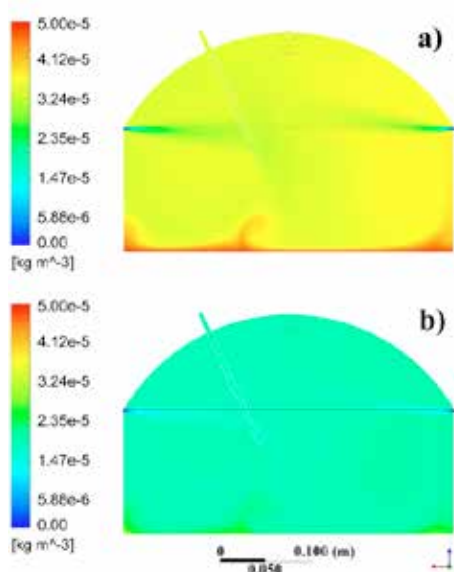


Figure 4 - Vertical profile of H₂S concentration for (a) concentration as boundary condition at interface and (b) flux as boundary condition at interface.

Table 1 presents the emission rate calculated at outlet sampling probe, using Equation 3, and the values found by Prata Jr. et al. (2016) in an experimental campaign and CFX modeling. The simulation considering a constant concentration was about 20 % lower than the experimental value. The results with a flux used as boundary condition generates an emission rate at the sampling probe much lower, compared with the other values, what may show a limitation of the Mackay and Yeun (1983) equation for lower friction velocities and compounds that are dependent primarily on liquid phase turbulence (large values of the Henry constant), as H₂S.

Table 1: H₂S emission rate at outlet sampling probe.

	E ($\mu\text{g m}^{-2} \text{s}^{-1}$)
Constant concentration as boundary condition	22.2
Flux as boundary condition	12.6
Prata Jr. et al. (2016) - experimental	27.7
Prata Jr. et al. (2016) - CFX	20

Figure 5 shows the time evolution of the emission rate calculated at the sampling probe. In the first 20 min (4 residential times) the emission rate increases. From 20 to 30 min, the change with time is slight, but still significant. After 30 min, a small increased of the emission rate was observed, with the stead condition reached in 50 min. Therefore, six residential times (30 min in this flux chamber) shows the minimum time to wait before proceeding the measurements.

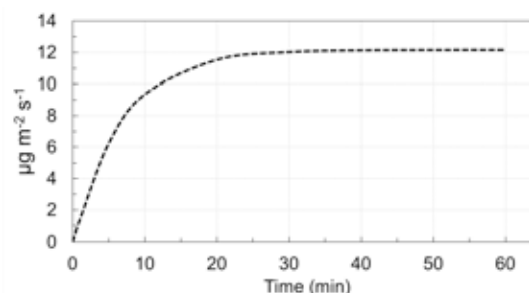


Figure 5 - Time evolution of H₂S emission rate calculated at outlet sampling probe.

CONCLUSIONS

The numerical simulation showed a pattern of complex flow inside the flux chamber. It was observed that the air flow inlet may reach the sampling probe, what may influence the concentration measured. The concentration field indicated that the flux chamber may be not well mixed. Therefore, a device, as a small fan, may be necessary to increase the mixing inside the chamber. It is recommended six residential times prior to start the measurements. The use of other equations to represent the mass flux at interface is necessary to investigate their impact in emission rate estimative, which may improve the results.

ACKNOWLEDGEMENTS

Authors acknowledge CAPES, CNPq, and FAPES.

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DEVELOPMENT OF A SENSITIVE METHOD FOR ASSESSING OF THE ODOUR CONCENTRATION IN A SLAUGHTERHOUSE, COLOMBIA

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Abstract: Odour is an important impact caused by human activities, and it is necessary to provide a method for assessing its extent of annoyance. (Bockreis & Steinberg, 2005). The odour characterization may be evaluated by sensory and analytical methods, but the sensory method is considered a response to environmental conflict produced odours. The sensory method involves the ability to perceive humans and this method evaluate the odour like a mixture of substances, in other words, it does not segregate by elements or compounds. Considering the above, the present article describes the application of the methodology of Dynamic Olfactometry UNE EN 13725 in composting process realized in Central Sacrifice Frigovito SA, Pasto, Colombia; to know the concentration of said odour emitting source. Finally, the result was 279, 15 OUE / m³ compared to other composting process, it is determined that on emission concentration does not represent a high concentration value.

Keywords: Dynamic olfactometry, emission, European Odour Unity (OUE), composting plant.

INTRODUCTION

In Colombia, with resolution 1541 of 2013 made by the Environment Ministry, since this time, the topic of dynamic olfactometry has been taken into account. In this methodology, human evaluators are used as sensors and the characteristics of odors allow determining concentration odour. (IDEAM, 2011). In this regulation, a great variety of emission sources were identified that can generate offensive odors. The slaughterhouses are important due to the sanitary and environmental impact that currently generate more than 70% of the Colombian population. (MINAMBIENTE, 2013).

The current problem with the dynamic olfactometry is its application has been sectorized towards the big industries located in the main cities. The possible cause of this problem is high costs due to sophisticated equipment and supplies are used. This problem has generated few measurements in small industries, but these types of industries must be considered due to the environmental impact can't be associated with extension of industries. In other words, a small source doesn't always generate a small impact on the population, it will be better to take preventive measures and avoid the possible impact that can be generated.

As noted above, it was decided to carry out all the necessary instrumentation to the application of the dynamic olfactometry methodology (European Sensory Technical Norm UNE-EN 13725) in a small slaughterhouse in San Juan de Pasto; a small municipality of southern Colombia. The research problem was: ¿What is the critical odor concentration (OUE) generated in the Frigovito S.A. slaughterhouse according to Colombian Resolution 1541 of 2013?, associated with the following hypothesis: "the measurement odour concentration exceeds the permissible level for the treatment and disposal system of hazardous waste and transfer stations: > 3 OUE/m³ according to the Colombian resolution 1541 of 2013 exceeds".

METHODS

Initially, the sampling site was in the slaughterhouse in Pasto, a township of Nariño, Colombia. The data collection techniques were applied in the slaughterhouse to determine the critical issue of offensive odour and thus determine the sampling point.

Then, it was decided to build a simulation system that allows making dilutions of an odour sample with odour-free air required to render it barely detectable by an odour observer, according to the provisions of Colombian Technical Standard NTC 5880; the common name of this device is olfactometer.

Odour concentration is typically expressed in terms of odour units per cubic meter of odour-free air (OUE/m³). This is the amount of odour necessary to contaminate 1 m³ of clean, odour-free air to the threshold level of the observer. The number of dilutions to threshold, otherwise known as the dilution factor, Z, is computed as: (Castro, 2011)

$$Z = \frac{(F1 + F2)}{F2}$$

Equation 1. Dilution factor. F1: flow of odour-free air (m³). F2. Flow of odorous air (m³). In this study, F1 was obtained of air compressor and F2 was odour sample of composting plant.

The odorous air was collected and contained in chemically inert sampling bags with 10 liters capacity. (Nalophanth) (Sironi, et al. 2014)

Panelists are selected strictly based on the observers' sensitivity towards a standard reference odorant, in other words, each potential panelist must be tested to N-butanol (Concentrations used: 80 g/m³, 20 g/m³ y 11 g/m³) on the olfactometer. The individual's average threshold measurement of N-butanol must be in the range of 20 - 80 ppb. The

antilog of the standard deviation must be less than 2.3 (Valor et al, 2003)

The odor dilutions are presented to the panelists, who are the people that have been selected according to your olfactory capacities and had been training for detecting the odor present in different dilutions of the sample, this methodology is known as “force-choice” (Denis,2012) and statistical approach of increasing levels of sample presentation is called “ascending concentration series”. The analysis of olfactometry was a period of 30 h between sampling and olfactometry, due to possible errors in the sample. (Sironi, et al. 2014)

So, the odor unit is calculated from the number of times that a gas sample must be diluted in order to be detected by a percentage of 50% of a group of the panel. Overall, all methods of this research were based on European standard UNE EN 13725.

FINDINGS AND ARGUMENT

The dynamic olfactometer was development with manual components, for instance, stainless steel rotameters and air valves. These components allow controlling pression and flow of odour-free air and odorous air in each dilution. (see Figure 1) and complete system to evaluating odour samples was shown in the Figure 2. The olfactometer was designed with large dilution range $2^7 - 2^9$.



Figure 1. Dynamic olfactometer.

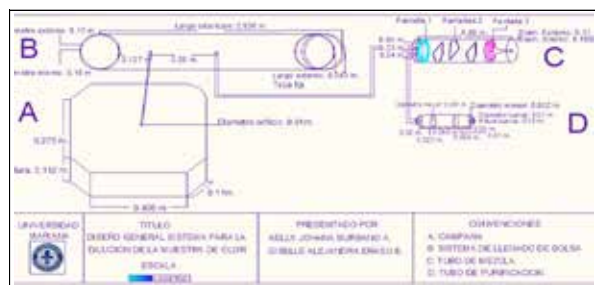


Figure 2. System to evaluate odor samples.
Section A: Hood to capture the odor in the point of measurement. Section B: Filling bag tube. Section C: Tube for mixing the sample odor with odour-free air. Section D: Filter to clean the air of dilution. (Burbano, Eraso,2015).

To define the point sampling firstly, visits were realized in the slaughterhouse to know the procedures carried out and the possible sources of emission of odour. Subsequently, the workers were surveyed considering the idea that these people are continuously exposed to different odors of slaughterhouse due to the fact they can determine if there was an odour more annoying than another, that is to say, workers gave information about the perception of the hedonic tone of the odors in slaughterhouse. In total, the number of surveys was 37, which are formed by twelve questions.

According to statistical analysis, 94% of the workers surveyed consider that some of the activities of the plant generate offensive odors and that these are possibly causing negative effects on your health; leading to conclude that workers of the plant identified as an offensive odor that they generate an olfactory discomfort or as damage to their health or the environment of their workplace. (MINAMBIENTE, 2013). Pearson statistical tests were made to establish if the workers do not get used to smelling slaughterhouse's odours according to the number of years they work in the company. The decision of the test was to accept the null hypothesis: there is independence between the intensity of the odor and the working time of the workers. In other words, workers didn't get used to these odours, even though they are in direct contact with this type odour emissions. In addition, workers still perceive unpleasant odors with the same intensity.

Finally, 40% of the operators identified that the area where the most unpleasant odor generated in composting plant, also the perception of odour presented every day and it was more intense from 6:00 a.m. to 12:00 p.m. The composting has different stack due to the fact it was very difficult to cover the entire emission area during sampling. As a result, the hood was changed its position in all stacks while the bag was filled. The number of samples was tree.(See Figure 3).



Figure 3. Description of the sampling site in the composting plant (Ubicated. East: 975850.South: 621821. Altitude: 2770 m.a.s.l).March 27, 2015.

The group of panelists was formed by four people, who evaluated the odour sample. The result of composting plant odor emission was 279, 15 OUE/m³. This value couldn't be compared with Colombian legislation, because these laws consider immission values and this researcher got the odor emission value. Emission value corresponds to the odour pollution of the source or slaughterhouse generates, not the odor concentration that is dispersed; as a result the hypothesis of present research is null.

The value obtained was less than other literature values of composting plants, for instance, a composting system of a wastewater treatment plant with an odor concentration of 27554 OUE/ m³. (LABQUA, 2011). This value is high compared to the value obtained in this investigation, the difference between the previous values can be associated to the type of raw material used in each composting activity (slaughter and wastewater treatment plant), as well as the by-products of the raw material associated with anaerobic biological decomposition (Moreno, J. 2007) and finally to the treatment carried out in each composting. (Jacobs, 2007).

CONCLUSIONS

The concentration of odor generated by the composting of the Frigovito S.A slaughterhouse corresponding to 279,140 OUE / m³. This value does not allow determining compliance or non-compliance with Colombian Resolution 1541 of 2013; because this normativity is framed in evaluating characteristics of immission and dispersion of odour. For this reason, the hypothesis of the investigation was annulled. It is important considered that this odor concentration value has high uncertainty associated with the tools used in taking the odor sample and its analysis.

The determination of the critical measurement point included the participation of the workers who evaluated the hedonic tone of the odor emissions generated in the plant; this characteristic allowed to include in the research the topic of offensive odors.

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PROTOCOL FOR EVALUATION OF SORPTION PROPERTIES OF BUILDING MATERIALS FOR VOCs IN INDOOR ENVIRONMENT

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Abstract: Increasing energy costs and indoor air pollutant concentrations has become a concern for the decision makers over the past few years. Currently, efforts are made to use innovative materials with specific properties to reduce the energy costs along with low emission of indoor air pollutants. Among the indoor air pollutants, Volatile Organic Carbons (VOC's) are found to be showing significant adverse effect on the health of the residents. The experimental setup has been setup for estimating the interaction/behavior of materials with Indoor VOCs especially. However, these experiments have many limitations, time consuming and expensive. This paper focuses on evaluating the ability of VOC's to adsorb/desorb pollutants in a given indoor environment using a combined approach of experiments and mathematical modelling using linear Langmuir model. As a part of this study, the adsorption and desorption coefficients for Toluene, limonene and dodecane for Medium Density Fibre (MDF) board have been estimated. It has been observed that MDF behaves similarly with limonene and toluene showing immediate re-emission. However, MDF adsorbs Dodecane rapidly and re-emits it slowly during desorption phase. Based on these observations made in the experimental chamber along with the mathematical modeling results, a protocol for evaluating the sorption properties has been developed to estimate sorption properties of the material. This protocol has been formulated considering the experiments conducted in two Liter chambers and 30m³ chambers (room size chamber).

Keywords: Indoor VOC, Building Materials, Sorption Properties, Experimental Monitoring, Emission Modelling

1.0 Introduction

The Indoor air quality in buildings is dependent on both the nature of air movement within the building systems and the nature and location of contaminant sources. Emission of pollutants like volatile organic compounds (VOC's) have direct influence on people's well-being and health. High exposure of VOCs concentration may cause conjunctival irritation, nose and throat discomfort headache, allergic skin reaction, dyspnea declines in serum cholinesterase levels, nausea, emesis, epistaxis, fatigue and dizziness (USEPA, 2017). Higher concentration of indoor air pollutants may cause various health problems that may result into 'sick building syndrome'. The Indoor air pollutants can originate from outdoor sources (e.g., traffic and other forms of combustion (CO, NO_x, SO₂) or from indoor sources, such as occupants and their activities, tobacco smoke, electronic equipment, cleaning products or heating, ventilating, air-conditioning (HVAC) systems and building and furnishing materials. The sources of VOCs in indoor may be paints, wood preservatives, aerosol sprays, cleansers and disinfectants, moth repellents and air fresheners, stored fuels and automotive products and building materials (USEPA, 2017). The VOCs emission of from building materials, especially those which develops from the viewpoint of energy conservation is one of the major sources of indoor air pollution which needs to be accessed accurately (Yang et al., 2001, Xu and Zhang, 2003). However, the properties of building materials can also influence the transport and the removal of indoor VOCs by sorption and desorption. The re-emission (desorption) of sorbed VOCs may increase the VOC concentrations in the indoor environment for months or years after a source event (Tichenor et al., 1991, Zhang et al., 2002). The adsorption and desorption properties of a material may influence by the chemical properties of VOCs in the form of strength of interaction (van der Waals) between material and pollutant (interaction between two polar molecules, between polar and nonpolar molecules, and induced-dipole/induced-dipole interactions between non-polar molecules). The material surface roughness can strongly affect the sorption capacity of the material. The greater the specific area, the larger the equilibrium coefficient which results higher adsorption capacity of materials. Additionally, temperature, relative humidity and air velocity can also influence the sorption properties of the material. The current strategies to reduce formaldehyde emissions from building materials are derived from reducing the use of formaldehyde at the product manufacturing stage (i.e. through the use of novel formaldehyde free resins for the panels industry). Additionally, the suppression of VOCs may be achieved by ventilation, the specification of low emission materials or the use of materials with high air purification properties, all of which improve IAQ. The present article provide an integrated approach based on monitoring and modelling to evaluate the adsorption and desorption properties of building materials for VOCs.

2.0 Methods

The methods of studying characteristics of VOC sources and sinks mainly fall into two categories: experimental investigation and emission modeling (Zhu et al., 2001, Zhao et al., 2002; Gulia et al., 2016; Chinthala et al., 2016). In principle, the experimental measurements provide the most realistic results than the modeling results. However, it require expensive and well-controlled instrumentation along with space and time. The experiments are setup using a small-scale or a full scale stainless steel or glass chamber to measure the sorption properties of a test material. The tests are usually conducted under a set of specific environmental conditions (e.g., 25°C, 50% RH, and 1 ACH). The experiments are generally completed in two

phases, the dynamic adsorption phase and the dynamic desorption phase. Figure 1 shows a general experimental setup of a small scale chamber.

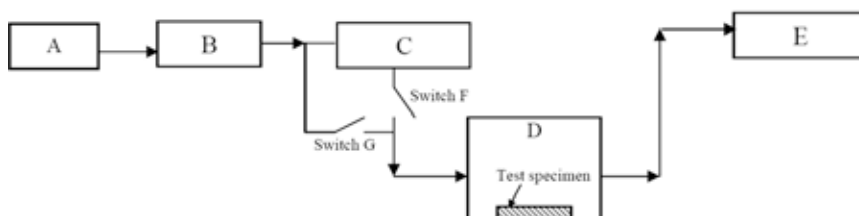


Figure 1: Experimental setup of a small scale chamber (Zhang et al., 2002)

where

A: Clean air supply system; B: Airflow, temperature and humidity controller; C: Temperature controlled VOC generator (e.g. VOC permeation tubes); D: Test chamber assembly; E: Air sampling system at the chamber exhaust.

In adsorption phase, the compounds generated from the pollutant generator (C) are carried by the conditioned, clean air from the conditioner (B) to the chamber containing the test specimen. The pollutants concentration in the chamber is measured by analyzing air samples taken from the chamber exhaust (E). After the system reaches an apparent equilibrium (the concentrations at the chamber exhaust does not increase any more), the dynamic desorption phase starts whereby the pollutant supply is stopped and the chamber is continuously flushed out by the clean air. Owing to the limitation of the experimental approach, many researchers have addressed the importance of simulating VOC emissions from building materials and furnishings using mathematical models. In literature, the sorption model are generally two types, i.e., first order adsorption/desorption rate models and equilibrium-interface models (Zhang et al., 2002). The linear Langmuir model is probably the most widely used sorption model. It is based on physisorption process and considers only the relatively fast surface sorption process. It does not consider the slow diffusion of pollutant inside the material. The linear Langmuir model is described by following equation - (i) (Tichenor et al., 1991).

$$\frac{dM}{dt} = k_a C - k_d M \text{ ----- (1)}$$

where,

dM/dt = net mass rate of change of VOCs adsorbed on the material surface ($\mu\text{g m}^{-2} \text{h}^{-1}$); C = concentration in chamber ($\mu\text{g}/\text{m}^3$); k_a = adsorption rate coefficient (m h^{-1}); k_d = desorption rate coefficient (h^{-1}); M = mass of pollutant per unit area on material surface ($\mu\text{g m}^{-2}$).

It is difficult to measure the value of k_a and k_d by experimentally. However, researchers used statistical tools to estimate the value of these coefficients based on monitoring data of concentration and emission rate.

3.0 Findings and Arguments

This method has been used to evaluate the adsorption and desorption properties of medium density board (MDF) for VOCs like Toluene, Limonene and Dodecane. The VOCs concentration has been monitored by using experimental setup for 2 litre micro test chamber as described in Figure 1 in Building Research Establishment (BRE), UK laboratory as part of ongoing ECO-SEE project (www.eco-see.eu). The k_a and k_d coefficients values have been estimated using the least square curve fitting method. For this, a curve-fitting software SCIENTIST (Micromath Software, 2015) has been used to estimate k_a and k_d values by fitting the Langmuir equation with experimental VOC values in the adsorption and desorption phase (Figure 2). Table 1 describes the experimental data used for curve fitting to estimate k_a and k_d values. The dosing concentration of Toluene, Limonene and Dodecane were 2169, 2397 and 2754 $\mu\text{g}/\text{m}^3$ respectively. The surface area of the MDF, test specimens were 0.016 m^2 .

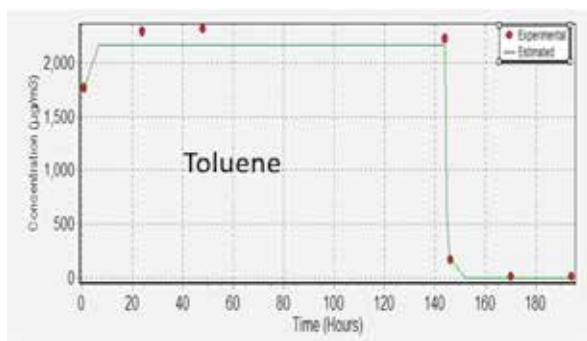


Figure 2: Curve fitting plots of toluene for MDF- an example
Table 1. Experimental data and estimated k_a and k_d values

S. N.	Parameters	Control MDF

		Toluene	Limonene	Dodecane
1	Chamber Volume, V_0 (m^3)	0.002	0.002	0.002
2	ACH, N_0 (1/h)	6	6	6
3	Sink Area, A_0 (m^2)	0.016	0.016	0.016
4	Dosing concentration, C_0 ($\mu g/m^3$)	2169	2397	2754
5	T_{stop} (Hours)	144	144	144
6	Estimated (k_a), m/h	0.398	0.2	0.297
7	Estimated (k_d) 1/h	1.297	0.382	0.2

The k_a and k_d values of 0.398 m/h and 1.297 1/h, respectively of MDF for Toluene indicate that MDF re-emits toluene suddenly in the chamber. It behaves similarly with limonene, having k_a and k_d values of 0.200 m/h and 0.382 1/h respectively. However, values of k_a (0.297 m/h) are higher when compared to k_d values (0.20 1/h) for Dodecane, which indicates that MDF adsorbs Dodecane rapidly and re-emits it slowly during desorption phase. It indicates that MDF behaves as a sink for Dodecane (Gulia et al., 2016). The results obtained above have been validated using a 30m³ chamber constructed in Building Research Establishment, London. The flow rate in the chamber has been controlled through various control mechanisms. The material has been placed on a wall perpendicular to the wall where inlet and outlets are located. The inlet and outlet of the chamber have been located in the opposite walls. The flow patterns and the concentration of the pollutants in the 30m³ have been simulated using the software FLUENT in order to check the performance of the material in the full scale model (Chinthala et al., 2016). Building construction materials play an important role in defining the indoor air pollution levels. The materials with high adsorption capacity may capture VOCs and thus reduce the ambient indoor concentration levels; however, materials possessing high desorption capacity may re-emit the VOCs suddenly and thus increase indoor concentrations. This approach can be used to evaluate the adsorption and desorption properties of bio based materials in Indian conditions which help to define the material as Source or Sink for VOCs. The protocol shall be developed by incorporating the results of 2L chambers, 30m³ chamber and real size test house data as shown in the figure 3.

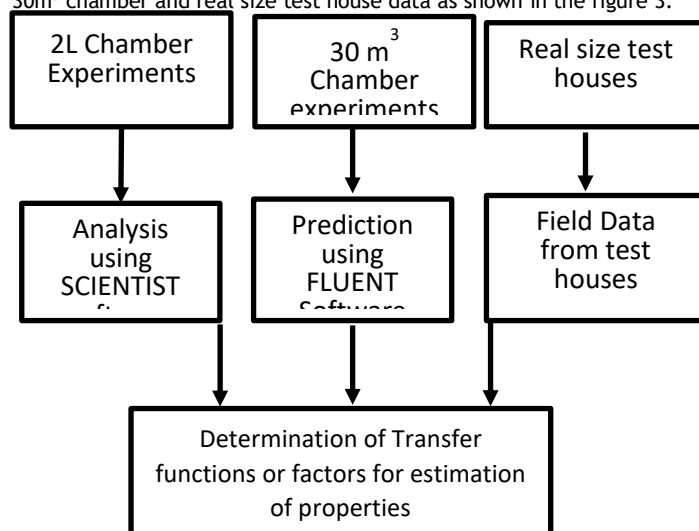


Figure 3: Protocol for evaluating the sorption properties of building materials for VOCs in Indoor Environment

4.0 Conclusions and Recommendations

The present study focused on the development of a protocol for estimating the sorption properties of material w.r.t. different VOCs using integrating approach of monitoring and modelling. The following conclusions can be drawn from this paper.

1. Due to the limitations and complexities involved in experimental approach, mathematical modelling for estimating the properties of the materials using linear Langmuir model gives satisfactory results.
2. MDF can be used as a sink for Dodecane as it adsorbs rapidly and desorbs slowly.
3. The adsorption and desorption properties of many bio-based materials are still not known properly. Hence the protocol can be implemented effectively to investigate the same.
4. The development of transfer functions for estimation of properties of materials should be carried out by using the combined data of experiments conducted on chambers of different sizes.

ACKNOWLEDGEMENTS

The results presented in this paper are part of the ECO-SEE project which has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no 609234 (www.eco-see.com).

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ARIA VIEW™ - CONTINUOUS MONITORING SYSTEM OF ODOR DISPERSION IN CELLULOSE PLANTS

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Abstract: The assessment of air quality conditions is necessary in the planning of industrial activities, where there is the possibility of occurrence of environmental impact. A widely disseminated strategy for assessing air quality conditions is based on the pollutant dispersion modeling, in which a variety of factors, such as representative meteorological patterns of the region of study, representation of the surface assessed and characteristics of atmospheric pollutant emissions from the activities implemented or to be implemented, are taken into account.

Given this need, ARIA has developed an operating system, called ARIA View™, which provides to the industry the continuous monitoring of the atmospheric pollutants dispersion in the region influenced by the industrial plant.

ARIA View™ system is configured to import data generated by emission measurement sensors from the chimneys and weather station installed in the plant. This data is collected at regular intervals from the data management system, which integrates and makes it available in average values for the system. The integration of the online data provided by data management systems allows the ARIA View to consolidate itself as a tool to support the management of the real-time impact of industrial activities on the atmospheric environment.

The system integrates the Micro SWIFT SPRAY (MSS) model developed by ARIA Technologies. Micro SWIFT SPRAY is a microscale Lagrangian dispersion model that reproduces scenarios in high spatial resolution with a lower computational time demand. The system allows the calculation of the dispersion of conventional atmospheric pollutants (SO₂, NO_x, PM, CO₂, Dioxin and etc.) and other parameters, such as odor.

In Brazil, the pulp and paper market is one of the main industrial sector interested by such type of technology. ARIA View™ allows a better understanding of the dispersion conditions and the increase of concentrations in the area of influenced in real time, contributing to a fast and efficient response to the possible complaints of the neighboring population.

Keywords: Modeling, Odor, Dispersion, Lagrangian Model.

INTRODUCTION

The installation and maintenance of sources emitting pollutants requires careful studies of air quality impact, combining monitoring and computational modelling techniques (U. S. EPA, 2005). In order to obtain the knowledge of the impact of the atmospheric emissions of a given activity, it should be considered the transport of these into the atmosphere to know the location of the regions most affected by the pollution plumes, the level of the concentration of pollutants present in the impacted regions, and the group of sources with the highest contributions in the final concentration.

The AriaView is an on-line system devoted to industrial chronic impact due to pollutant emissions. It is built to integrate emission and meteorological information. The aim is to allow environmental managers to monitor, in real time, the evolution of air quality in the industrial plant surroundings and the continuous monitoring of the dispersion of atmospheric pollutants emitted by the plant activities.

The AriaView system uses the coupled Micro-SWIFT and Micro-SPRAY calculation modules. These modules were applied and evaluated (Sontowski et

al, 2006) for continuous emissions installations (Moussafir et al, 2007).

METHODS

The system operation is based on routine modeling cycles every 30 minutes and on two input data available from the site: meteorological and emission. Every 30 minutes, the system collect these information, from the data management system, which integrate them and make it available in average values.

The figure 1 represents the operating scheme of the ARIA View System.



Figure 1: Representative scheme of the ARIA View system

• Meteorology input and treatment

First, the meteorological data from a weather station located on the facility is used to create 3D meteorological fields, including wind, temperature and turbulence every thirty minutes. This step is performed by the Micro-SWIFT model. In order to increase precision, Micro-SWIFT could run on three nested domains, i. e. with a resolution of 25 meters for the innermost domain which includes the facility, 100 meters for the industrial zone surrounding the facility and 200 meters for the larger domain, for example. These resolutions may be easily tuned to be applied to any industrial zone.

• Emission definition

In parallel, concentration values over the sensors network installed on the chimneys are downloaded from the PI system, through a WebService, of the facility. Also, in case of non-operation of the sensors, an offline inventory is configured with the physical and chemical parameters of the emitting sources to be considered.

• Dispersion of pollutant

Using the source emissions and the meteorological 3D fields, the dispersion Lagrangian model Micro-SPRAY calculates the average of the dispersion of the plume for the time-step (30 minutes). The model uses the same three nested domains to calculate pollutant concentration distribution. The complete calculation cycle (data acquisition, meteorological 3D fields and dispersion) is achieved in five or ten minutes depending on hardware availability.

• Meteorological and Dispersion Models Description

Micro-SWIFT is a 3D wind field model for complex terrain. It produces a mass-consistent wind field using data from a sparse meteorological network. Temperature and humidity fields can also be interpolated with Micro-SWIFT. This module generates also the turbulent components which are used by the dispersion module.

Apart from the static data (topography, land use, buildings, reconstruction of a wind field with Micro-SWIFT requires data from at least one measuring site and one vertical structure. In the case that no meteorological vertical structure exists, profiles of wind and temperature are extrapolated from the surface stations according to the stability of the atmosphere. This stability is derived from the available physical meanings (temperature profile, solar radiation, cloud cover, ...). Several interpolation procedures can be used, depending on the amount of available data. Variations in the stability coefficient can be considered by entering one or more temperature profiles.

The results of the meteorological model are stored in binary files accessible to the dispersion module and postprocessors.

Micro-SPRAY is a three-dimensional Lagrangian particle dispersion model developed by Arianet S.r.l. in collaboration with Aria Technologies SA. This code reproduces the transport, dispersion, dry and wet deposition and radioactive decay of airborne chemically inert species released in meteorological complex conditions (low wind speed, flow over complex topography), often marked by spatial and temporal inhomogeneities of the meteo-diffusive variables (e.g., vertical wind-shear, breeze due to the presence of terrain discontinuities). In addition, it is also possible to reproduce the dispersion of particulate emissions, considering the gravitational vertical settling phenomenon. Micro-SPRAY can integrate emissions from point, area or line sources, continuous and discontinuous, as well as to exploit the available wind and turbulence measurements provided by advanced meteorological instruments. In addition, Micro-SPRAY may calculate 3D dispersion in domain including obstacles (as buildings).

• Results Display

The AriaView System includes two types of display for the results:

- 1) A desktop interface (Figure 2) where the user may examine the plume for the different time steps of the simulation, animate, adapt the color scale and levels, and more. As the results are stored, it allows the user to come back to previous time step.

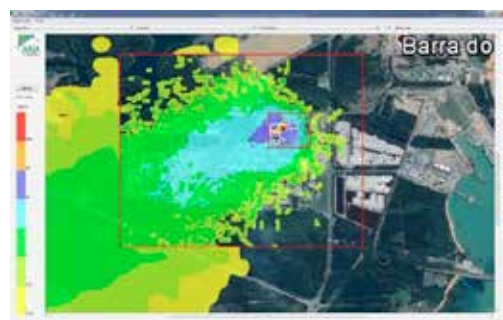


Figure 2: Example of desktop display

- 2) A Web interface, which may be available in the LAN of the facility to inform everyone involved in the management of the situation.

FINDINGS AND ARGUMENT

The ARIA View real-time system is actually installed and operational on 6 pulp and paper plants in Brazil and 1 in Uruguay. It was developed aiming the

applicability to any industrial site. The modularity of the software allows to adapt it to various data acquisition systems. The parallelization for the calculation enables a better than real-time characterization of the situation (Oldrini et al, 2011).

This tool allows the manager to regularly visualize the results of the dispersion of atmospheric pollutants from the industrial plant (map of concentrations - Figure 3, deposition and succinct reports - Figure 4); Obtain the calculated values at the receptor points, provide concentration and deposition maps for the periods (daily, monthly and annual); Store maps and meteorological data for a full year period (machine configuration must be in accordance with storage requirements); Display chronological series of wind speed and direction for the previous day, the roses of the monthly winds; and Quickly access useful data for the monitoring program.

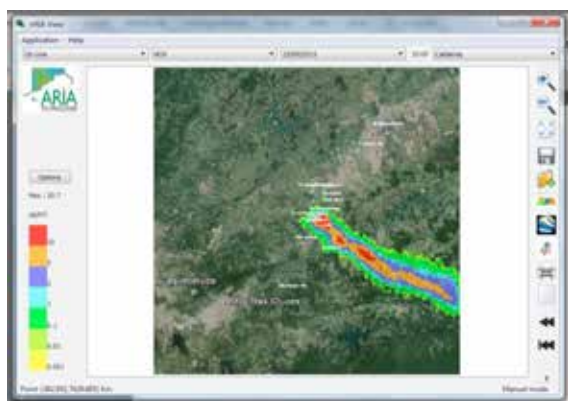


Figure 3: Example of desktop display



Figure 4: Report available on ARIA View™ system

The managers use the results presented to respond to the situations of complains of odors, for example, in case of accentuated values of concentration for TRS. In this way, they can respond if the complaint is applicable or not.

CONCLUSIONS

This system, developed by ARIA Technologies, is a solution for the monitoring and management of continuous atmospheric dispersion modeling for Total Reduced Sulfur (TRS), NO_x, SO_x, CO and PM₁₀

pollutants in industrial facilities. Although such type of solution is not usually required for operation license, it represents a proactive tool for the companies interested in environmental footprint reduction.

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Application of atmospheric dispersion modeling to evaluate the ammonia emissions of a refrigeration system

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Abstract: The disorderly urban occupation results in conflicts of residential use with other forms of use, such as industrial, commercial and provision of services. The environmental impacts of these activities are generally accentuated when the urban occupation next to the enterprise is predominantly residential. Thus, the objective of this work is to evaluate if atmospheric emissions of ammonia from the refrigeration system of a slaughter fridge installed in the city of Belo Horizonte, with a residential neighborhood, have the potential to cause atmospheric pollution.

For this, the Lagrangian dispersion model of atmospheric pollutants Micro Swift Spray - MSS was used, from which plumes were generated. The meteorological data were obtained from the nearest meteorological station belonging to the National Meteorological Institute (INMET).

Topography data were obtained from level curves of the city of Belo Horizonte, as well as land use data from the study region. In order to consider the interaction of ammonia with water droplets, which may significantly hinder the dispersion of the gas, the water vapor plume was simulated in the same period. The two plumes were overlapped. The rate of ammonia emission was estimated from values recorded in portable measurers in the enterprise and the water vapor was estimated by means of an isokinetic sampling report from the boiler chimney. The quantity of ammonia replacement in the system was considered equivalent to the amount released into the atmosphere as fugitive emissions, considering that the system is closed. For the evaluation of the environmental impact in the neighborhood, the 5 ppm ammonia concentration was used as the reference value, which is the minimum for the perception of its odor.

The plume's analysis and the concentration values generated by the model showed that the enterprise interferes in the air quality in the surroundings. Although, more research is necessary to prove that ammonia emission can cause atmospheric pollution in the region.

Keywords: plume dispersion, ammonia, Micro Swift Spray (MSS), atmospheric pollution.

INTRODUCTION

The disorderly growth of metropolitan cities in developing countries leads to problems of land occupation, mainly conflicts of use. Areas located in regions that are most suitable for industrial use, such as industrial districts, roadside borders, among others, may have buildings and residential homes.

Thereby, the discomfort related to atmospheric emissions, more specifically odors, is potentialized. Even if the facility meets emission standards and doesn't significantly interfere with the air quality in the region, there may be discomfort related to odoriferous substances in the neighborhood.

Caputo, Gimenez and Schlamp (2003), apud Barbon and Gomes (2010), emphasize the special importance attributed to the possible risks to which the population is subjected during the atmospheric dispersion of pollutants generated by several industrial sources and that models are being developed for the assessment of emissions impacts, constituting useful tools to advise studies of risk minimization and management of available resources in case of accidents.

Schlink et al. (2006), apud Barbon and Gomes (2010), highlight that a fundamental aspect to be considered in atmospheric research involving the dispersion of pollutants is the preservation of human health, that is, the development of knowledge for the application in benefit of the health and well-being of the human.

According to Barbon and Gomes (2010), it can be stated that the use of a dispersion simulation tool in atmospheric environment is very useful because it allows forecasting the concentrations of a given pollutant and can offer the population an opportunity to avoid exposure to high concentrations; can allow the companies a prediction of investment in equipments that can reduce atmospheric emissions; and public agencies, the possibility of questioning new enterprises whose atmospheric emissions contribute to the degradation of air quality conditions.

In the city of Belo Horizonte there are in operation industries with different typologies. Some of these, such as the manufacture of frozen pasta, beverages and slaughterhouses/refrigerators, require refrigeration systems, which in turn use refrigerant fluids.

Among them, ammonia is widely used because of its high latent heat of vaporization and low cost. This substance has excellent heat transfer, which makes it possible to operate with higher evaporation temperatures or lower condensing temperatures.

Due to its characteristic odor, it is easy to notice the occurrence of leaks. It also has high toxicity, a property that must be taken into account in relation to impacts in the surroundings.

Its main consequences for the health of the worker were summarized in Technical Note n 03/DSST/SIT (Brasil, 2004): The gas is a powerful irritant of the respiratory tract, eyes and skin. Depending on the time and level of exposure, effects may range from mild irritation to severe bodily injury.

It is easily detected from low concentrations (5 ppm) in the air by its *sui generis* smell. Contact with eyes at low concentrations (10 ppm) results in eye irritation and tearing.

According to CETESB (Environmental Company from State of São Paulo), ammonia is an irritating gas to the eyes and, if inhaled, it can be toxic.

Ammonia leaks can be perceived over long distances and in low concentrations. Moreover, due to the formation of hydrogen bonds, ammonia has a great interaction capacity with droplets of water vapor, which favors its permanence in the places of supposed annoyances due to its lower mobility in the atmosphere as a particulate matter.

Atmospheric pollutant dispersion models use computational mathematical calculations to simulate atmospheric behavior in a defined geographic domain and then calculate the concentration of the pollutants after they interact with the atmosphere.

In this context, the present work aims to model the fugitive emissions of ammonia from a refrigeration system of an industry, as a case study, in the city of Belo Horizonte and analyze its interference in environmental quality.

METHODS

For modeling, the MSS (Micro Swift Spray) model system, developed by ARIA Technologies, was used. The system uses the Micro Swift model, which generates the local scale wind field and the Micro Spray, a Lagrangian dispersion model. The MSS is suitable for calculating the wind field and pollutants at complex terrain sites, although do not consider interactions between the simulated species.

The simulations were done on the interfaces produced by the company ARIA Technologies. These include topography preprocessors, land use, wind field and pollutant dispersion (MSS).

For the relief was created a digital elevation model (MDE) from a file containing shape file of level contours of the city. The topography preprocessor of the interface generated a topography file with resolution of 30 meters. From this file, was defined the domain for modeling, an area of 2,25km² (1,5x1,5km).

The land use data was obtained from a satellite image *Landsat 8* with 30 meters of spatial resolution and a classification file containing geophysical parameters such as albedo, soil roughness, Bowen ratio, among others.

The meteorological data is from the INMET (National Institute of Meteorology) and belong to the nearest meteorological station of the defined domain. The parameters entered were time data of temperature, precipitation, direction and wind speed, humidity, radiation and atmospheric pressure. Of these, the software estimated other

parameters necessary for simulation, such as cloudiness. Figure 1 shows the wind rose for the simulated period.

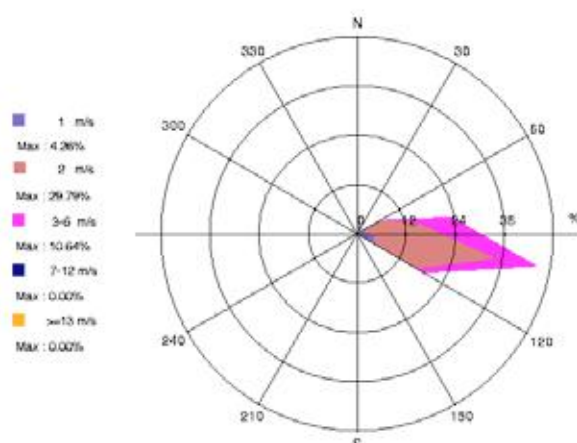


Figure 1. Wind Rose (09/05/2019-10/05/2019)
(Reference: Personal collection)

The parameters used to differentiate the species emitted were the density, dry deposition velocity (m/s), wet deposition coefficient (1/s), was applicable only on for NH_3 , and particle diameter (μm), was applicable only for the steam (particle).

In the enterprise under study, in addition to the refrigeration system whose refrigerant used is ammonia, there is a wood burning boiler. The burning of this fuel generates water vapor, which, because it is a particulate matter and interacts with the ammonia, can hinder its dispersion.

In order to verify if the gas interacts with the water, emissions of water vapor from the company's boiler were also modeled. The source of energy of the boiler is the combustion of the wood, from which it can be generated up to 6% of water vapor, according to the isokinetic sampling reports from the boiler's chimney (Pelanda, 2016).

As water vapor and ammonia plumes were generated over the same period, they were compared in order to evaluate the interaction of ammonia with the water droplets resulting from the vapor and to verify the possibility of nuisance in the vicinity.

Since the droplet of water vapor isn't a common substance for modeling, its parameters have been estimated and calculated. According to Barbosa (2014), the diameter of water vapor droplets can range from 5 to 30 microns. For the present study, the value of 15 micrometers (μm) was used. According to ALVES (2011), one of the most used models for calculating the rate of deposition of larger particles is from Noll and Fang (1989), which

is applied to particles of approximately 4 to 100 μm . The model defines that the deposition velocity is the sum of the gravitational sedimentation and the velocity of inertial deposition. The calculated value was 0.57m/s. The washout coefficient was canceled, as it was considered that there would be no increase of steam deposition under precipitation conditions, as occurs with the other particles.

In the case under study, the refrigeration system is confined in an engine room where the leaked NH_3 escapes through an opening. Thus, the engine room opening was defined as a point source, not area, with horizontal flow, to better reflect the actual conditions. For the emission rate, measured values with the use of calibrated portable meter (SP2nd- NH_3 SENKO model) of ammonia were used, in the opening of the engine room at a time of normal operating conditions, and at another moment in which significant leak occurred. The values measured by the equipment were obtained in PPM (parts per million), converted to concentration (mg/Nm^3) and, from a flow value defined in the calculation files of the design of the site exhaust system provided by the company, the emission rates were defined. The exit velocity of the NH_3 emission was calculated from the already defined flow rate and the exit area (opening of the engine room). The temperature value of the emission used was the hourly average of the two simulated days.

As for the steam, the emission values were obtained from an isokinetic sampling report made in the chimney of the slaughterhouse's boiler. The parameters and values used to define the emission sources of this work are found in Table 1.

Table 1. Parameters of emissions values

		NH_3	Steam (H_2O)
Rate (kg/h)	Normal conditions	4,825	654,23
	Leak	383,0	
Velocity (m/s)		0,40	12,85
Temperature ($^{\circ}\text{C}$)		18,5	167,8

Reference: Personal collection

The simulated period was 48 hours. Fugitive emissions were considered in the normal operation of the refrigeration system and during accidental leakage, with modulation of the concentrations, simulating the actual situation occurred, in which there were episodes of odor perception in the neighborhood, which is predominantly residential.

The statistical calculation used was the worst situation (highest concentration) for the simulated hours. Based on the immediate neighborhood, 3 receptor points were defined for the analysis of maximum results. Afterwards, to make possible a spatial analysis, the plumes were overlapped. However, it should be emphasized that the

modeling used does not predict the interaction of ammonia with water vapor droplets.

FINDINGS AND ARGUMENT

The model generated concentration maps of the evaluated substances. Figure 2 shows the result of ammonia dispersion in the defined domain. The displacement of the plume occurred mainly in the east-west direction, predominant direction of the wind, as can be seen in Figure 1. From a visual analysis of the plume, it is possible to notice that the highest concentrations vary between 60-80 $\mu\text{g}/\text{m}^3$, which indicates that is inside the area of the enterprise. In the immediate neighborhood concentrations of up to 40 $\mu\text{g}/\text{m}^3$ were reached, while in the more distant areas were registered up to 20 $\mu\text{g}/\text{m}^3$.

All concentration results found are below the ammonia odor thresholds established by technical studies (Brasil, 2004). However, the odors from this refrigeration system when there is a leak have been perceived by the neighborhood. In this scenario, stands out the previously mentioned hypothesis that the ammonia gas has its dispersion difficulty due to its interaction with the water droplets resulting from the steam from the chimney.

Figure 3 shows the result of the plume of water vapor from the boiler, where it is possible to verify the similarity of behavior when compared to the ammonia dispersion plume, in relation to the direction of east-west displacement.

In Figure 4, it can be seen that the plume of NH_3 gas was contained in the water vapor plume dispersion area, reinforcing the hypothesis that the ammonia would have its dispersion hampered by being adhered to the water droplets, causing the perception of odors in the neighborhoods.

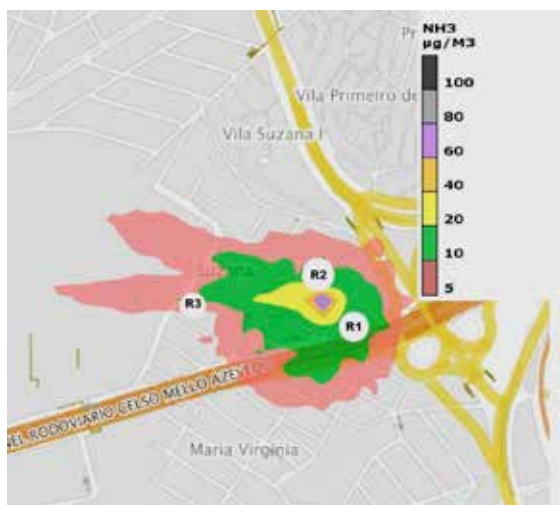


Figure 2. Ammonia plume
(Reference: Personal collection)

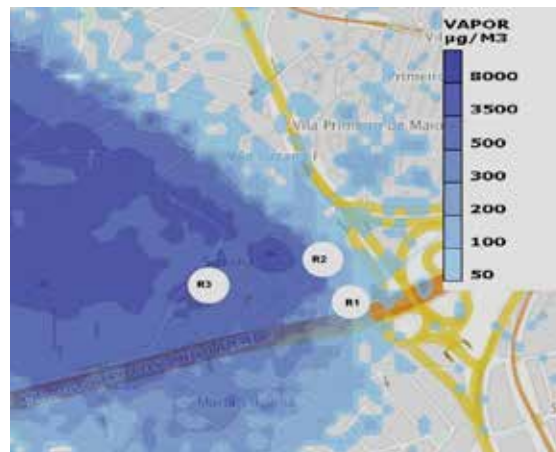


Figure 3. Water steam plume
(Reference: Personal collection)

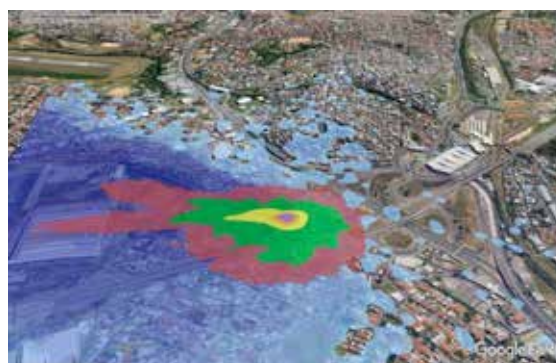


Figure 4. Ammonia and water steam overlapped plumes
(Reference: Personal collection)

CONCLUSIONS

The analysis of the plume and the concentration values generated in the atmospheric emissions modeling in the meteorological conditions of the simulated days showed that the project interferes with the ambient air quality. However, the reference value of 5 ppm (about 3,500 $\mu\text{g}/\text{m}^3$ of NH_3 at 25 °C) for odor perception was not achieved.

The water vapor generated in the boiler can interfere with the dispersion of ammonia in a leakage incident because the NH_3 molecule, impregnated with water vapor, has less mobility due to its behavior as a particulate, a situation that could not be evaluated using modeling as a tool. This interaction may be an explanation for the increase of its concentration to the levels that were perceived in the vicinity, when the ammonia leak occurred and its discomfort due to the odor.

More studies are needed to prove that the emission of ammonia can cause atmospheric pollution in the region. Future studies can be carried out using dispersion models that consider the interaction of ammonia with water vapor droplets. In addition, the calculations for the estimation of the emission rates for a more real simulation of the leakage can be improved, using information about the consumption of ammonia by the company in a certain period

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ANALYSIS OF THE AERODYNAMIC PERFORMANCE OF A PORTABLE WIND TUNNEL FOR ODOUR MEASUREMENTS

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Abstract: Special sampling methods, like the wind tunnel, are adopted to perform the estimation of the emission rate of odorous compounds in quiescent area sources. The wind tunnel was designed to reproduce a fully developed boundary layer and thus provide better results than the other device largely used for this purpose, the dynamic flux chamber. However, further investigation is still necessary to study its aerodynamic performance. In the present work, Computational Fluid Dynamics (CFD) was used to investigate the flow inside of a portable wind tunnel and the following cases were tested: (i) changes in the geometry of the wind tunnel in order to evaluate the flow pattern inside this device for a smooth surface and (ii) use of different rough surfaces to represent the real conditions for the original design of the wind tunnel. The main parameters investigated were the velocity profiles and streamlines of the flow in the main section and the friction velocity distribution on the solid/liquid interface. The friction velocity is the key variable to represent the shear caused by the atmospheric flow and should reproduce the real atmospheric conditions inside a measuring device. Two geometry modifications were tested and they improved the velocity distribution, suggesting that modifications in the geometry can lead to considerable improvements on its aerodynamics. For the original wind tunnel design, four surfaces were evaluated with roughness heights varying from 0.0003 m to 0.3 m. The numerical results showed values of friction velocity (averaged over the liquid/solid interface) close to the reality (from 0.11 to 0.27 m/s), and, according to this parameter, this wind tunnel can be considered suitable to be used over different surfaces.

Keywords: Wind tunnel, Odour emission rate, CFD, Friction velocity, Roughness.

INTRODUCTION

The emission of gases coming from quiescent liquid area sources, i.e, large liquid surfaces with a low degree of disturbance are major sources of odorant compounds (Latos et al., 2011). Such compounds may cause a great number of deleterious effects to the human being including discomfort, malaise, stress, headaches, sleep and appetite disorder (Durmusoglu et al., 2005).

The estimation of odorant gases emission rate can be performed by different approaches. The most used techniques are: (i) indirect methods that combine micrometeorological measurements and dispersion modelling and (ii) direct methods that use a device that enclosure a portion of the source. Although the higher reliability associated with the indirect methods (there is no perturbation to the emission process), the high cost and elevated time involved with the great number of samples needed makes this technique unfeasible to odorant gases emission assessments.

In contrast, several sampling devices are being used and studied, among them, the two most commonly used are the US-EPA Dynamic Flux Chamber (DFC)

and the UNSW Portable Wind Tunnel (PWT) (Hudson and Ayoko, 2008a).

Several authors have studied the aerodynamics inside monitoring equipment, among them Saha et al. (2011) worked with the effect of the geometrical aspects of the portable wind tunnel, Andreão et al. (2017) evaluated the influence of micro fans on the flow inside a DFC and concluded that it does improve the mixing and Capelli et al. (2009) proposed a new design for a portable wind tunnel based on uniform velocity profiles and good agreement with boundary-layer theory.

The principle of the direct techniques consists in determining the concentration of the emitted compound on a sampling surface where the aerodynamics of the air flow inside the device and the flow rates are controlled. The emission rate is obtained as a product of this concentration and the flow rate (Jiang et al. 1995). Despite the uncomplicated principle for odorant gases emission assessments, Hudson and Ayoko (2009) showed that the results provided by the DFC and PWT may be quite different. Hudson and Ayoko (2008), based on literature review and theoretical considerations, noticed several problems with the use of the

dynamic flux chambers. Odorant compounds can accumulate inside the hood of a flux chamber, raising its concentration in the gas phase. The wind tunnel, due to the more intense turbulence of the air flow, did not appear to be affected by this problem. In addition, the ability to relate emission rates obtained through the wind tunnel and those derived by micrometeorological techniques supports the use of wind tunnel measurements to be used as input data for dispersion models (Hudson and Ayoko, 2008b).

The wind tunnels are portable open-bottom equipments that are placed over the emitting surface. In its operation, clean air is introduced inside the equipment where the volatilization of the odorant compound occurs, simulating the action of the natural wind flow on the surface (parallel air flow to the emitting surface without vertical mixing). The concentration measured at the apparatus is directly dependent on the volatilization process. The phenomenon of mass transfer depends on several factors. The main factor that determine odorant gases emission rate are the gradient of concentration between the two phases (liquid and gas). Other parameters presenting important effects on the volatilization process are: (i) magnitude of the Henry's Constant (k_h) and (ii) turbulence in the liquid or air phases, in special for those with small values of k_h , which is the case for the most part of the odorant gases (Hudson and Ayoko, 2008b).

The capacity of the wind tunnel in represent the atmospheric flow in the liquid surface is essential for the accurate measurement of the odour emission rate (Jiang et al, 1995). In this context, the aim of this work is to analyse the air flow inside the PWT model designed by the University of New South Wales (UNSW) in Australia. The UNSW wind wunnel was projected to create in its inside a well-developed boundary layer environment, seeking to simulate a simple atmospheric condition of flow parallel to the emitting surface (Wang et al., 2001). Numerical simulations were conducted to investigate the influence of different geometry configurations and surface roughness on the flow behaviour.

METHODS

Tested cases

In order to analyse the aerodynamics of the UNSW PWT the authors have tested the influence of inflow conditions (three geometries for a smooth surface) and surface roughness (four types of surface for the original geometry).

The reference case (Case A) is shown in Figure 1 and it was built exactly as the wind tunnel firstly proposed by Jiang et al. (1995) and modified by

Wang et al. (1995). This geometry was used to simulate the different surface roughness, however, the flow conditioner and the extended outlet were not considered in this case.

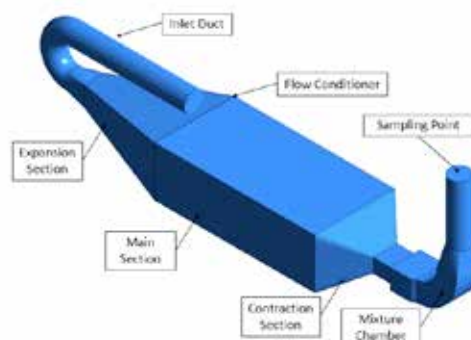


Figure 1. Schematic drawing of the original wind tunnel (Case A)

The first modification of the reference case is shown in Figure 2 (Case B). The curved pipe at the inlet was changed by an extended straight duct of 2 meters. In the second modification, shown in Figure 3 (Case C), the curved pipe at the inlet was maintained but with an additional flow conditioner downstream from the curve and upstream the expansion section. The idea behind the modifications was to diminish the undesirable acceleration at the bottom caused by the curve in the inlet duct.



Figure 2. Schematic drawing of the modified geometry: extended straight inlet (Case B)

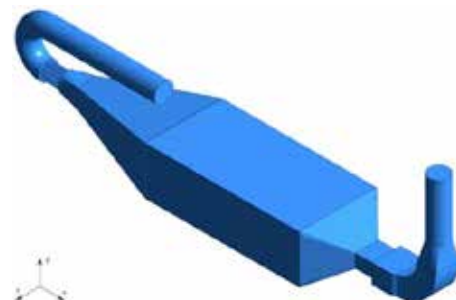


Figure 3. Schematic drawing of the modified geometry: flow conditioner downstream the curve (Case C)

Additional numerical simulations were performed with four different values of roughness at the bottom surface of the tunnel with the objective to represent solid surfaces, as the ones found in landfill sites, and quiescent liquid surfaces, as the ones found in wastewater treatment plants. The roughness values were chosen according to Seinfeld and Pandis (2006), that presents roughness lengths values for various surfaces. The values are (in meters): 0.3 (lawn), 0.03 (sand), 0.003 (smooth water) and 0.0003 (smooth surface). It is worth to notice that the effects of surfaces roughness were evaluated for Case A without flow conditioner and the extended outlet.

Mathematical Modeling

The aerodynamics of the wind tunnel was described based on the governing equations of fluid flow. The flow of an incompressible and Newtonian fluid is described by the Navier Stokes equations. Since the flow in the wind tunnel is turbulent, we used the Reynolds Averaged Navier Stokes (RANS) approach. The equations of mass and momentum conservation with the appropriate statistical treatment are:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (1)$$

$$\bar{u}_i \frac{\partial \bar{u}_j}{\partial x_i} = -\frac{\partial \bar{P}}{\partial x_j} + \frac{\partial}{\partial x_i} \left[(\nu + \nu_T) \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right] \quad (2)$$

Where u_i is velocity vector [m/s], P is the pressure [Pa], ν is the kinematic viscosity [m^2/s], ν_T is turbulent kinematic viscosity [m^2/s], and x_i is the position vector [m/s]. The model used to solve the both equations for our case was the $k-\omega$ SST proposed by Menter (1994).

The boundary conditions were: (i) imposition of an uniform velocity equals to 3,82 m/s, providing a mean velocity of 0,33 m/s in the main section, as explored by Jiang et al. (1995), (ii) at the outlet atmospheric pressure was considered and the derivate of the other variables with respect to the normal direction is zero and (iii) at the walls a non-slip condition is used. The flow is air, so $\mu = 1,79 \times 10^{-5}$ Pa.s. The set of the governing equations was solved using the commercial software ANSYS Fluent 17.0 which uses the Finite Volume Method.

FINDINGS AND ARGUMENT

In order to analyse the influence of the geometry modifications in the aerodynamic behaviour of the wind tunnel, we analysed: (i) the streamlines for the reference case (Figure 4) and (ii) the velocity distribution at the beginning of the expansion section, as shown in Figure 5.

Figure 5 shows the streamlines throughout the entire wind tunnel for the reference case (Case A). One can notice that the flow conditioner (perforated plate) placed at the beginning of the main section causes a recirculation in the flow and such recirculation makes the flow pattern distant from the expected, a fully-developed or close to an atmospheric boundary layer condition flow. In addition, the acceleration caused by the curve in the inlet duct helps the recirculation effect to be accentuated, justifying the proposed modifications. The friction velocity distribution at the gas-liquid(solid) interface resulted in very small values of its mean, 0.031, 0.033 and 0.036 m/s for Cases A, B and C, respectively. It does not represent a friction velocity of an atmospheric boundary layer flow.

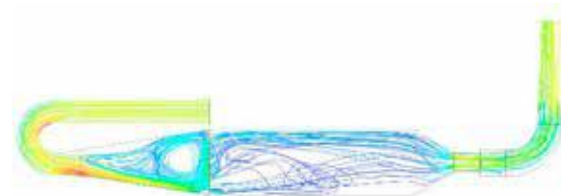


Figure 4. Streamlines for the Case A

Figure 5 shows the velocity distribution at the entrance of the expansion section for the tested cases. The higher velocities are concentrated in the distribution for the Case A, more specifically near the bottom. This result shows that the curve in the inlet duct is the main reason of the undesirable acceleration of the flow near the bottom.

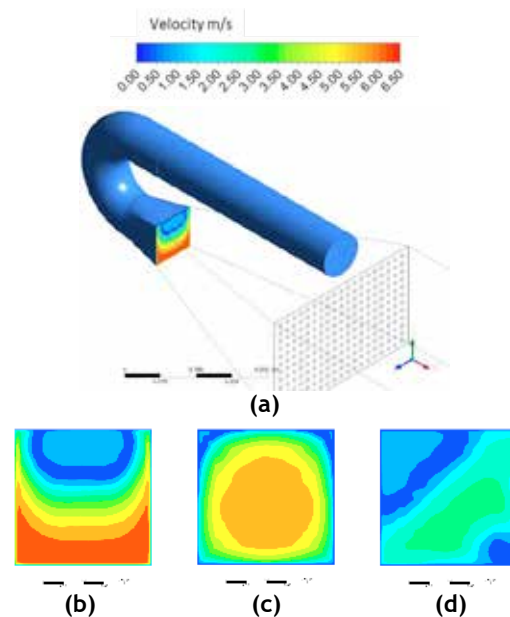


Figure 5. (a) Location of the plane used to analyze the velocity distribution at the beginning of the expansion section for (b) Case A, (c) Case B and (d) Case C

Case C (Figure 5(d)) was the one that presented the lowest velocity values although it did not achieve an ideal velocity distribution and the mean friction velocity value was not as expected. On the other hand, Case B (Figure 5(c)) managed to considerably minimize the effects of the curve, but the friction velocity value was still too low.

Figure 6 shows the velocity vectors and the distribution of friction velocity at the bottom surface of the wind tunnel. It is worth notice that the influence of the roughness height was evaluated for the reference case (Case A) without flow conditioner and the extended outlet. The velocity vectors show a very similar pattern of the flow inside the main section for all the roughness heights. The high concentration of vectors indicates high velocity values. This condition can be seen in every case with a slight reduction of the recirculation zone as the roughness height is higher. It means that the type of surface is modifying the accelerated pattern near the bottom observed for the original geometry simulated (case A).

The friction velocity is the main parameter related to the volatilization of gaseous compounds from liquid or solid surfaces. The mean values of friction velocity at the liquid-gas interface (bottom of the main section) are shown in Table 4. These values are in agreement with the mean values of friction velocity normally considered for the atmospheric flow over liquid or solid surfaces. Santos et al. (2012), for example, used friction velocity values varying between 0.11 m/s and 0.27 m/s to estimate the H_2S overall mass transfer coefficient from quiescent surfaces at wastewater treatment plants. Additionally, in Figure 6 we see the distribution of friction velocity. For the higher roughness heights (Figure 6(a), (b) and (c)) almost the half of the surface presented friction velocity greater than 0.25 m/s with a maximum of 0.50 m/s.

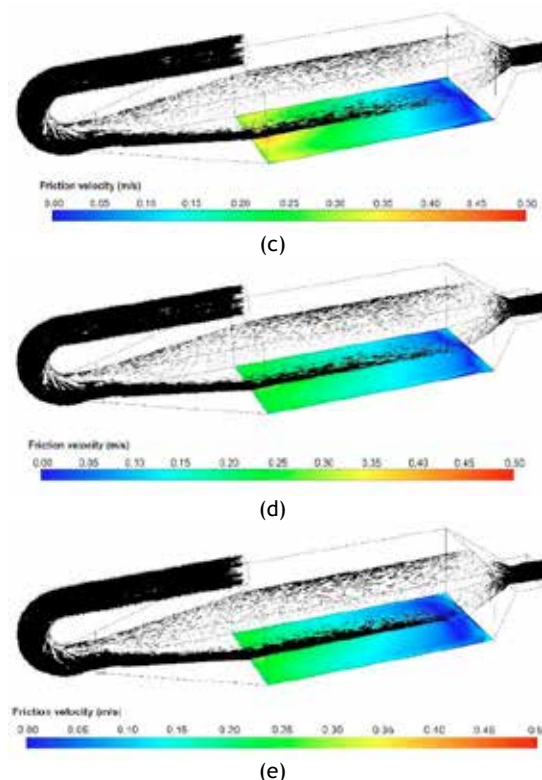
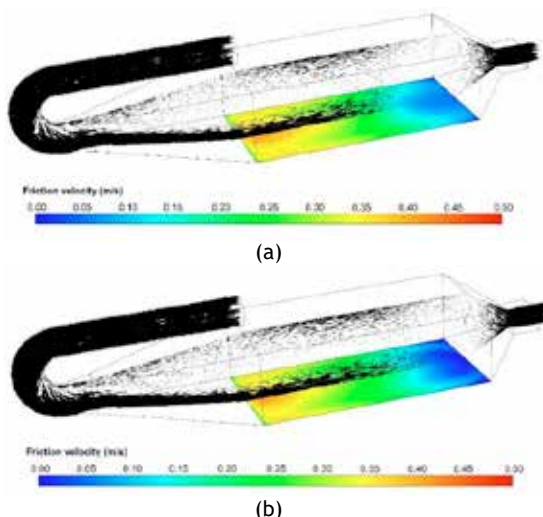


Figure 6. Velocity vectors and friction velocity distribution for different roughness heights [m]: (a) 0.3, (b) 0.03, (c) 0.003, (d) 0.0003 and (e) smooth

Table 1. Tested roughness heights and mean friction velocity obtained through the numerical simulations

Roughness height [m]	Friction velocity [m/s]
0.3	0.25
0.03	0.23
0.003	0.20
0.0003	0.17
Smooth	0.15

CONCLUSIONS

The present work had as objective to investigate the air flow inside the portable wind tunnel developed by the UNSW. The tool used to do it was the computational numerical simulation of the air flow inside the tunnel. The continuity and the momentum conservation equations were solved using the Ansys Fluent software, which is based on the finite volume method. The turbulence was treated with the model $\kappa-\omega$ SST, used to solve RANS equations.

Two modified geometries were proposed in addition to the reference case, one with an extended straight inlet and the other with a flow conditioner just after the inlet curve. These modifications led to less disturbed profiles (compared to the

reference case). In particular, the addition of the flow conditioner after the inlet curve led to the elimination of almost all the negative velocities at the tested positions. However, the mean friction velocity values were very small at the interface, 0.031, 0.033 and 0.036 m/s for Case A, B and C, respectively.

The numerical results showed various vortices inside the tunnel. This can be a good indication that the flow inside the tunnel is well mixed. However, an acceleration at the bottom surface after the inlet curve could cause an overestimation when measuring odour components; since higher flow velocities cause a low resistance to the mass transference at the surface, consequently increasing the odour emission. So, further investigation is necessary to understand the volatilization process inside the tunnel.

According to the results, the smoother the surface, the longer and with less intensity are the vortices inside the tunnel. A different behaviour is seen with turbulence intensity; the smoother the surface, the more intense the turbulence gets. Although differences in the tunnel's flow behaviour can be seen between the surfaces, the variation among the friction velocities is small and the values found represent the values found in reality, according with the presented by Santos et al. (2012). This indicates that the tunnel is suitable to be used with different surfaces as wastewater treatment plants and landfill sites once the friction velocity over the emitting surface is directly related with the emission of odorant compounds.

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ODOR IMPACT ASSESSMENT IN A RENDERING PLANT USING FIELD AND DYNAMIC OLFACTOMETRY AND DISPERSION MODELLING

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Abstract:

The impact caused by odor emission in the environment is a growing issue for many industries. In many cases, the capital costs of odor abatement systems is high, and its installation is complex. Therefore, it is important to conduct a quantitative odor source assessment to aid in the selection of the best technology for management and control of these emissions. The scope of this study is an animal rendering plant (which processes animal subproducts from a slaughterhouse), located close to a residential area. The goals are to do the assessment and ranking of odor emission sources, and suggest control actions. The odor control system in use in the plant is a biofilter, where monitoring of odor emissions was conducted. The sampling plan divided the biofilter area in 18 parcels, where gas velocity and temperature were measured to analyse the biofilter's homogeneity. 3 parcels with the highest flux were selected for collection of 2 samples in each. The sampling followed VDI 3477:2004, and the samples were analyzed by dynamic olfactometry according to EN13725:2003. Then the resulting odor emission rate was calculated. The results showed variation in velocity, temperature and odor concentration in the exiting gas throughout the biofilter, which led to low treatment efficiency.

Afterward, the odor atmospheric dispersion was modelled using AERMOD. The biofilter was represented by an area source, while the rendering plant building was represented by a fugitive volume source. The calibration of this fugitive source's emission rate was performed through reverse modelling, using as input odor data concentration at the receptors, obtained by field olfactometry. The results of odor dispersion modelling were evaluated based on international criteria, specific for this kind of activity: 5 ouE/m³ for the 98-percentile (JORF, 2003). This methodology contributed to correct decision-making on the odor management and control technology to be implemented on-site.

Keywords: Odor dispersion modelling; rendering plants, biofilters, field olfactometry, dynamic olfactometry.

INTRODUCTION

The animal rendering industry is very important and closely connected with the meat industry. All the byproducts of slaughter are transformed into protein that can be used in the animal feed industry, or others. Nevertheless, the process of rendering produces odor that can become a nuisance if not managed properly.

The scope of this study is an animal rendering plant which processes swine and poultry, located close to a residential area. The goals are to do the assessment and ranking of odor emission sources, and suggest control actions to adequately direct the investment toward minimizing the industry's impact on its surrounding community.

METHODS

The evaluation includes 5 basic phases: 1) the qualitative assessment of individual processes inside the rendering plant to verify the gas collection system's efficiency in taking the odorous gases to the odor control system (biofilter); 2) Monitoring biofilter odor emissions; 3) Field olfactometry in the vicinity; 4) Odor dispersion modelling using reverse modelling to assess the impact on the community, and 5) Suggestion of odor emission prevention and control measures.

1) Assessment of gas collection system

All the processes were analyzed and ranked in high, medium and low relevance for odor control

based on the following criteria: use of direct vapor; batch or continuous process; presence and efficiency of gas collection system.

2) Monitoring biofilter odor emissions

The biofilter was also identified as a relevant odor source, and therefore was subject to odor monitoring. The sampling plan divided the biofilter area (14 x 26,3 m = 368,2m²) in 18 parcels, where gas velocity and temperature were measured to analyze the biofilter's homogeneity. 3 parcels with the highest flux were selected for collection of 2 odor samples in each. The sampling followed VDI 3477:2004 using a hood, and the samples were analyzed by dynamic olfactometry according to EN13725:2003, within the period of 30 hours. Then the resulting biofilter odor emission rate was calculated according to Brancher (2013).

3) Field Olfactometry

This method was used to assess the odor perception inside and outside the industry's limits. The Nasal Ranger® field olfactometer was the selected tool. 29 monitoring points were defined, being 19 external (distances between points varying between 250 and 300m, covering a 2km radius) and 10 internal to the plant boundary. Two monitoring campaigns were carried out, in a total of 5 days and 131 measurements. The choice of monitoring points prioritized sensible locations such as schools, health care establishments and residential areas. The results were mapped and

used to aid in calibration of dispersion modelling emission rate.

4) Odor dispersion modelling

Odor atmospheric dispersion was modelled using AERMOD. The biofilter was represented by an area source, while the rendering plant building was represented by a fugitive volume source. The calibration of this fugitive source's emission rate was performed through reverse modelling, using as input maximum odor data concentration at the receptors, obtained by field olfactometry, using meteorological data collected during the odor field campaigns. After calibration, odor dispersion was simulated again considering a longer meteorological database (5 complete years). The results of odor dispersion modelling were evaluated based on international criteria, specific for this kind of activity (existing rendering plants): 5 ouE/m^3 for the 98-percentile (JORF, 2003).

FINDINGS AND DISCUSSION

1) Assessment of gas collection system

The analysis revealed many processes that had relevant odor emission potential (had use of direct vapor and were batch processes with high flowrate and odor emission at the end of each batch), but had no gas collection system, or the system was inefficient. This fact contributed to fugitive emissions that were not treated by the biofilter. The highest priority was given to the swine digesters; all other processes were ranked in order of relevance for the odor control.

2) Monitoring biofilter odor emissions

The results showed variation in velocity, temperature and odor concentration in the exiting gas throughout the biofilter (as shown in Table 1 and 2), which led to low treatment efficiency, high odor concentration and emission rate (Table 3).

Table 1. Velocity and temperature on the biofilter surface.

Data	v biofilter (m/s)	Temp. (°C)
Average	0,027	41,2
Std. deviation	0,011	4,8

Table 2. Odor concentration in different parcels.

Source Biofilter	Odor Concentration (ouE/m ³)		
	SampleA	SampleB	Geo. mean
Parcel 2	3.069	3.866	3.445
Parcel 8	1.149	1.448	1.290
Parcel 16	5.468	6.502	5.963

Table 3. Odor concentration and flowrate on biofilter surface.

Odor average concentration (C_m)	3.865 ouE/m ³
Odor emission rate (TE_m)	38.267 ouE/s

Table 4. shows a comparison of results obtained on the biofilter, and reference parameters.

Table 4. Comparison of results on biofilter and reference parameters

Data	Result	Reference parameters
Empty-bed residence time (EBCT)	22 to 92s Avg. 45s	360 s (EUROPEAN COMMISSION, 2005)
Temp. (°C)	31,8 - 48,3°C Average 41,2 °C	20-50°C (LIU, 2015)
Flowrate	Avg: 0,027 m/s Std.Dev.: 0,011 m/s	Uniform flowrate through all area (GROSKREUT, 2004)
Flowrate/area	96,8 m ³ /m ² .h	60-100 m ³ /m ² .h (CHERNICHARO, 2011)
Media Porosity and Humidity	Unknown	40-60% (LIU, 2015)

3) Field Olfactometry and Odor dispersion modelling

The results of fields olfactometry are in Table 4.

Table 4. Field olfactometry odor results.

Odor	Odor ranges (D/T)						
	<2	2	4	7	15	30	60
N	76	13	9	6	6	0	0
Freq.(%)	69	12	8	5	5	0	0

In total, 11% of measurements in the external area were above the recommended criteria (equal or above 7 D/T).

Odor dispersion modelling considered two sources: the biofilter (whose results are shown in Table 2), and the rendering plant building, represented by a fugitive emission source. Its emission rate was determined by reverse modelling, a useful technique for particulate and odor fugitive source quantitative determination. It is done by running multiple simulations with different emission rates, and comparing model results with field olfactometry measurements (MALHEIROS et al, 2016). The final result of calibration is in Table 5.

Table 5. Calibration result of reverse modelling.

	Average concentrations on the most impacted area	
Method	Field measurements	AERMOD
Result	8 UO/m ³	11 ouE/m ³

Using this method, the odor emission rate for the rendering plant was 38.267 ou_E/s.

Finally, the resulting odor dispersion plume for the whole period showed that the odor criteria, 5 ou_E/m³ in the 98 percentile (JORF, 2003) was exceeded in a area reaching 1.800m to the west, and 300 m on the other directions. This was mostly influenced by local topography and sources's location.

4) Odor control measures

The results of the previous phases of the study all confirmed the odor impact in the neighbouring community. Therefore, the following control and mitigation measures were suggested:

Control measures on the rendering plant building:

- Implementation of a efficient exaustion and gas collection system in order to really conduct the odorour gas to treatment in the biofilter, and keep a slightly negative pressure in the building;
- Conduct a cost-benefit analysis of a pre-treatment phase before the biofilter to reduce temperature, and/or condensate part of the gases to reduce concentration (condenser or scrubber);
- Homogenize the flow from both swine and poultry processing, which nowadays arrives at biofilter by 2 separated ducts;
- After improving the collection system, monitor new emission parameters (flowrate, temperature, humidity, odor concentration, and H₂S and NH₃ concentration), in order to supply data to control system design.

Control measures on the biofilter:

- Assess the need and applicability of a pre-humidifier before the biofilter;
- Improve gas distribution inside the biofilter bed, removing less-resistance paths;
- Collect samples to analyze humidity and porosity of biofilter media, in order to adjust them according to literature parameters, for example VDI 3477;
- Follow the Best Management Practices for animal subproducts industry (EUROPEAN COMMISSION, 2005).

CONCLUSIONS

The work displayed the important role of a comprehensive assessment in order to truly define the relevant odor sources in a rendering plant. The results clearly show that fugitive emissions are an important part of the plant's total emissions, and must not be taken for granted.

Another important aspect is the verification of incorrect design and operation of the biofilter, which led to poor efficiency and high odor emission rates. Therefore, in conclusion this methodology contributed to correct decision-making on the odor

management and control technology to be implemented on-site.

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MEASUREMENT AND MATHEMATICAL MODELLING OF ODOR GASES IN A COLLAGEN AND GELATINE PLANT

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Abstract: The objective of this work was to identify and quantify odor sources throughout the production process of a gelatine and collagen factory located in the interior of Paraná State, Brazil. At the same time, an atmospheric dispersion model was used to identify the radius of coverage and the frequency of perceived values of odor around the company and, thus, propose improvements of control systems or installation of new systems. The NH₃ (ammonia) and H₂S/CH₄S gases (hydrogen sulphide/methyl mercaptan) were measured during 7 consecutive days around emission sources and throughout the company's production process. Thus, the monitoring was performed on the arrival of the trucks with the used raw material (bovine hides), loading of storage hopper, storage shed and effluent treatment station. Electrochemical, automatic and continuous measurement Cairpol's sensors were used. This equipment records the measurements in ppb (part per billion) every minute and stores them in an internal data logger. During the monitoring period, an anemometer was installed to record wind direction and wind speed data every 5 minutes to correlate with gas measurements. After identification and quantification of odors sources the atmospheric dispersion mathematical model AMS/USEPA AERMOD was implemented. For this, the Aermom View software developed by Lakes Environmental. The model was applied to evaluate the spatial range of perceived odors in the company surroundings, as well as for simulated future scenarios with reduced emission of odoriferous gases. The model requires the following input data: meteorological, topographic, soil use of the study region, and gases emission rate for emission sources. The emission rates of non-point sources were estimated using a reversed modeling method. The results of gases measurement showed that the largest sources of emissions are concentrated in the storage hopper, storage sheds, industrial effluent treatment plant and the biofilter outlet used to treat the gases from one of the storage sheds. The mathematical simulation showed that under unfavorable conditions for pollutants dispersion, it is possible to smell H₂S/CH₄S within a radius of approximately 5 km from the company. For the NH₃ this radius is 1.5 km for all people with average sensitivity to odors. A hypothetical scenario was created considering a reduction of 80% in the emission of the gases from the biofilter, process and storage and of 50% from the treatment plant, based on the propositions made for adjustment and implementation of new control systems. This future scenario indicated a decrease in the NH₃ perception radius to approximately 200 meters from the company and 4 km for h₂s/ch₄s in the worst conditions of gases dispersion for the simulated period.

Keywords: odour, odour monitoring, mathematical air dispersion modeling, odour sensors.

INTRODUCTION

Odor emitted by industries are the major sources of environmental pollution related claims for air pollution (Henshawet et al., 2006). Odor is the olfactory response of humans to odorous gases, indicating that it is a subjective sensation, with individual characteristic. Odor emissions are a nuisance to neighboring communities due to bad smell and potential health hazards. However, they are rarely monitored on an ongoing basis due to the limitations of the techniques and the lack of legislation. Odoriferous substances can usually be grouped into three groups: sulfur compounds (hydrogen sulphide, mercaptans), volatile organic compounds and nitrogen-containing compounds (ammonia, amines) (Schiffmann, 2001). In several processes some compounds are dominant over the odor, indicating the total odor concentration, as they are present in higher concentrations than other odorants and can be detected in low concentrations through continuous measurement equipment (Karageorgos, 2010). Hydrogen sulfide (H₂S), mercaptans (CH₄S) and ammonia (NH₃) are

predominant odoriferous gases in processes using animal raw material, such as gelatine and collagen factories and industrial wastewater treatment plants. H₂S is a corrosive, colorless, extremely toxic gas with odor of rotten egg. The California Environmental Protection Agency cites that in population terms the average odor threshold of this gas in outdoor environments is in the range of 30 to 50 ppb, for this reason it limits the concentration in the air to 30 ppb, considering the hourly average. Ammonia (NH₃) is a colorless gas with an irritating and poisonous odor if inhaled in large quantities (EPA 456, 1995). Nagata (2003) determined the olfactory limit of ammonia, evaluated in the laboratory through the "triangle odor bag" method, at 1,580 ppb. Alberta (Canada) legislation, based on the perception of odors, set the limit of 2,000 ppb for the hourly average of NH₃. The objective of the study was to identify and quantify the odor emission sources of NH₃ and H₂S/CH₄S odor gases throughout the production process of a gelatin and collagen factory. After the emission sources were evaluated, the mathematical model AERMOD was used to define the radius of odor coverage in the

surroundings of the company and propose improvements or installation of new control systems in odor emission sources.

METHODS

Area of study is located in Maringá city, state of Paraná (Brazil). The measurements of the gases were carried out with the Cairpol sensors, electrochemical, automatic and continuous measurement. This equipment records the measurements in ppb (part per billion) every minute. All sources of odoriferous substances emitted from the company's production process were monitored as places around the sources too. All measurements were performed for seven days in a row. The emission sources monitored were: on the arrival of the trucks with the used raw material (bovine hides), loading of storage hopper and washing of raw materials, storage sheds, effluent treatment station (ETS) and biofilter outlet. Figure 1 shows the 28 gas monitoring points.

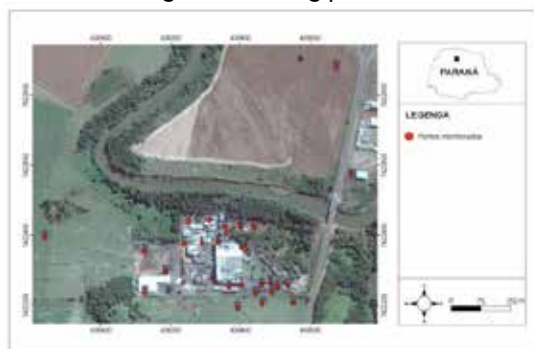


Figure 1: Monitoring points.

During the monitoring period, an anemometer was installed to record wind direction and wind speed data every 5 minutes to correlate with gas measurements. The mathematical modeling of odor dispersion was performed using the AERMOD View. The meteorological input data for the model was obtained for the period from 2013 to 2017 from the meteorological station installed in Maringá city. The terrain data was obtained from the SRTM30, land use data an online database, available at www.webgis.com. The emission data of the sources were estimated based on the gas measurements carried out in the field. A square grid of receivers with a size of 10 km x 10 km was defined in two levels of refinement. The first level had dimensions of 2 km x 2 km, spaced every 100 meters and the second level with receivers spaced every 500 m. Two scenarios were simulated: the first one contemplated the real emissions, which were estimated through field measurements. The second scenario considered reductions in H_2S/CH_4S and NH_3 emissions, with improvement in the design and operation of the biofilter and implementation of new systems for odor control in odor sources,

suggesting the installation of gas scrubbers and activated carbon filters. For the biofilter, production process and storage of raw material was considered an 80% reduction of emissions. For the ETS and yard of trucks, as they are open areas, the solution for odor reduction is the use of neutralizers of ambient odor, therefore considered reduction was of 50%.

FINDINGS AND ARGUMENT

GAS MONITORING

The results of the monitored maximum values of H_2S/CH_4S and NH_3 were interpolated and superimposed on the aerial image of the study area. Figure 2 shows the maximum monitored concentrations of H_2S/CH_4S . The maximum values are located throughout the ETS and close to the hopper (beginning of the raw material processing). The maximum measured concentration was 1000 ppb (maximum scale of equipment used).

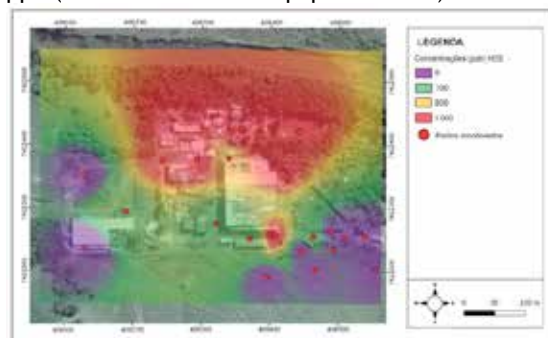


Figure 2: Results for H_2S/CH_4S

Figure 3 shows the maximum concentrations of NH_3 monitored. The maximum values are located in the unloading of the trucks and entrance of the hopper and near the biological filter. The maximum monitored value was 3,079 ppb, near the hopper.

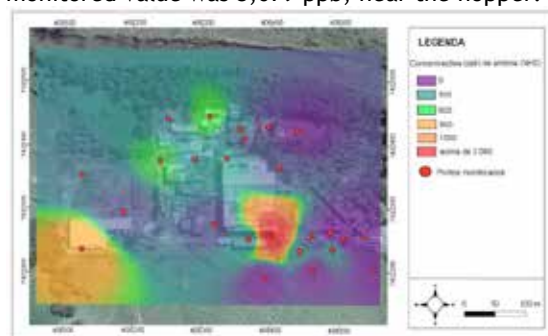


Figure 3: Results for NH_3

The results of the monitoring in the sources of emission indicating the sites of greater emission and allowed the calculation of the emission rate of the odor sources through reverse modeling, which was used as input data in the mathematical model.

MATHEMATICAL MODELING

Scenario 1 - H₂S/CH₄S

The results of the maximum concentrations of H₂S/CH₄S are shown in Figure 4.

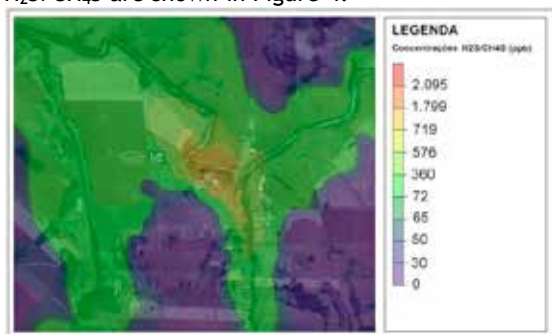


Figure 4: Results for H₂S/CH₄S - Scenario 1

The highest concentration of H₂S/CH₄S was 2,095 ppb, near the ETS. This simulation showed that in the northwest and southwest directions the concentrations could be higher than 30 ppb at distances higher than 5 km of the company, while in the other directions, the maximum distance is approximately 2.5 km.

Scenario 1 - NH₃

The results of the maximum concentrations of NH₃ are shown in Figure 5.

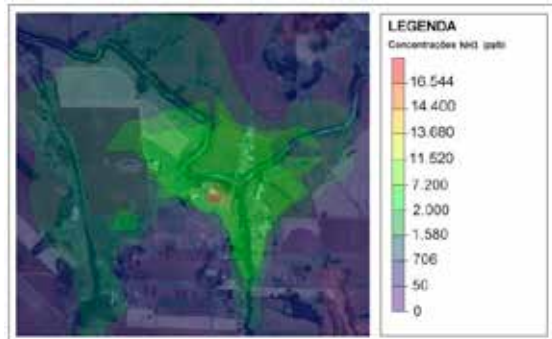


Figure 5: Results for NH₃ - Scenario 1

The odor perception range for NH₃ is concentrations above 1,580 ppb (Nakata, 2003), while Alberta (Canada) legislation sets the limit of 2,000 ppb. The highest concentration of ammonia was 16,544 ppb, close to the truck yard. In a radius of approximately 1.5 km, the concentrations were less than 1,580 ppb, whereas the concentration of 2,000 ppb was restricted to an average radius of approximately 1 km of the company.

Scenario 2 - H₂S/CH₄S

The maximum hourly concentration of H₂S/CH₄S was 934 ppb, close to ETS, indicating a reduction of 55% about scenario 1. The simulation of scenario 2 showed that in the northwest, southwest and east directions the concentrations can be higher than 30 ppb at distances higher than 4 km of the company, while in the other directions, the maximum distance

in which concentrations are still higher than 30 ppb is less than 2,5 km.

Scenario 2 - NH₃

The highest ammonia concentration was 3,340 ppb, less than 20 meters from the truck yard. This concentration is 80% lower than the maximum concentration in scenario 1. Concentrations above 2,000 ppb were restricted to a distance of approximately 160 m from the company and concentrations of 1,580 ppb at a distance of about 220 m.

CONCLUSIONS

The main emission sources identified after the monitoring were: ETS, beginning of the raw material processing and storage of the raw material, besides the exit of the Biofilter. The dispersion study showed that in scenario 2 (future) there is a decrease in the NH₃ perception radius to approximately 200 meters of the company in the worst conditions of gas dispersion of the simulated period. For H₂S/CH₄S the reduction of the maximum distance of odor perception was not so significant. The main source of emission of this gas is the ETS, which was attributed a reduction of 50% of its emission, because being an open source its odor control should be by means of encapsulators, which do not allow an efficiency as high as the other control systems. The H₂S/CH₄S concentration showed a reduction of 55% from scenario 1 to 2. With the simulations carried out, it is possible to conclude that the improvements in the control of emission sources will avoid the annoyance and complaints in the neighboring community and sanctions of the environmental agency.

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NUMERICAL MODELLING OF ODOUR DISPERSION BY A SOLID WASTE LANDFILL EMISSIONS IN GRANDE VITÓRIA - ESPÍRITO SANTO, BRAZIL

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Abstract: Odour compounds are one of the most important pollutants related to nuisance complaints in the environmental agencies. This study presents the Dispersion Modeling (AERMOD) of Odorous Gases emissions from a landfill of Grande Vitória/Espírito Santo, Brazil, to evaluate the impact of its operation.

Odour perception is very subjective and perceived in very low concentrations (ppb) above the perception limit (that varies between individuals - gender, age, smoker or non-smoker). Thus, is very important to work with models that can solve mass transport equations in time intervals less than an hour to be possible to catch peaks concentrations.

The scientific problem discussed in this abstract resides in the application of a gaussian model (such as AERMOD) to treat odour peak events in time intervals less than an hour. The potential law described by Duffee et. al (1991) was applied to obtain peak concentrations required to identify odour complaint episodes.

As secondary objectives of this study, the construction of an emission inventory with the most representative sources, a better understanding of the dispersion phenomena of odorous gases emissions and to create fundamentals for discussions about the impact on air quality in regions neighboring the plant. The computational domain was defined as a square with 400 km². Meteorological data was obtained from the Vitória/ES airport station (SBVT). The data presented was imported into the METAR code. The topographic data were extracted through the digital elevation model: SRTM3, MDE S21W041 and land use data from the region were obtained through the Environmental Agency of the State of Espírito Santo (IEMA, 2015).

The emission rate for each source type were calculated by different approaches: i) The United States Environmental Protection Agency (USEPA) literature (AP-42) was consulted to obtain emission factors related to the activities that generates odorant compounds; ii) LandGEM *software* (Landfill Gas Emission Model) was used to obtain emission rates for landfill cells; iii) for leachate ponds the method proposed by the EPA (AP-42, Chapter 4) was also used, however, referring to the sources associated with evaporative losses in the collection, treatment and storage of wastewater; iv) the composting unit emissions were determined by emission factors proposed by Sironi et. al (2006).

It was possible to establish a relation of odour concentrations between the meteorological and topographic parameters: proximity of the main sources, difference of altitude between the sources and the receptor points, the predominant direction of the wind and the conditions of atmospheric stability. It is not possible to establish a predominant year period with the most critical results, since this analysis is related to the location of the receiver in question, but considering the population to the south of the enterprise, the months of May to August tend to present the worst results, depending on wind direction and atmospheric stability in those periods.

It was possible to evaluate AERMOD application in odour management due to combined applications with potential law. The obtained results directly from AERMOD in peak concentrations events were able to be identified. The most significant emissions of odours were those of cells in operation due to large areas and constant waste stream. The simulations showed the maximum hourly increase is was up to 12,20 OU/m³ converted to 2 OU/m³ in a 10 minutes averaging period.

Keywords: Atmospheric dispersion, landfill emissions, odour modelling, emission factor, odour management.

INTRODUCTION

Odour perception is very subjective and perceived in very low concentrations (ppb) above the perception limit (that varies between individuals - gender, age, smoker or non-smoker). Thus, is very important to work with models that can solve mass transport equations in time intervals less than an hour to be possible to catch peaks concentrations. The application of a Gaussian model (AERMOD) to treat peak odour events at time intervals of less than one hour. The potential law described by Duffee et. al (1991) was applied to obtain peak results to identify episodes of odour complaint.

The methodology usually adopted to establish odour perception patterns defined by Australian Standard AS/NZ S4323.3 (2001) Stationary Source Emissions Part 3, which an odour unit is conceptualized as the concentration of certain compound sufficient that at least 50% of the odour panel can detect its presence. This response is called the odour detection threshold and defines an odour unit per cubic meter (UO/m³). Thus, an odour of less than 1 UO/m³ is theoretically an irrelevant impact on olfactory perception (FAZIO, 2015).

The operation of the landfill in the present study occurs in the presence of a total of 8 cells, to which solid wastes are deposited. Only one cell was considered to be still in operation. It was considered that for the capture of the biogas in the cells of the landfill we use drains implanted during the construction of the cells. The storage system of leachate material from the sanitary landfill has six ponds, totaling 6313.80 m². The treatment of the effluent of septic tank has an area of 2510.7 m², with four ponds, two for the storage of the raw effluent and the others for the treated one. The landfill composting system was also considered as an odour source.

METHODS

To perform the mathematical modeling of the dispersion of particles in the atmosphere and to evaluate the increases in environmental concentrations and changes in air quality, the computational domain was defined as a square with 400 km². The 2013, 2014 and 2015 meteorological data from the Vitória Airport Station (SBVT) were used to perform the analysis. The land area was characterized by the different occupations present in the study region.

The emission rate for each source type were calculated by different approaches: i) The United States Environmental Protection Agency (USEPA) literature (AP-42) was consulted to obtain emission factors related to the activities that generates odorant compounds; ii) LandGEM software (Landfill Gas Emission Model) was used to obtain emission rates for landfill cells; iii) for leachate ponds the

method proposed by the EPA (AP-42, Chapter 4) was also used, however, referring to the sources associated with evaporative losses in the collection, treatment and storage of wastewater; iv) the composting unit emissions were determined by emission factors proposed by Sironi et. al (2006).

After the emissions are estimated, the conversion factor for odorant units proposed by Lucernoni (2016) was considered, from the following equation:

$$C_{odor} = 0,21 \times C_{CH_4} + CH_4^0$$

Where the odour concentration of the generated gas (C_{odor}) UO/m³ corresponds to the product between the conversion factor obtained through experimental studies (0,21) and the concentration of methane (C_{CH_4}) ppm plus the odour concentration considered when the methane concentration is zero (CH_4^0) UO/m³.

The output data of the AERMOD model were also converted to average more suitable for the desired analysis. To convert the hourly averages into more adequate averages of time, the Potential Law, described by Duffee et al. (1991) was used:

$$C(t) = C(t_0) \times \left(\frac{t_0}{t}\right)^{0,2}$$

In which the concentration in time t ($C(t)$) corresponds to the product between the concentration in time t_0 ($C(t_0)$) and the ratio between the concentration in the average of one hour t_0 .

By obtaining the emission factors related to the main activities that generate odorant compounds, it is possible to determine the propagation of landfill odours using the AERMOD software in its standard conditions for the sources.

FINDS AND ARGUMENT

Figure 1 shows the contribution in total emissions of the sources of odorant compounds considered. The largest contribution made by the cell in the operation of landfill waste solids urban (18175,72 UO/s, 64,89% do total) and the lowest contribution is generated by the composting unit (381,23 UO/m³, 1,36% of the total).

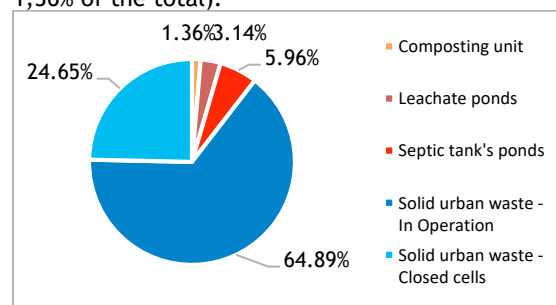


Figure 1: Emissions generated by different sources in modeling.

Through the modeling, the scenarios vary according to the adopted temporal average. Table 1 presents the maximum daily increase and mean annual increase for study sources.

Table 1: Mean and maximum values contributions different emissions groups.

Source	Mean (UO/m ³)	Maximum (UO/m ³)
Solid waste cells	0,09	12,20
Leachate ponds	0,02	1,90
Septic tank's effluent pond	0,001	0,29
Composting unit	0,00033	0,064
Synergy between all sources	0,10	12,20

The dispersion plumes of the odorant gases presented make it possible to verify that some receptors located near the project are more affected by the activities of the landfill. Figure 2 and Figure 3 represent the location of the discrete receptors, with the maximum daily concentrations and mean annual concentrations respectively.

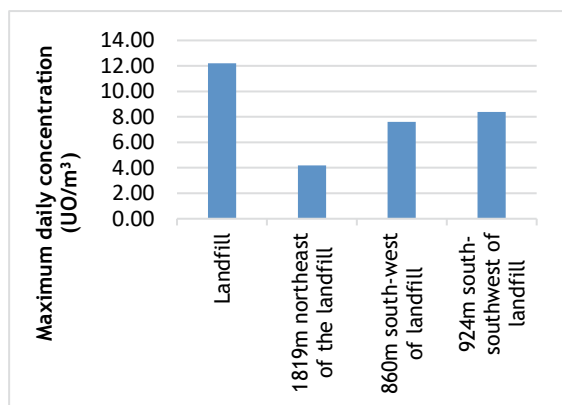


Figure 2: Maximum daily concentrations.

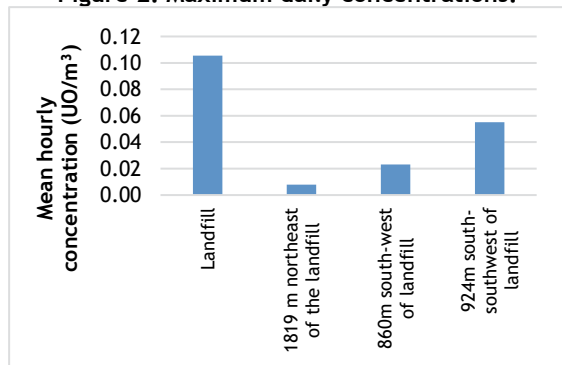


Figure 3: Mean annual concentrations.

CONCLUSIONS

By the analysis of the inventory of emission and the mathematical modeling is possible to verify that the

highest contribution to the odour emissions comes from the cells still in operation (64.89% of the total), since they are constantly fed with solid waste and it is not possible to burn the generated gases.

It was possible to establish a relationship between the meteorological and topographic parameters with the presence of higher odour concentrations: the proximity of the main sources: the difference of elevation in the sources and the receptor points, the predominant wind direction and the conditions of atmospheric stability that can be considered decisive factors to determine the way in which the population around the landfill will be impacted by the odorant emissions.

It was possible to evaluate the application of AERMOD in the handling of odours due to applications combined with the potential law, in order to compare them with limits established in legislation that take into consideration periods of exposure less than 1 hour. The most significant emissions of odours were those of cells in operation due to large areas and constant waste stream. The simulations showed that the maximum hourly increase was of 12,20 OU/m³ converted to 2 OU/m³ in an average of 10 minutes.

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MODELLING OF ATMOSPHERIC DISPERSION OF HYDROGEN SULFIDE EMITTED FROM DRAINAGE SYSTEM CHANNEL IN DROUGHT AND RAINY PERIODS

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Abstract: Dispersion models can aid policy-makers to focus on local air quality problems and how to address them, making air pollution 'quantifiable' for community. Sanitary sewage systems emit compounds that can lead to air pollution in form of odorant gases. They often influence the population living close to a sewer process unit as the emission of odors affects the quality of any human being's life and health, resulting in environmental and social problems. In Brazil, there are two network systems separating rainwater and wastewater. However, the rainwater drainage channels represent a source of odorant compounds due to improper domestic sewage releases, which mixed with rainwater, mainly during periods of drought, offer anaerobic conditions similar to those of wastewater in the arrival of a treatment plant. In the present study, to describe a source of odor emissions in a drainage channel it was necessary to look closer on how this sanitary system works as a source of hydrogen sulphide (H₂S). The methodology used tried to adapt Rainwater Drainage Systems subjected to illegal connections into the quantification of emission rate proposed by the Wastewater Treatment Plants mathematical modelling (Water9 developed by the United States Environmental Protection Agency). The sulphide concentration in liquid phase, after chemical analysis, was taken as an input data for the mathematical emission model. Furthermore, emission rates for drought and rainy periods were compared and used to model the atmospheric dispersion. The dispersion process of H₂S was investigated using the U.S. EPA recommended Gaussian dispersion model for nearby applications, AERMOD. Therefore, a map of dispersion, based on the concentration and perception was created. This study can assist further works related to disturbance caused by odorant pollutants to neighbor populations.

Keywords: Dispersion modelling, Exposure Assessments, Odour, Annoyance.

INTRODUCTION

In wastewater treatment system there is emission of gaseous pollutants as odorant gases, causing impact on the community that lives nearby. This emission affects human's well being and health, resulting in social issues (GOSTELOW; PARSONS; STUETS, 2001).

In Brazil, there is emission of hydrogen sulphide (H₂S) coming from drainage systems when illegal disposals of domestic sewage are cast, mixing with rainwater. It happens mostly in drought periods, due to the anaerobic conditions on drainage channels, behaving as an anaerobic plant of wastewater treatment.

The identification of the source of emission and the extension of its impacts facilitate the monitoring of the pollutants diffused in the atmosphere. When a material is dispersed in the atmosphere, it is carried by the wind and diluted by the turbulence present in the atmosphere, depending on meteorological conditions. This process produces a plume of polluted air that can be described mathematically by the Gaussian equation (SHERIDAN et al., 2004).

This paper aims to develop an approach to model the atmospheric dispersion of H₂S emitted from diffused sources and then determine its impact on the community. It was necessary to study emission factors to quantify the compounds and then set regions based on the concentration of perception of H₂S.

METHODS

The area of study is a drainage channel located in Praia da Costa, Vila Velha - ES (see red line in Figure 1), named after the neighborhood, Praia da Costa channel.

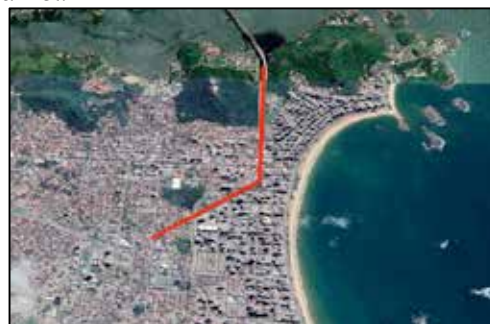


Figure 1. Overview of a drainage channel in Praia da Costa, Vila Velha - ES
Reference: Google Earth (2019)

Praia da Costa channel (see Figure 2) is part of the urban drainage system, built to collect rainwater. It is considered an area source for mathematical modelling, because of its shape and due to the fact that emissions occur all over its extension.



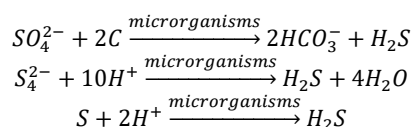
Figure 2. Praia da Costa channel

The methodology used to determine sulphide in wastewater uses precipitation of Zinc sulphide (ZnS) when a sample (diluted 1:10) of the channel reacts with Zinc Acetate. The precipitate is filtered then washed to clean any dirt. The solid part is transferred to an erlenmeyer and then it reacts with an Iodine solution (I_2) in acid solution (HCl). The Iodine exceeded is titrated with Sodium Thiosulphate which starch as an indicator (ALPHA, XXXX). The volume of Sodium Thiosulphate is used to calculate the concentration of sulphide with the following equation:

$$\frac{(0.025V_{I_2} - V_{Na_2S_2O_3}) \times 16000}{V_{sample}}$$

Where V_{I_2} is the volume of Iodine used, $Na_2S_2O_3$ is the volume of Sodium Thiosulphate titrated and V_{sample} is the volume from the sample collect after diluted. The result was 76 mg/L of sulphide.

The main biochemical reactions occurred in sanitary systems, where sulfur compounds are reduced by microorganisms, according to the EPA (2017):



H_2S emissions can occur through diffusion or convection. The diffusion happens due to the difference of concentration between the liquid and the gas, as in the equation of desulphation, where microorganisms react with the sulphate dissolved in the liquid, turning it into hydrogen sulphide on the gaseous part. To apply this methodology it was necessary to choose a suitable equation for this case. A drainage channel can be considered like non aerated system, biologically active, no oil film layer and flowthrough (EPA, 1977). The equations chosen were:

- Liquid phase mass transfer coefficient:

$$K_l = 2,78 \cdot 10^{-6} \cdot \left(\frac{D_w}{D_{\text{éter}}}\right)^{2/3} \quad \text{for } 0 < U_{10} < 3,25 \text{ m/s}$$

- Gas phase mass transfer coefficient:

$$K_g = 4,82 \cdot 10^{-3} \cdot (U_{10})^{0,78} \cdot (Sc_G)^{-0,67} (d_e)^{-0,11} \quad \text{where}$$

$$Sc_g = \frac{\mu_a}{\rho_a \cdot D_a}$$

$$d_e = \left(\frac{2 \cdot A}{\pi}\right)^{0,3}$$

- Overall mass transfer coefficient for transfer of constituent from liquid phase to gas phase:

$$K = \frac{K_l \cdot K_{eq} \cdot K_g}{K_{eq} \cdot K_g + K_l} \quad \text{where}$$

$$K_{eq} = \frac{H}{RT}$$

- Emission:

$$N = K \cdot C_L \cdot A \quad \text{where}$$

$$C_L = \frac{[-b + (b^2 + 4a \cdot c)^{1/2}]}{2 \cdot a}$$

$$a = \frac{K \cdot A}{Q + 1}$$

$$b = K_s \cdot \frac{K \cdot A}{Q + 1} + \frac{K_{max} \cdot b_i \cdot V}{Q \cdot C_o}$$

$$c = K_s \cdot C_o$$

AERMOD is very helpful for modeling air quality impacts of pollution sources. Sources emission rates can be treated as constant throughout the modeling period or optional periods of variation. The AERMOD model utilizes a file of surface boundary layer parameters and a file of profile variables including wind speed, wind direction, and turbulence parameters. These two types of meteorological inputs are generated by the meteorological preprocessor for AERMOD, which is called AERMET (EPA, 2004). It creates vertical profiles of meteorological data, wind velocity and direction, turbulence and temperature gradient. The characteristics of the surface of the terrain as rugosity, Bowen and Albedo values are necessary to build a similarity profile of the relevant parameters on the limit sheet (CIMORELLI, ALAN J; PERRY, STEVEN G. et al., 2004).

The region had to be divided in sectors (see in Figure 3 regions) in order to gather Bowen, Albedo and rugosity values depending on the kind of terrain use.



Figure 3. Sectors of the domain
Reference: Google Earth (2019)

FINDINGS AND ARGUMENT

Despite the tabled values, the flow rate and the velocity were calculated and the width and depth (W and D) were measured using a measuring tape. The length of the channel was measured using Google Earth. After gathering all these values, the Co was calculated using the Sulphide Method. The emission was calculated using Water9 model from EPA. Table 1 contains all the values obtained.

Table 1. Tabled, measured and calculated values for Emission rate

Measured values in the channel			
A	23868.79	m ²	Superficial area
D	3.50	m	Depth
V	83540.76	m ³	Volume
Q	0.062	m ³ /s	Wastewater flow rate
C_0	0.307	mg/L	Sulphide concentration
d_e	174.37	m	Effective diameter
Tabled values			
U_{10}	4.64	m/s	Wind velocity over 10m
T	298	K	Wastewater temperature
b_j	50	g/m ³	Biomass concentration
F/D	61.14	-	Fetch to depth ratio
Air, water and H ₂ S properties			
D_w	0.0000161	cm ² /s	H ₂ S diffusivity in water
D_a	0.176	cm ² /s	H ₂ S diffusivity in the air
H	0.023	atm .m ³ /gmol	Henry's law constant
K_{max}	0.00000299	g/g .s	Maximum biorate constant
K_s	6.329	g/m ³	Half saturation biorate constant
ρ_a	0.00120	g/cm ³	Air density
μ_a	0.000181	g/cm.s	Air viscosity
D_{ether}	0.00000850	cm ² /s	Ether diffusivity in water
R	0.0000821	atm.m ³ /gmol	Universal gas constant
Sc_G	0.857	-	Schmidt number on gas side

Mass transfer coefficient			
k_l	0.00000860	m/s	Liquid mass transfer

k_g	0.0100	m/s	coefficient Gas mass transfer coefficient
Global mass transfer			
k_{eq}	0.940	-	Equilibrium constant
K	0.00000859	m/s	Overall mass transfer coefficient of H ₂ S from liquid phase to gas phase
Emission of H ₂ S			
a	4.29	-	
b	226.91	-	
c	-1.94	-	
C_L	0.00856	g/m ³	Concentration of H ₂ S in the Liquid phase
N	0.00176	g/s	Emission rate

The wind rose obtained after using AERMET was from 2015 data (see Figure 4). It was created with WRPlot.

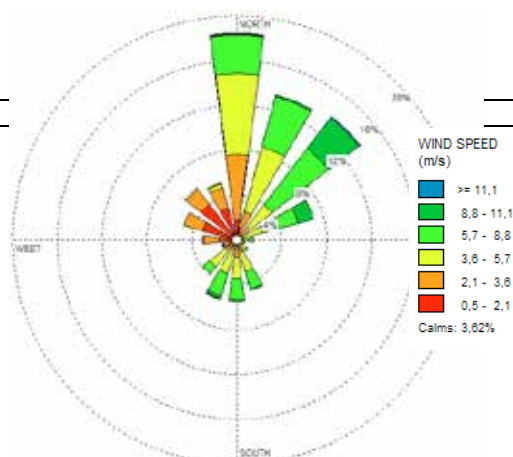


Figure 4. Wind Rose from 2015

AERMAP created a terrain model, using coordinates of the domain. A Digital Elevation Model was created also using WRPlot (see Figure 5).

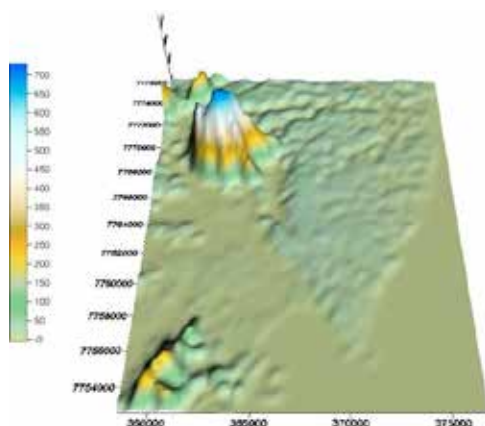


Figure 5. Digital Elevation Model

AERMOD generates a file that provides data to create a map of concentrations, based on two-peak mean. The peak was considered as 5 seconds (the period of a human breathe) and the result given per hour was transformed according to the peak concentration felt in 5 seconds. The minimum value is the 0 and the maximum is 15 OU/m³, where OU is Odorant Unit, that allows a better view of the map (see in Figure 6), identifying what concentration is felt by humans. In this case, the threshold for humans is 11,25 OU/m³.

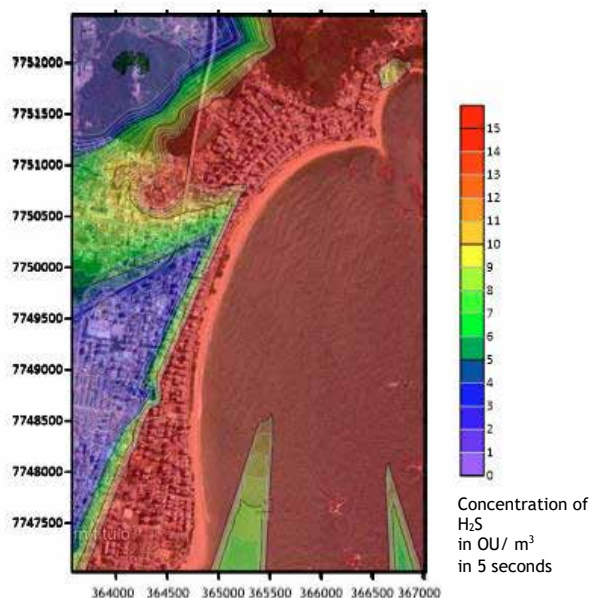


Figure 6. Concentrations of H₂S in the studied region

CONCLUSIONS

After gathering information about how the emission of H₂S from the drainage system behaves, it was possible to apply Water9 that is actually used for wastewater treatment plants.

As for the dispersion of the pollutant in the atmosphere, AERMOD facilitated the creation of a Wind Rose to consider wind direction and velocity influence - AERMET - the Digital Elevation Model - AERMAP - and the concentration of H₂S throughout the region.

It was a very worrying result, since the threshold for human perception is 11,25 OU/s and there was a huge area presenting concentration above it. The concern on this issue should be presented to the authorities as a scenario of impact on the population's health and welfare. If those illegal releases could be diminished, there would be a possibility of reducing the concentration of sulphide in the water and consequently the concentration of H₂S in the atmosphere.

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THE REVISION OF THE STANDARD EN 13725 - DETERMINATION OF ODOUR CONCENTRATION BY DYNAMIC OLFACTOMETRY AND ODOUR EMISSION RATE FROM STATIONARY BY SOURCE

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Abstract: The original Standard EN 13725, launched in 2003, established well defined procedures for odour measurement including sampling and laboratory analysis. After 16 years of its implementation, this new revision, still in draft format for enquiry comments, expanded and detailed additional points related to health and safety, sampling and emissions measurement, the use of additional reference materials and the assessment of overall uncertainty.

Keywords: odour, odor, dynamic olfactometry, human assessors, EROM.

INTRODUCTION

The standard method EN13725 *Air Quality Determination of Odor Concentration by Dynamic Olfactometry* was originally issued in 2003 by CEN - EUROPEAN COMMITTEE FOR STANDARDIZATION and has since been used in the countries of the European Community for objective determination of the odor concentration of gaseous samples emitted by a wide variety of sources, using dynamic olfactometry with human assessors. This standard has been the basis for several regulatory frameworks related to limiting odor impacts in European countries. National standards identical or largely identical to the EN13725 have been issued in Australia/New Zealand (AS/NZS 4323.3:2001), Chile (NCh3190:2010) and Colombia (NTC 5880).

After 12 years of its application, the positive vote in the 4-year CEN revision cycle confirmed the need to improve and complete this standard based on the experiences derived from its use. Several modifications were proposed and discussed for its improvement.

The purpose of this paper is to present briefly the main concepts and aspects of the standard issued in 2003 and the most relevant modifications being proposed and already consolidated in the draft developed by the Technical Committee and submitted to CEN Enquiry. By the time of this publication, the last draft for public comment was issued on June 24, 2019.

BASIC CONCEPTS

The scope of this standard includes odour measurement by delayed olfactometry, in which a sample of odorous gas is collected in a sample container, which is subsequently analysed for determining the odour concentration of that sample.

The human nose is used as the sensor to detect the odours of a gas sample. The method is based on the dilution of the sample with neutral air (without odour) for its evaluation by qualified human assessors (panel of experts). The odour concentration is determined from the number of dilutions with neutral air (without odour) that are applied to the sample until reaching a certain physiological response (threshold of detection) to the members of a panel whose olfactory capacity has been previously certified and calibrated with a reference gas (n-butanol), so that it meets the requirements of the standard. The odour concentration is measured by determining the dilution factor required to reach the detection threshold. The odour concentration at the detection threshold is, by definition, 1 ou_E/m³.

The European Odour Unit (ou_E) is the amount of odorant(s) that, when evaporated into one cubic metre of neutral gas at standard conditions, elicits a physiological response from a panel (detection threshold) equivalent to that elicited by one European Reference Odour Mass (EROM), evaporated in 1 m³ of neutral gas at standard conditions. The primary reference odorant is n-butanol (CAS-Nr. 71-36-3). The conventional quantity value for 1 EROM is 123 µg n-butanol. Evaporated in 1 m³ of neutral gas this produces a concentration of 0,040 µmol/mol or 40 ppb/v.

SAMPLING

Health and safety issues during sampling operations shall be considered, in compliance with EN 15259 and with relevant legal requirements. Requirements for working areas, working platforms and measurement sites are specified in EN 15259.

Appropriate materials shall be used for those parts of the sampling equipment that are in contact with

the odorous gas sample. The following materials are appropriate (the list is not limitative):

- PTFE (polytetrafluoroethylene),
- tetrafluoroethylene hexafluoropropylene copolymer (FEP),
- polyethyleneterephthalate1 (PET, Nalophan),
- titanium,
- aluminium (sampling hoods),
- stainless steel with suitable coating to avoid significantly reduced recovery, in particular of H_2S and reduced sulphur compounds.

Sampling methods include: lung method, direct sampling with positive pressure in the case of ducts with positive pressure and direct sampling of open air in rooms. As condensation of the collected gases affects the odour concentration, procedures are described in this standard to prevent condensation during sampling and transport of the bags to the lab. Those procedures are based in pre-diluting the samples with nitrogen or neutral gas.

The interval between sampling and analysis shall not exceed 30 hours, by convention, in order to minimize degradation of odour concentration due to diffusion and other phenomena. Care should be taken in relation to temperature, humidity and exposure to solar radiation of the samples.

Sufficient samples should be collected to ensure that the stream of odorous gases is properly quantified, taking into account the precision of the measurement method and the confidence level required to reach a valid conclusion in the study at hand. Increasing the number of replicate odour measurements reduces the measurement uncertainty. For example, Standard EN15259 requires a minimum number of $n=3$ for sampling stable emission sources.

Sampling of a point source, or ducted waste gas source can be done using a sampling train consisting of a probe, a delivery tube and an optional particulate filter before the sample collection system (Ex: lung method system). Appropriate standards should be followed when measuring the volume flow rate in order to obtain a reliable odour flow rate (ou_E/s).

Area sources should be sampled in different ways depending on if it is an active or passive area source. Area sources with an exit velocity $v > 0,008$ m/s are considered to be active area sources and are to be sampled accordingly. Area sources with lower exit speeds are considered to be passive area sources.

Samples from active area sources can be taken with the help of a sampling hood as shown in Fig.1.

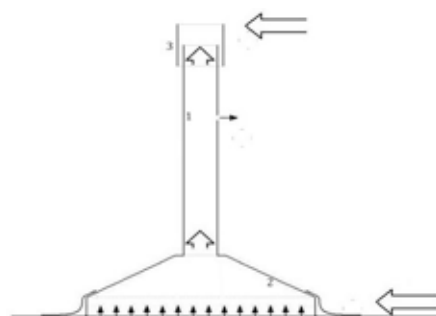


Figure 1: Sampling Hood for Active Area Source

Other ways of sampling active area sources include full and partial coverage of the area source. Depending on the size of the active area sources, the number of sampling cells varies from 9 to 30 for areas larger than 100 m^2 . Homogenous active area sources require a smaller number of sampling cells.

The specific odour emission rate (SOER) from passive area sources (without outward flow) has been measured in practice by covering a part of the surface with a ventilated hood, in order to attain a degree of standardisation of the mass transfer conditions. Different methods exist, such as flux hoods and wind tunnels. The specific odour emission rate (SOER) expressed in the measurement unit $ou_E/m^2/s$ is the combined outcome of the distinct transfer rates of each of the odorants making up the odorant gas emission. Because sampling hoods are typically used for sampling a small fraction of the total area, the sampling plan shall take into consideration that the area sampled is representative for the entire emission from the area source.



Figure 2: Example of Passive Area Source Sampling

OLFACTOMETRIC ANALYSIS

Different modes of presentation and choice can be used to obtain an individual threshold estimate using an olfactometer. In the Yes/No mode, the assessor is asked to evaluate gas presented from a specific port and to indicate if an odour is perceived (Yes/No). The assessor is aware that in some cases blanks (only neutral gas) is presented at a random sequence. In the Forced Choice Mode the assessor is presented with two or more ports, of which one presents the stimulus and the other(s)

neutral gas. The location of the stimulus in consecutive presentations is randomly distributed over the two or more ports. The assessor is asked to indicate which of the ports is the one with the stimulus.

Presentations in one dilution series shall be presented in ascending order of stimuli. The olfactometer shall be capable of producing a dilution range from less than 2^7 up to at least 2^{14} , with a range of at least 2^{13} between the maximum and minimum dilution.

Materials used in dynamic dilution systems shall not cause the recovery of known odorants to be reduced to less than 80%. The recovery and instrumental response time of olfactometers can be demonstrated with measurements of at least the following components: H_2S , n-butanol, propanoic acid, dimethyl sulphide.

To ensure correct dilution characteristics, the settings of the olfactometer shall be calibrated using a suitable tracer, and a monitor that has a proven accuracy of an order of magnitude better than the required level of accuracy for the dilution equipment. The appropriate calibration frequency shall be based on the performance history of the equipment, but shall be at least once a year.

Three types of room may be used for olfactometric analysis: stationary permanent laboratory, mobile units as those built into a truck, van or container and specially adapted rooms at or near testing sites, which have been put at the disposal of the testing team for a limited time. The working environment for assessors shall be comfortable and odourless. In order to ensure the thermal comfort of the assessors, the temperature of the olfactometry room air shall be within $\pm 2^\circ C$ around the set-point temperature. The minimum set-point temperature shall be $21^\circ C$. The relative humidity in the room shall be within the range $20\% < RH < 80\%$. Sufficient ventilation is ensured by the requirement that the CO_2 volume fraction in the olfactometry room shall be less than 0,15%.

The panel selection process include at least 12 individual threshold estimates (ITE) for the reference odorant. As a reference the primary reference odorant n-butanol or a reference material with known EROM value shall be used. The data for each assessor shall be collected in at least 3 sessions on separate days with a pause of at least one day between sessions. The geometric mean of the individual threshold estimates ITE substance, expressed in mass concentration units of the reference gas, has to fall between 0,5 times and 2 times the conventional quantity value for that reference material (for n-butanol $62 \mu g/m^3$ to $246 \mu g/m^3 \equiv 0,020 \mu mol/mol$ to $0,080 \mu mol/mol$). The antilog of the standard deviation

S_{ITE} calculated from the logarithms ($\log_{10}$) of the individual threshold estimates, expressed in mass concentration units of the reference gas, has to be less than 2,3. The panel size in any measurement of odour concentration shall be no less than four. A code of behaviour shall be followed. The test leader shall be informed about any potential toxicity of the substances that are presented to the assessors and in cases of known concentration of the components, the current occupational exposure limits for those components shall be assessed in relation with the proposed dilutions



Figure 3: Example of Olfactometer and Panel

Precision, here defined as repeatability, shall comply with $r \leq 0,477$ and accuracy shall be $A \leq 0,217$. Procedures for calculating overall uncertainty are well defined in this new version both within one laboratory and between laboratories. Uncertainty can be assessed on primary or secondary reference odorants with a known EROM value, or using a combination of a reference odorant and duplicate analysis of 'real world' odour samples using panels of different composition.

CONCLUSION

The use of the EN13725 standard for over 16 years has brought benefits in measuring something as complex as odour. The need for some improvements was identified from the experience and the regular review process has addressed these optimisation needs. This first revision contains modified and additional clauses on health and safety, sampling and emissions measurement, the use of additional reference materials and the assessment of overall uncertainty.

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**PROCEEDINGS OF THE
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Session 10
**Management of Gaseous
Emissions in Sewage
Treatment Plants**

MOLECULAR APPROACH TO EVALUATE BACTERIAL COMMUNITY FOR H₂S TREATMENT IN BIOREACTOR

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Abstract: Concern about odorant emissions from sewage treatment systems has been prominent in recent years. As a way of treating these odorant emissions, biological processes have emerged as an alternative because of their economic and environmental appeal, being one of them the biofilters, which are worldwide spread due to the low cost and operational facility. Although this treatment system is well established, there is still little knowledge about the dynamics and identification of the microbial community in these systems. Thus, the objective of this study was, therefore, to identify the microbial community responsible for the H₂S treatment in a biofiltration system, as well as its temporal and spatial dynamics. Sampling and analysis were conducted for 180 days covering different climatic seasons and spatial distributions in the filter bed. The H₂S concentration was measured with the Jerome® gas analyzer, model 631-X (Arizona Instruments). The High-throughput 16S rRNA sequencing analysis MiSeq® Illumina was used to characterize the microbial community. Removal efficiencies reached 100% for the majority of the running time at an empty bed retention time (EBRT) of the 30s, and air flow was about 720 m³.h⁻¹. It was observed a difference in the dynamics of the bacterial community before and after the startup and the main bacterial genera found were *Acidothermus*, *Telmatobacter*, *Rhizomicrobium*, *Bryobacter*, and *Methylovirgula* representing the genera that are possibly involved in the transformation of H₂S into this system.

Keywords: Wastewater odor, biofiltration, hydrogen sulfide, bacterial community, high-throughput 16S rRNA sequencing.

Introduction

In recent years, there has been a growing concern about potential impacts on public health and wellbeing due to exposure to environmental odor [BRANCHER et al., 2019]. The emission of malodorous gases by wastewater treatment systems is one of the major concerns of the people who live near these areas [ALLIEVI et al., 2017; ALFONSÍN et al., 2015]. The biological processes applied to odor treatment have been diffused in the last decades, becoming attractive treatment alternatives for odors coming from wastewater systems. Biological techniques operate under normal conditions of temperature (between 10 and 40°C) and atmospheric pressure, and are capable of treating large gas flows with low concentrations of pollutants [FULAZZAKY et al., 2014]. Besides these characteristics, biological processes have advantages such as being eco-friendly, not generating toxic byproducts, and having low operating costs and energy requirements [ALFONSÍN et al., 2015]. Biofiltration technology based on microbial degradation and assimilation is used for the removal of malodorous compounds [KITAMURA et al., 2016]. Biofilters are complex systems whose efficiency depends on many factors, such as temperature, pH, filter medium, filter bed humidity, the supply of nutrients, and many others [DELHOMÉIE; HEITZ, 2005]. The physicochemical and biological reactions happen in a fixed filtration medium, in which a biologically active layer, the biofilm, grows. In this layer, the adhered microorganisms biologically oxidize the polluting

compound, transforming it into less toxic compounds such as carbon dioxide, water, sulfate, and nitrate that are ecologically safe [FULAZZAKY et al., 2014]. But for these reactions to happen, the system needs to maintain constant performance despite fluctuating environmental conditions. Thus, this is a primary interest, but it is highly challenging because the mechanisms that drive the response of microbial communities to disturbances still have to be elucidated [CABROL et al., 2015; BRIONES et al., 2003]. In summary, the malodorous gases' treatment is intimately linked to the microorganisms that make the compounds' conversion, that is why the knowledge of the bacterial community structure present in those systems, as well as the linking of this community with the physical-chemical and environmental factors, is crucial in comprehending the processes that occur inside these systems [FERRERA; SANCHEZ, 2016]. Furthermore, knowledge of the bacterial community can be used to improve the bioaccumulation of desirable organisms, increasing the degradation of specific pollutants; it can also help in the modeling, monitoring, and operation of full-scale systems [CYDZIK-KWIATKOWSKA; ZIELIŃSKA, 2016]. Studies about microbial fauna in these systems have grown exponentially; however, further studies are still needed to understand the dynamics on molecular ecology to monitoring microbial population while H₂S is removed [LI et al., 2013]. The major studies about biofilters to H₂S removal evaluated biofilters in lab scale or pilot scale; there are a few researches about

biofiltration systems in full-scale [CHOUARI et al., 2015; OMRI et al., 2011].

In this framework, this work aimed to assess microbial community through identification of the dominant species involved in the H₂S treatment in a full-scale biofiltration system.

Material and methods

Biofiltration system

A full-scale biofiltration system was set up at the wastewater pumping station (WPS) installed in a residential zone in Florianópolis, Santa Catarina, Brazil. The odor emitted by the pumping station was not a controllable parameter and was characterized mainly by the presence of sulfide gas in concentrations that varied in the range of 0.01 and 8.88 mg H₂S.m⁻³.

The biofilter has a rectangular structure, closed with a working volume of 6 m³ and was operated in the upward flow mode and equipped with sampling points at the inlet, the middle and the outlet of the filter bed. Peat (virgin) was used as the filter material up to a height of 1 m in the filter. Regarding the empty bed retention time (EBRT), it was about 30 seconds, and the air stream was about 720 m³.h⁻¹.

The biofiltration system was irrigated in the upper area of the peat, which provided the necessary humidity for the microorganisms' growth while the peat, organic matter, provided the essential nutrients. The peat has a porosity of 60%, pH of 4-6, moisture content of 60-80% and bacterial concentration of 7×10⁸ UFC/mL.

Gas collection and analyses

The analyses carried out in this study included the H₂S concentration, at the inlet and outlet of the biofilter system. The gases were analyzed with the Hydrogen Sulfide Analyzer Jerome® (631-X - Arizona Instruments) device. Sampling was done in triplicate, and the mean of concentrations was considered for calculation of the system efficiency. The removal efficiency (RE) was calculated with Equation 1.

$$(1) \quad RE = \frac{C_{inlet} - C_{outlet}}{C_{inlet}} \times 100$$

RE, removal efficiency; C_{inlet}, H₂S inlet concentration; C_{outlet}, H₂S outlet concentration.

Microbial community analysis

Sampling

Samples pools for molecular analyses were collected with the spatial differences within the biofilter: in depth - 0.15 m (upper) and 0.75 m (bottom) - of the filter bed; at two sites at a distance of 2 m from each other and at 0.50 m from the walls of the biofilter; and seasonal

differences - winter (W) and summer (S). Winter and summer seasons were studied because the biofilter is located in an area with a subtropical climate, where the seasons are well defined, which can cause a considerable difference in the bacterial community. Different depths were studied because the difference in the bacterial community could be explained by the temperature, which is higher in the upper part of the biofilter since it receives more solar incidence than the bottom part. Besides that, the bacterial community can have differentiation due to the direction of the gas flow, since the sulfuric gas first comes into contact with the bottom of the biofilter. Information on the sampling is presented in Table 1.

The analyses for this study were carried out after two years of the startup of the biofilter operation; thus, the bacterial community was considered stable.

Samples	Code
Pool Upper / Winter	PUW
Pool Bottom / Winter	PBW
Pool Upper / Summer	PUS
Pool Bottom / Summer	PBS
Peat Filter bed	Peat

Table 1 - Information on the sampling points used to collect and display data.

DNA extraction and high-throughput 16S rRNA sequencing

Genomic DNA was extracted from a pellet of a concentrated effluent sample using the Power Soil™ DNA Isolation Kit (Mobio, laboratories, Inc., Carlsbad, CA), according to the protocol recommended by the manufacturer, with slight modifications. The quality of the extracted DNA was verified by a 1.5% agarose gel run, and after verification, the DNA was quantified by the Invitrogen QUBIT®.

All 16S rRNA reads were analyzed using the sequencing of the V3-V4 region on the extracted DNA. The universal primers 341F 5'-CCTACGGGGRSGCAGCAG-3' [WANG; QIAN, 2009] and 806R 5'-GGACTACHVGGGTWTCTAAT-3' [CAPORASO et al., 2011] were utilized since this pair has good taxonomic coverage in Bacteria and Archaea [TAKAHASHI et al., 2014]. The high-throughput sequencing was performed by the company Neopropecta Microbiome Technologies, Inc. (Florianópolis, Brazil) using the Miseq platform (Miseq™, Illumina Inc., USA). The data were processed using mothur, version 1.33.3 [SCHLOSS et al., 2009], following the MiSeq standard operating procedure (SOP) (http://www.mothur.org/wiki/MiSeq_SOP) [KOZICH et al., 2013]. Sequences were clustered into operational taxonomic units (OTUs) at 0.03 (97% similarity) and classified using SILVA Database release 119 [QUAST et al., 2013].

For the alpha diversity analysis, samples were normalized to the lowest number of sequence reads obtained. Alpha diversity was estimated using Chao1, Good's coverage, and the Shannon diversity index. The MicrobiomeAnalyst software determined a comparative analysis of different samples, and then the graphic of Principal coordinate analysis (PCoA) was conducted.

Results and Discussion

Removal efficiency of hydrogen sulfide

Figure 1 shows the H₂S inlet and outlet concentrations and the removal efficiency by the biofiltration system over 180 days of monitoring. During this period, inlet concentrations ranged from 0.011 to 8.880 mg.m⁻³ and outlet concentrations from 0.000 to 0.098 mg.m⁻³. The removal efficiency reached more than 99% over 150 days of the monitoring period.

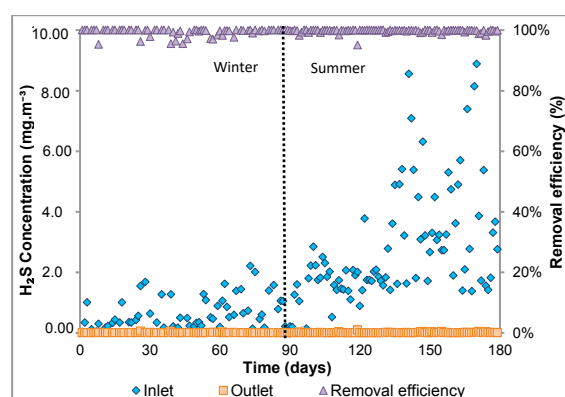


Figure 1. Biofiltration system performance during 180 days; Inlet and outlet concentrations, and removal efficiency.

The increase of temperature that occurs in the summer can favor an increase in the H₂S concentration in sewage transport pipes due to the growth of the microbial activity in anaerobiosis and consequently higher production of hydrogen sulfide. This behavior can be observed in Figure 1, where the concentrations of hydrogen sulfide at inlet during the season summer are higher than during the winter. Despite the difference in concentrations between summer and winter, it is possible to observe that the biofiltration system remained efficient and stable, even with higher H₂S concentrations.

16S rRNA sequencing of the microbial community

Diversity and estimated richness

A total of 204,581 sequences for five samples from the biofilter system were retrieved from the high-throughput 16S rRNA Illumina MiSeq™ sequencing platform, and after quality control by mothur to

remove low-quality reads (Phred <24) and chimera, a total of 129,639 high-quality sequences remained for further analysis.

Among the samples evaluated, the sample that showed the highest estimated richness (Chao1 index) was PUS (from the upper part of the biofilter collected during the summer period), and the fewest Chao1 was Peat, as shown in Table 2. This result comes from what we know about the influence of temperature on the richness of a bacterial community. The low Chao1 index found in the peat may have been due to its chemical and biological composition. Peat is a type of humic coal resulting from accumulations of uncarbonized plants and formed mainly by Sphagnum (sphagnum, group of mosses). In summary, the bacterial community estimated richness illustrated showed values not so distinct for the samples and, in general, the highest values were to samples the upper of the filter.

Samples	Raw reads	Effective	Norm ^(*) Reads	OTUs	Norm ^(*) Chao1	Norm ^(*) Shannon	Norm ^(*) Good's (%)
Peat	61928	41387	1530	173	174	3.55	99.98
PUW	36239	22945	1530	418	420	4.89	99.90
PBW	23806	15304	1530	393	395	4.86	99.98
PUS	46446	27246	1530	426	428	4.92	99.98
PBS	36162	22757	1530	354	356	4.57	99.92

* Normalized

Table 2. Number of sequences analyzed, OTU richness (Chao1, ACE), Shannon diversity index, and Good's coverage obtained.

According to the Shannon index, the bacterial diversity didn't present an apparent variation, indicating certain homogeneity in the samples. However, the highest Shannon index (4.92) and the fewest (3.55) was for the PUS and Peat samples, respectively, in the same way as for the Chao1 index. Together with the results of H₂S removal, we can infer that the diversity of the bacterial community remained stable regardless of the season. This stability is an important result because when we look at Figure 3, we notice the apparent difference in the concentrations of H₂S between winter and summer. The concentrations of H₂S at the inlet of the system during summer season reached values up to 4 times higher than the inlet concentrations during the winter season, and yet the system remained stable and efficiently above 99%.

Principal coordinates analysis (PCoA), based on the Bray-Curtis and Jaccard distance metric, were applied to evaluate the patterns of similarities of the samples and how the samples group according to metadata information (Figure 2).

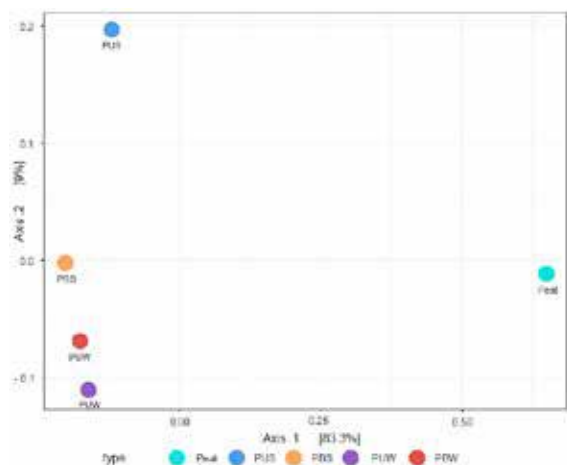


Figure 2. Principal coordinate analysis (PCoA) plot using Bray-Curtis distances.

The results of PCoA showed a pattern of distribution according to the season of the year. It was also possible to observe that the winter samples are closer to each other, which may indicate that the diversity of the bacterial community in this period is smaller due to the influence of temperature. Moreover, the difference of the Peat sample about the other samples was evidenced.

Spatial and temporal bacterial community structure

Phylum and genus were used to illustrate the spatial and temporal variation of the diversity of the bacterial community in the biofilter tested. The relative abundance of the selected taxa for all samples is depicted in Figure 3 and Figure 4.

At the phylum level, sequences derived from all samples were distributed among 11 distinct phyla and can be observed in Figure 3. The most abundant phyla in all samples were Proteobacteria, Acidobacteria, Bacteroidetes, Actinobacteria, Candidate_division_TM7, Verrucomicrobia, and Nitrospirae.

At the genus level, *Acidothermus*, *Telmatobacter*, *Rhizomicrobium*, *Bryobacter*, and *Methylovirgula* were the most abundant genera in the samples availed, except for Peat sample, which showed different structural diversity than the others, with the predominance of *Chitinophaga* genus. The relative abundance on the genus level is shown in Figure 4.

The genus *Chitinophaga* was the most abundant in the peat sample (56.73%) after the system startup, the relative abundance of this genus decreased dramatically to 0%. The genus *Chitinophaga* belongs to phylum Bacteroidetes. This genus is frequently found in soils where dead fungal mycelia are being actively decomposed they are capable of degrading chitin, fungal cell wall constituent (Larsbrink et al., 2017; Weon et al., 2009).

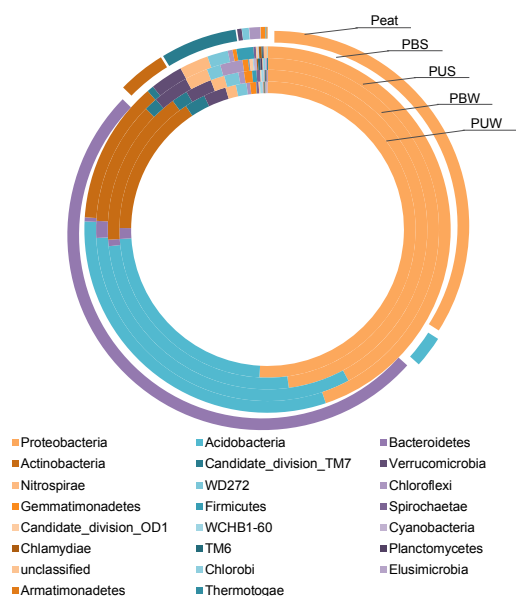


Figure 3. Relative abundance at the phylum level found in the dataset of the biofilter.

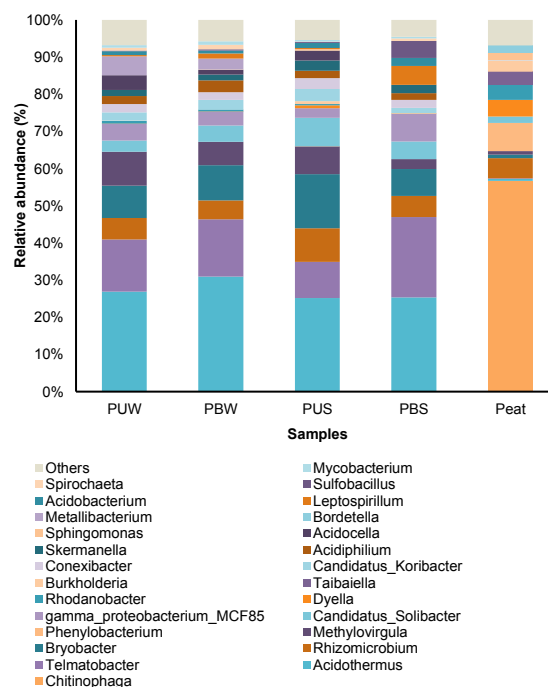


Figure 4 - Relative abundance at the genus level found in the dataset of the biofilter.

Acidothermus was the most representative genre in the system. Belonging to the group of gram-negative bacteria, it is considered obligate aerobes and grows in thermophilic temperatures (Mohagheghi et al., 1986). In the virgin peat, this genus was found with 0.50% of relative abundance; however, after the H₂S injection, the relative abundance increased reaching values up to 30% remaining stable over time. In this way, we can

infer that this genus played a key role in the decomposition of H₂S.

Telmatobacter was the second most abundant genus, as can be observed in Fig. 4. This genus was also not identified in the virgin peat sample at significant values, but when the biofiltration system came into operation, the relative abundance increase in a range from 9% to 19%, depending on the seasonal and spatial distribution. The genus *Telmatobacter* isn't widely studied but is commonly found in soils, and it's related to nutrients cycle (Li et al., 2013). Pankratov et al. (2012) classify this genus as being gram-negative, facultatively anaerobic chemoorganotrophs, which grow in acidophilic and mesophilic media.

Concerning the *Rhizomicrobium* was the only genus that maintained stable since before the system startup until the H₂S injection, i.e., wasn't affected by H₂S over time. However, the genus *Bryobacter* showed structural variation from the injection of sulfuric gas. At the peat sample, the relative abundance of this genus was about 1%, after the system startup, the relative abundance had an increase, reaching values between 6,65% to 14,48%. The major value was found in the PUS sample. The highest values in the PUS sample indicate that the genus *Bryobacter* was affected by temperature, being favored at higher temperatures. Bacteria of this genus are strictly aerobic, gram-negative, acid tolerant, and mesophilic and are found in different soil types (Kulichevskaya et al., 2010). The same behavior was found for the genus *Methylovirgula*.

The stability of the bacterial community is also observed in the relative abundance of microorganisms at the phylum and genus levels, Figures 3 and 4, respectively. In spite of the temperature difference between the seasons and also the concentration of H₂S at the inlet, the bacterial community did not have a significant change, and the same genera appeared in all the samples. Thus, we can conclude the *Acidothermus*, *Telmatobacter*, *Bryobacter*, *Methylovirgula*, and *Candidatus_Solibacter* were genera linked with sulfide gas treatment in this biofiltration system since when the system came into operation, the bacterial community changed completely with the predominance of these genera.

Conclusions

In this study we can conclude that the temperature variation in the environment interferes with the H₂S concentrations entering the system due to the degradation of the faster organic matter in the sewage pipes, however, despite the significant difference in the inlet concentration, the system operated efficiently above 99% for most of the monitoring period.

The bacterial community changed drastically after system startup. This microbial differentiation

allows to infer that the microorganisms found in the seasonal samples may be related to the degradation of hydrogen sulphide, once the molecular biology analysis was performed after the biofilter was operating for two years.

Molecular biology analyzes bring us a new look within the bioreactors for the treatment of odors coming from a sewage plant, since they can help us accumulate desirable microorganisms, to increase the degradation of pollutants without losing efficiency. Besides, the knowledge of microorganisms can help in the modeling and operation of real-scale bioreactors, which are still scarcely explored in terms of research.

Acknowledgements

The authors acknowledge the financial support of Coordination of Improvement of Higher Education Personnel of Brazil (CAPES) and Multiágua Environmental Engineering Company and Wastewater Company (CASAN) for giving the space for installing the biofilter.

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ASSESSMENT OF H₂S EMISSION AND DISPERSION: A CASE STUDY IN A FULL-SCALE ANAEROBIC-BASED SEWAGE TREATMENT PLANT IN BRAZIL

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Abstract: Anaerobic-based sewage treatment processes lead to formation of odorous compounds, as hydrogen sulfide (H₂S), which can cause nuisance and impact the health and nearby residents. Mathematical models can be used for estimating emissions of gases to the atmosphere from specific units within sewage treatment plants (STP). Dispersion models are the commonly used to evaluate the concentration of volatile pollutants near the emitting sources. In this work, mathematical models, based on AP-42, were applied to estimate hourly emissions of H₂S in two specific units (post-anaerobic reactor flow distribution units and trickling filters) in an STP in Minas Gerais (Brazil) in July 2018, based on H₂S concentrations in the liquid phase. CALPUFF Modeling System was used to investigate H₂S dispersion and to estimate its concentration in the neighborhood. For the scenario with the highest one-hour average concentrations, the limit value of H₂S perception (5 ppb) reached 6 km south/southwest from the STP, according to wind direction. The highest hourly average concentration obtained with the model was 1.68 ppm. The scenario considering the monthly average concentration, the maximum value of H₂S obtained was 0.04 ppm. Values of 5 ppb could be observed at a distance of 4.5 km to the south and east of the STP, but such exposure occurred in a low concentration, which does not lead to health risks. These results show the importance of controlling odorous gas emissions, by applying corrective actions to reduce their impact in communities that live near STPs.

Keywords: hydrogen sulfide, sewage treatment plants, emission, dispersion, CALPUFF.

INTRODUCTION

Projects related to sewage treatment plants (STP) face the need to evaluate their odorant gaseous emissions, in order to reduce the possible impacts on the environment and the nearby community. The emission of odorous gases can have a real impact on people and their well-being.

In order to estimate the emission of odorant gases, one of the most used approaches refers to the use of mathematical models, as AP-42. This estimation is based on several equations, which consider aspects relate to the concentration of the compound in the liquid phase, wind speed and the type of treatment unit, for example.

Once emitted, the odorant gases begin to disperse through the atmosphere, reaching different regions. The atmospheric dispersion modeling of pollutants is a tool that allows to investigate the possible areas most affected by these emissions. Among the existing mathematical models, the California Puff Model (CALPUFF) stands out as the US EPA regulatory model recommended for the odorant gases modeling (SCIRE, 2000).

This work presents an estimative of hydrogen sulfide (H₂S) emissions in two specific units (post-anaerobic reactor flow distribution units and trickling filters) in an STP in Minas Gerais (Brazil) for July 2018. After, the CALPUFF Modeling System was used to investigate H₂S dispersion and to estimate its concentration in the neighborhood.

METHODS

The estimative of H₂S emissions were carried out for July 2018, when campaigns were conducted to collect samples to determine the concentration of H₂S in the liquid phase in post-anaerobic reactor flow distribution units.

Each module of the secondary effluent treatment system of the STP evaluated is composed by four UASB reactors, one Post-UASB Flow Distribution Unit (CDV 4), two trickling filters (FBP) and two decanters. In July 2018, two of the three modules were in operation, with each module operating with only three of the four UASB reactors, according to Figure 1. From the sulfide concentration values in post-UASB reactors it was possible to estimate the H₂S emissions in the two post-UASB flow distribution units (CDV 4-1 and CDV 4-2) and in four trickling filter (FBP 1 and 4). These two units generally present the highest emissions in STP with similar operating units.

In the period evaluated, each flow distribution unit received the effluent from three UASB reactors. In each CDV, the effluent of each UASB reactor arrives in an antechamber of 1 m² of area, pouring in a fall of 0.543 m. Then, the effluent from UASB 1 flows to a second spillway with a 0.233 m drop. The effluents from UASB 3 and 4 are mixed in the CDV and then are directed to a spillway with a drop of 0.233 m. After the second spillway, the effluent from UASB 1 is directed to FBP 1, while the effluent from UASB 3 and 4 are directed to FBP 2. The second operating

module, shown in the right side of Figure 1, follows the same flow scheme of the first module (left side).

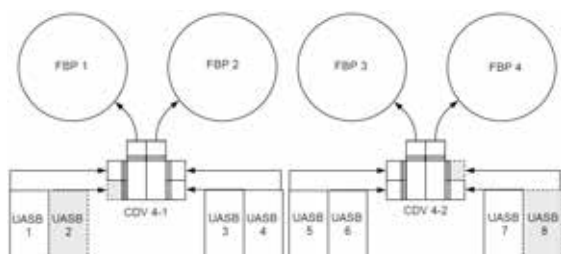


Figure 1 - Simplified schematic of the first module (left) and second module (right) of the STP. The UASB reactors 2 and 8 were not operating.

The average flow of July from 2013 to 2017, $0.330 \text{ m}^3 \text{ s}^{-1}$, was used to estimate the emissions. The effluent samples and the dissolved sulfide analysis were performed by the Companhia de Saneamento de Minas Gerais (COPASA). The samples were collected in the exit line of the six reactors in operation (UASB 1 and UASB 3 to 7) in five days of 2018: 06/29; 07/05; 07/12; 07/19; and 07/26. The methodology used to determine the sulfide concentration was from Spectroquant® Sulfide Test, which is analogous to EPA 376.2, APHA 4500-S2-D, ISO 10530, and DIN 38405-26.

Table 1 shows the sulfide concentration values (mg L^{-1}) found at the exit of each reactor. These values are used to estimate the H_2S emission. Each H_2S concentration value was used to estimate H_2S emissions in the week of collection.

Table 1: Sulfide concentration [mg L^{-1}] pos-UASB (liquid phase).

Date	UASB 1	UASB 3	UASB 4	UASB 5	UASB 6	UASB 7
06/29	2.96	2.07	3.18	3.53	2.21	2.66
07/05	1.83	0.71	0.63	1.25	0.84	0.72
07/12	0.77	0.72	0.74	0.59	0.79	0.66
07/19	1.53	3.30	9.96	2.79	2.75	8.92
07/26	3.94	3.41	4.14	1.52	3.29	1.50

The emission estimative used emission factors and equations suggested in US EPA Compilation of Air Emissions Factors AP-42 (US EPA, 1998). In the CDV, the emission estimative was performed based on weir. The emissions in the trickling filters were calculated considering the filter distributors, as weir, and by the biological filter itself, calculated as a biological system with natural aeration.

For the dispersion analysis, CALPUFF Modeling System was used to investigate one-month H_2S dispersion, where meteorological data monitored by an Automatic Weather Station located about 1 km far from the STP were used as surface data. The vertical meteorological data was obtained from WRF model.

FINDINGS AND ARGUMENT

Figure 2 shows the estimated daily-average emissions for each CDV and trickling filter. The highest emissions occurred 07/19 and 07/25, when highest values of sulfide concentration in the liquid phase pos-UASB was observed. Between the days 07/26 and 07/31, CDV 4-1 showed higher emissions than CDV 4-2, also due to higher liquid sulfide concentrations. This higher concentration also reflected in the results found for FBP 2.

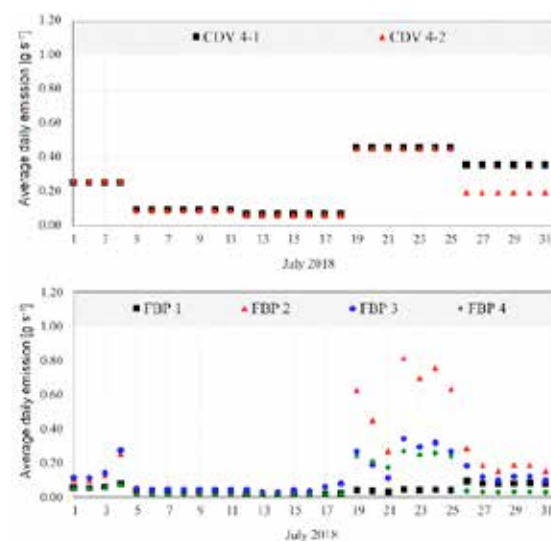


Figure 2 - Average daily emission of H_2S for CDV 4-1, CDV 4-2, FBP 1, FBP 2, FBP 3 and FBP 4.

The maps of H_2S dispersion scenarios from the STP are shown in Figures 3 to 7. The threshold of perceived odor varies depending on the individual. The minimum H_2S concentration that results in its perception of odor is around 0.005 ppm (5.0 ppb) (WHO, 2003).

For the scenario with the one-hour highest average concentrations (Figure 3), it was observed that the H_2S limit value of perception can reach 6 km south/southwest of STP, located in the north of the city. The highest modeled hourly average was 1.68 ppm.

The EPA defines 0.75 ppm as the 10-minute acute exposure limit (AEGL1), without irreversible harmful effects being observed (US EPA, 2019). Figure 4 shows the maximum concentration values found for the 10-minute peaks. The odor perception limit (0.005 ppm) reached 12.2 km in the southwest part of the city from the STP. However, values above 0.75 ppm were only observed inside the STP and its immediate surroundings (up to 625 m), with the maximum H_2S concentration reaching 2.4 ppm.

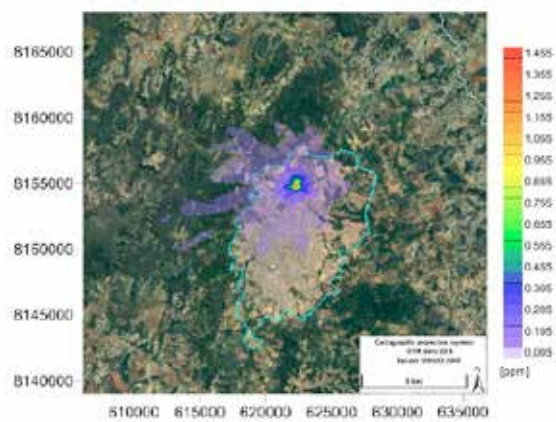


Figure 3 - Scenario of H₂S dispersion of the highest hourly means. The blue line represents the urban area.

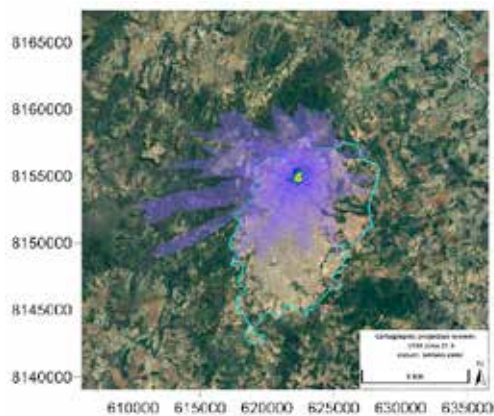


Figure 4 - Scenario of H₂S dispersion for 10-minute peaks. The blue line represents the urban area.

It was also performed a scenario considering a peak of exposure of 10 seconds, according to Figure 5. The highest H₂S averages calculated were 5.44 ppm in the STP. Concentrations of 0.005 ppm could be observed 15 km northwest of the STP and 21 km to the east.

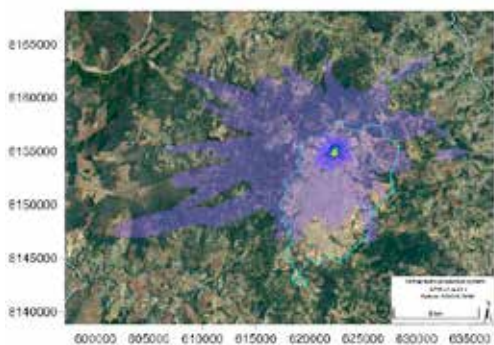


Figure 5 - Scenario of H₂S dispersion for 10-seconds peaks. The blue line represents the urban area.

Figure 6 shows the highest 24-hour averages. The minimum H₂S concentration for perception were observed 8 km south of STP. The highest average found was 0.123 ppm.

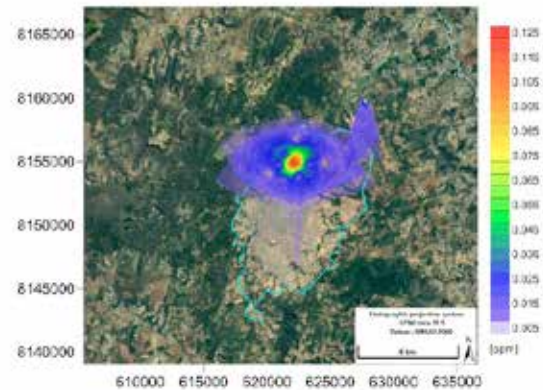


Figure 6 - Scenario of H₂S dispersion for the highest daily averages. The blue line represents the urban area.

The scenario considering the monthly average is shown in Figure 7. The highest H₂S value found was 0.04 ppm. Values of 0.005 ppm were observed 4.5 km to the south and east of the STP.

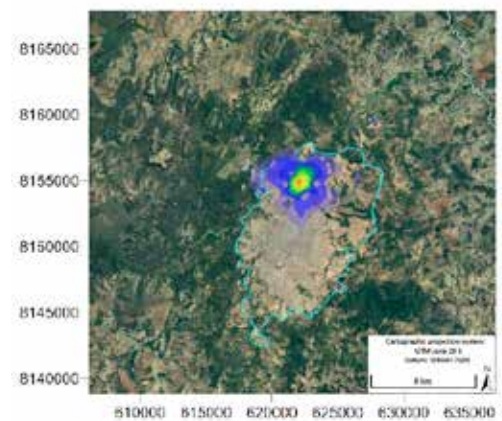


Figure 7 - Scenario H₂S dispersion for the monthly average. The blue line represents the outline of the urban area.

CONCLUSIONS

Overall, from the modeling it was possible to observe that the highest concentrations of H₂S occurred inside the STP. On the other hand, the minimum H₂S concentration so that the odor caused by this compound begins to be perceived (0.005 ppm) can lead to the annoyance of the surrounding populations, especially those in the neighborhoods surrounding the STP. However, such exposure occurs in low concentration, which does not lead to health risks.

ACKNOWLEDGEMENTS

Authors acknowledge CAPES and COPASA.

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BIOGAS UPGRADING INTO BIOMETHANE IN THE AGROINDUSTRY AND SANITATION SECTORS

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Abstract: Biogas is a methane-rich gas that is produced during anaerobic treatment of waste streams (methanization), and can be converted in biomethane, a gas with more than 96.5% of methane in its composition. This study aims to discuss and compare the main characteristics of the current technologies and methods for biogas upgrading in agroindustry and sanitation sectors in Brazil. Firstly, a table with the features, advantages and disadvantages of the selected methods was organized. Secondly, a quali-quantitative table was constructed, considering the following parameters: efficiency, costs, sustainability, operational complexity and developing stage of the technique. Each of these parameters was evaluated in numerous studies and the performance of each technique was accessed to define if the parameter was less or more favorable for biogas upgrading. Afterwards, the relevant techniques to Brazil were selected considering the main necessary characteristics to its reality, which are costs, operational complexity and developing stage of the technique. The results pointed to the physical absorption and the membrane contactors that better fit to Brazilian conditions.

Keywords: anaerobic, energy, methane, methanization, waste treatment.

INTRODUCTION

Biogas is a methane-rich gas that is produced during anaerobic treatment of waste streams (methanization or digestion). This process is widely applicable in developing countries since it is a simple operational technique, which requires low capital expenditure. Additionally, the Brazilian tropical climate helps to enhance the activity of microorganisms involved in the methanization. The biogas can be used as energy, supplying partially or totally the energy demanded by the waste stream treatment, resulting in a more sustainable cycle. The biogas has a variable composition since it depends on the waste stream characteristics and operational parameters of the digester. Usually, it contains 60% to 65% of methane (CH₄) and 35% to 40% of carbon dioxide (CO₂). In lower proportion, it also contains hydrogen sulfide (H₂S), nitrogen (N₂), and hydrogen (H₂). Besides that, there are also traces gases as oxygen (O₂), carbon monoxide (CO), ammonia (NH₃), argon (Ar), and volatile organic compounds (VOCs) (NOYOLA; MORGAN-SAGASTUME; LÓPEZ-HERNÁNDEZ, 2006). Most of these components decrease the calorific power of biomethane and are harmful to heat and power engines, resulting in corrosion, abrasion and even explosion (RYCKEBOSCH; DROUILLON; VERVAEREN, 2011). Moreover, health risks are associated with the exposure of humans to H₂S and NH₃ (e.g., tearing of the eyes and even death), as well as environmental problems like acid rain (MAINIER, 2007; ABATZOGLOU, 2009).

The CH₄ is a greenhouse gas that has a high global warming potential (PACHAURI et al., 2014). Therefore, when the energy use of biogas is not proposed during anaerobic treatment of waste

streams, it must be flared converting the CH₄ into CO₂. Biogas also can be converted in biomethane, that is a gas with more than 96.5% in CH₄. Since the biomethane has high calorific power, it can be widely used as an energy source, replacing natural gas, vehicular fuels and in industrial fuels (SUN et al., 2015). Despite the numerous benefits of using biomethane as an energy source, this technique is still underdeveloped in Brazil. This fact is due to economic barriers, lack of technology in the biogas plants, low operational control of the processes, and obstacles to legalizing the plants as energy producers, since usually the properly technology is not chosen (MINAS GERAIS, 2015). For this reason, it is necessary to study the current methods of biogas upgrading that fits better to the Brazilian reality. In this sense, this study aims to discuss and compare the main characteristics of the current technologies and methods for biogas upgrading in agroindustry and sanitation sectors in Brazil.

METHODS

In this study, a range of biogas upgrading technologies was studied. The physical techniques studied were: physical absorption (by water or organic solvents), adsorption, membrane contactors and cryogenic separation. Chemical absorption was the only chemical method considered in the literature review. Between the biological techniques, chemoautotrophic and photosynthetic technologies were studied. The methods were subdivided into three parts. Initially, the features, advantages and disadvantages of each biogas upgrading techniques were accessed. Therefore, a quali-quantitative

table was systematized considering the parameters and the classification for each technology. Each of these parameters was evaluated in some studies: Allegue (2012), Bahr (2013), Kao (2012), Luo (2013), Luo (2012), Muñoz (2015), Noyola (2006), Ryckebosch (2011), Sun (2015) and Tippayawong (2010). Therefore an average of the performance of each technique was calculated, analyzing how favorable a certain parameter was for the upgrading technology. Finally, the relevant methods to Brazil were selected considering the principal features to its reality: low cost, low operational complexity and advanced stage of technology development.

FINDINGS AND ARGUMENT

Table 1 presents the quali-quantitative parameters used to classify the technologies based on the referenced studies. Table 2 presents the quali-quantitative analysis of these techniques.

Considering the principal features to Brazilian reality, physical absorption and membrane contactors showed to be the better techniques among the studied. Firstly, the physical absorption is a technology in which the undesirable gases in biogas are transferred to a liquid phase by contact with water or an organic solvent. This process occurs inside a scrubber while the gas and the solvent enter in countercurrent. The water-based method is highly efficient, easily operated, low costly and there is no need for chemicals. On the other hand, it is not efficient in the H_2S abatement, it is highly water consuming and has a high footprint.

Secondly, the membrane contactors operate at a molecular scale and require a module of hollow fibers membranes. The biogas enters inside the hollow fibers and the undesirable gases (e.g., CO_2) pass through outside due to the molecular size, while the CH_4 is retained. This technique has a lot of advantages: low cost, energy-efficient and easy to operate. However, as the physical absorption, the H_2S must be previously removed.

CONCLUSIONS

Cost, operational complexity and developing stage of the techniques are the main barriers related to the implementation of biogas upgrading technologies in Brazil. The methods that better fit to the Brazilian reality were the physical absorption by water and the membrane contactors since both methods showed more favorable to these parameters.

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Table 1. Quali-quantitative parameters to classify the biogas upgrading technologies.

Classification	Parameters									
	Efficiency				Sustainability				Operational complexity*	Developing stage of the technique*
	CH ₄ concentration in biomethane (%v/v)	CH ₄ losses (%)	CO ₂ and H ₂ S removal from biogas (%)*	Energy efficiency (%)	Energy demand*	Water demand*	Waste streams production*	Costs (capital and operational)*		
●	>=96.5	<=2	low	>=90.9	low	low	low	low	low	low
●	90 a 96.5	2 a 7	medium	89 e 90.9	medium	medium	medium	medium	medium	medium
●	<=90	>=7	high	<=89	high	high	high	high	high	high

(*) Parameters were calculated by an average of qualitative information obtained in the articles: low = 1, medium = 2, high = 3.

Table 2. Quali-quantitative classification of the biogas upgrading technologies.

Method	Parameters									
	Efficiency				Sustainability				Operational complexity	Developing stage of the technique
	CH ₄ concentration in biomethane (%v/v)	CH ₄ losses (%)	CO ₂ and H ₂ S removal from biogas (%)	Energy efficiency (%)	Energy demand	Water demand	Waste streams production	Costs (capital and operational)		
Physical absorption	●	●	●	●	●	●	●	●	●	●
Physical absorption (organic solvents)	●	●	●	●	●	●	●	●	●	●
Adsorption	●	●	●	●	●	●	●	●	●	●
Membrane contactors	●	●	●	●	●	-	●	●	●	●
Cryogenic separation	●	●	●	●	●	●	●	●	●	●
Chemical absorption	●	●	●	●	●	●	●	●	●	●
Chemoautotrophic	●	-	●	-	●	●	●	●	●	●
Photosynthetic	●	-	●	-	●	●	●	-	●	●

ATMOSPHERIC DISPERSION OF HYDROGEN SULPHIDE FROM A WASTEWATER TREATMENT PLANT

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Abstract: The objective of this study was to evaluate the atmospheric dispersion of hydrogen sulfide from a WWTP located in the Metropolitan Area of Belo Horizonte, Minas Gerais, Brazil. The H₂S emission rates were calculated using AP-42 (USEPA) methodology, in a previous study carried out during 2017. Based on these data, associated with meteorological and topography information of the study region, the atmospheric dispersion of the emitted H₂S was evaluated for the same days that emissions rates were estimated, using the CALPUFF model (California Puff Modell) in a 50x50 km modeling domain. It was verified that the relief and the winds velocity and direction had large influence on the dispersion and concentration of H₂S for the different modeled scenarios. For one-hour exposure averages, the perception limit of hydrogen sulfide (0.0047 ppm) was observed at 5.15 km far from the WWTP. When 10 minutes exposure averages scenario were considered, maximum concentration of 0.069 ppm were observed respectively for each one of the campaigns performed. This verified concentration is lower than the acute exposure limit for 10 minutes defined by the USEPA (0.75 ppm). The CALPUFF use associated with emission rates estimation based on the AP-42 methodology was an important tool for the evaluation of the H₂S influence in populations surrounding Wastewater Treatment Plants.

Keywords: Hydrogen sulphide, Wastewater Treatment Plant, atmospheric dispersion, CALPUFF

INTRODUCTION

The accelerated and usually unplanned growth of cities has making urban populations increasingly inhabit areas closer to Wastewater Treatment Plants (WWTP). Due to the effluents and the treatment processes characteristics, these plants are responsible for odor emissions, which are mainly caused by hydrogen sulfide (H₂S), a compound that has a particular characteristic of rotten egg smell. This compound can cause, besides environmental impacts, damage to human health, such as nausea, loss of appetite, breathing problems, and even death (VINCENT, 2001). As consequence, legal and administrative complaints by the WWTP surrounding populations have grown over the last years (KIM *et al.*, 2014; ESTRADA *et al.*, 2015).

In order to evaluate the reach and influence of odor compounds emitted by WWTP in receptors, dispersion studies have large importance. This dispersion can be evaluated through different methods, such as field experiments, wind tunnel

and mathematical models. The last ones are alternatives to high costs of wind tunnels and difficult in variables control in filed experiments (MELO, 2011).

The US EPA recommends a list of dispersion models, which are based on solution of mathematical equations, such as AERMOD, CALPUFF, BLP and CALINE 3 (USEPA, 2017) of which the two firsts are the most used (GAO, 2014). AERMOD model is most indicated for dispersion evaluation in areas smaller than 50km, while CALPUFF is more recommended for long-range transport modeling since it is able to handle complex three dimension wind fields' regimes and variable reliefs (SILVA *et al.*, 2014). Although, studies carried out by Silva *et al.* (2014) and by Diosey *et al.* (2002) have shown a more conservative pattern for CALPUFF, even for smaller distances.

CALPUFF (Californian Meteorological Model) is a non-state Gaussian model of multipollutant

transport and dispersion in atmosphere multilayer. It is composed by three main components: CALMET, CALPUFF and CALPOST (GAO, 2014).

In the light of WWTPs importance for sewage treatment and the possible damage caused by odor released from these facilities, the objective of this study was to evaluate the atmospheric dispersion of hydrogen sulfide from a WWTP located in the Metropolitan Area of Belo Horizonte, Brazil.

METHODS

The study area is a Wastewater Treatment Plant located in the North region of Belo Horizonte City, Minas Gerais, Brazil. With 65.5 hectares of area, the facility treats 1.8 m³/s of sewage, through screens, UASB reactors (Upflow Anaerobic Sludge Blanket), trickling filters and settling tanks (COPASA, 2017).

The H₂S emission rates were calculated using AP-42 (US EPA) methodology in a previous study (MIRANDA, 2017), based on a campaign carried out in May 2017.

The H₂S dispersion was modelled in CALPUFF, version 6.0, in a 50x50 km modeling domain, based on surface parameters (land use and relief); meteorological parameters for Pampulha's and Cercadinho's stations (wind velocity and direction, atmospheric pressure, radiation, humidity, air temperature and cloud cover); and H₂S emission rated for the different units in the WWTP. More details can be verified in Miranda (2017).

Two scenarios were evaluated: one hour exposure and 10 minutes exposure. The human perception minimum concentration for H₂S (0.0047ppm) (SANTOS, 2007) and the acute exposure limit for 10 minutes (0.75ppm) defined by the US EPA (2010) were evaluated, based on wind speed and direction, for the two meteorological station - Pampulha's and Cercadinho's.

FINDINGS AND ARGUMENT

The dispersion scenarios of higher concentrations of H₂S to one-hour and 10 minute exposure are shown in Figures 1 and 2, respectively. The wind roses for Pampulha's and Cercadinho's meteorological Stations are shown in Figures 3 and 4, respectively.

The higher concentrations of H₂S, for both scenarios, were observed in Southwest direction, what is related to the smaller predominance and velocity of wind in this direction.

For the one-hour higher concentrations scenario, the minimum concentration of H₂S that is perceived by human smell (0.0047 ppm) was

observed at 5.15 km far from the WWTP. The higher concentration observed for this scenario was 0.049 ppm, for points inside the facility.

For the 10 minutes average scenario, the higher concentration was 0.069 ppm, inside the plant, which is smaller than the acute exposure limit of 0.75 ppm established by the US EPA, not representing though, risk for human health. For this scenario, the concentration of 0.0047 ppm was observed at 5.42 km from the center of the WWTP.

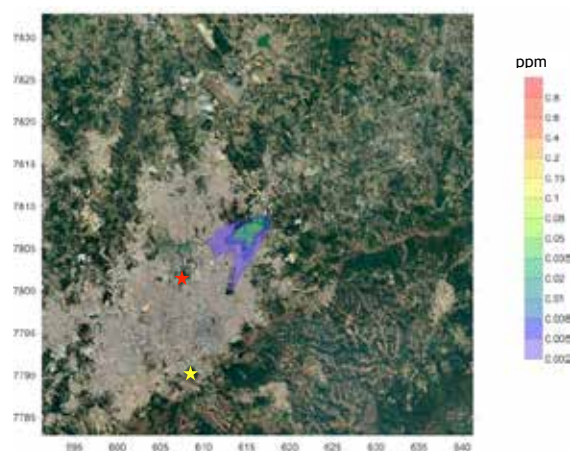


Figure 1. One-hour average exposure scenario.
Red star - Pampulha's Station; Yellow star - Cercadinho's Station

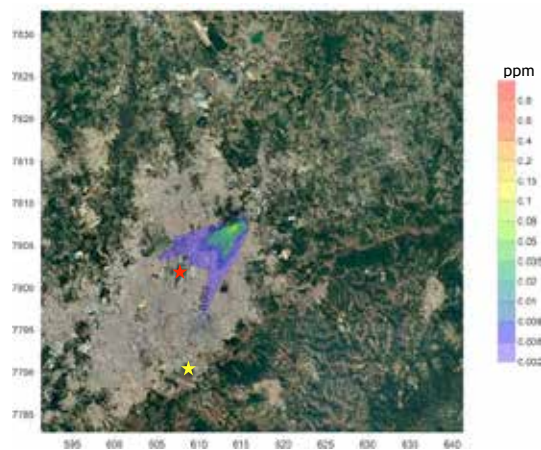


Figure 2. 10 minutes exposure scenario.
Red star - Pampulha's Station; Yellow star - Cercadinho's Station

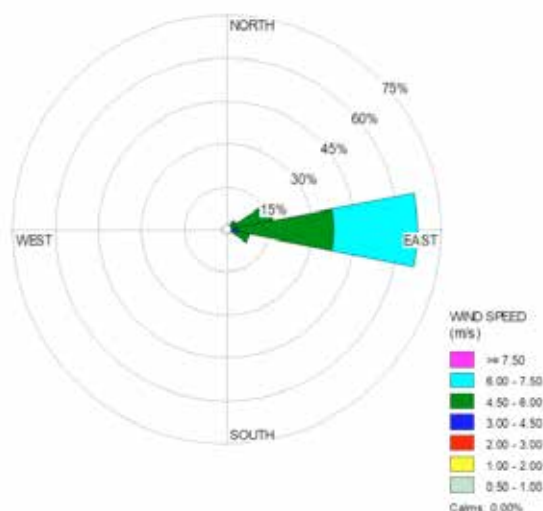


Figure 3. Pampulha's meteorological station wind rose for 05/19/2017.

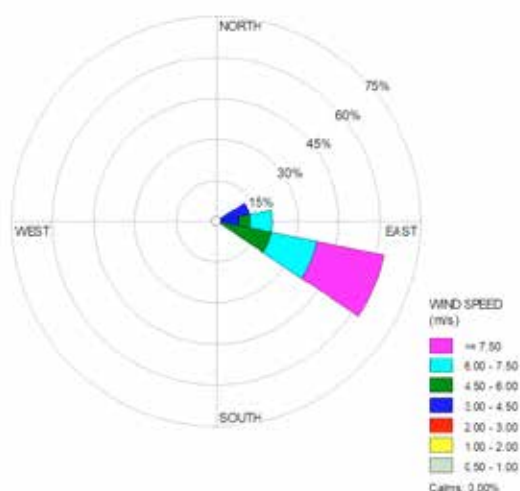


Figure 4. Cercadinho's meteorological station wind rose for 05/19/2017.

CONCLUSIONS

The developed study showed that the use of CALPUFF associated with emission rates estimation based on the AP-42 methodology is an important tool for the evaluation of the H_2S influence in populations surrounding Wastewater Treatment Plants.

The both analyzed scenarios, one-hour higher concentrations and 10 minutes average exposure, indicated that the H_2S smell can be observed over than 5 km far from the facility. However, the acute exposure concentration was not observed,

which do not represent risk for the surrounding population, at the studied day and at the meteorological specific conditions. For a more conclusive study, the modelling should be carried out during a longer period, mainly in winter, where the pollutant dispersion conditions are worse in the studied area.

ACKNOWLEDGEMENT

The authors acknowledge the National Council of Technological and Scientific Development (CNPq), the Research Support Foundation of the State of Minas Gerais (FAPEMIG), the Coordination for the Improvement of Higher Education Personnel (CAPES) and the Minas Gerais Sanitation Company (COPASA) for the support.

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ESTIMATION OF HYDROGEN SULPHIDE EMISSION RATES FROM A SEWAGE TREATMENT PLANT IN BELO HORIZONTE

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Abstract:

The aim of the present study was to estimate the emission rates of hydrogen sulfide from different units of a Sewage Treatment Plant (STP) located in the metropolitan region of Belo Horizonte. The concentrations of H₂S in the liquid and gas phases were determined in a campaign carried out during on May 2017, for the different units of the STP, among them: inflow box, post-screening, flow distribution box for the UASB (Upflow Anaerobic Sludge Blanket), UASB reactors, post-UASB collection box, trickling filters and secondary clarifiers. Based on the H₂S concentration in the liquid phase, the methodology established by the AP-42 (US EPA) was used to determine the odoriferous compound emissions rates for each of those STP analyzed units. Among the evaluated units, the post-UASB collection box was the one with the highest emission rate (3.45 g/s) followed by post-screening and trickling filters. The inflow box and the secondary clarifiers were the points of smaller emission, once they are systems with less turbulence. The H₂S emission rate for the whole STP were 7.5 g/s. The results obtained in the present study demonstrates the importance of evaluating H₂S emissions by of each unit and its influence on the total emission of the STP, what can support decision making in regards to emission control, besides subsidizing pollutant dispersion models.

Keywords: Sewage Treatment Plant, Hydrogen Sulphide, emission rate, AP-42.

INTRODUCTION

Sewage Treatment Plants (STP) release different types of odorant compounds, such as ammonia, acetones, acetic acids, hydrogen sulphide, methyl mercaptan, butyric acid and methylamine (LEWKOWSKA *et al.*, 2016). Among them, hydrogen sulphide (H₂S) corresponds for until 90% of a STP's atmospheric emissions (ESTRADA *et al.*, 2015).

The H₂S, which main characteristic is the smell of rotten egg, has low perception threshold (0.0047 ppm) (SANTOS, 2007), what results in human smell perception, even at low concentrations of the compound, which causes annoyances and increasing complaints related to STP by the population that surround this facilities. For health, H₂S is related to symptoms such as nausea, headache, and respiratory problems (ESTRADA *et al.*, 2015). Furthermore, hydrogen sulphide can be lethal in concentrations higher than 300 ppm, when its smell is no longer perceived anymore (VINCENT, 2001).

In STPs, different unities are responsible for H₂S emission, such as preliminary treatment, settling

tanks, activated sludge systems, anaerobic reactors, clarifiers, and sludge dehydration. However, the anaerobic treatment is the most important source of hydrogen sulfide, where concentrations of this compounds can reach 500 ppm (AUGUSTO, 2015; CHERNICHARO, *et al.*, 2010).

The estimation of the emission rates of H₂S by STPs is of high importance, since it becomes a subsidy for dispersion modelling and, consequently, establishment of the concentration of this pollutant at communities, besides being an important tool for decision making.

Different methods can be used to estimate H₂S emissions, among them laboratory experiments, direct sampling of gaseous phase and empirical mathematical equations. The last ones gather simplicity and lower cost, being the main reason for these equations to be widely used (SANTOS *et al.*, 2006; CARRERA-CHAPELA *et al.*, 2014).

The AP-42 is one of the empirical models of equations to determine odor compounds emissions.

The methodology, published by the US EPA is a compilation of emission factors for more than 200 emission sources of atmospheric pollutants (USEPA, 1995).

Considering this scenario, the objective of the present study was to estimate the emission rates of hydrogen sulfide from different units of a STP located in the metropolitan area of Belo Horizonte.

METHODS

The study area is a Wastewater Treatment Plant located in the North region of Belo Horizonte City, Minas Gerais, Brazil. With 65.5 hectares of area, the facility treats 1.8 m³/s of sewage, through screens, UASB reactors (Upflow Anaerobic Sludge Blanket), trickling filters and settling tanks (COPASA, 2017).

A sampling campaign was carried out on May 2017, to determine the concentration of H₂S in wastewater and in air around different units of the STP, among them: inflow box (Point 1), post-screening (Point 2), flow distribution box for the UASB (Upflow Anaerobic Sludge Blanket) (Point 3), UASB reactors (Point 4), post-UASB collection box (Point 5), trickling filters (Points 6 and 7) and secondary clarifiers (Point 8) (Figure 1).



Figure 1. Points of H₂S sampling

Based on the H₂S concentration in the liquid phase and on the methodology established by the US EPA AP-42 - Chapter 4 (Evaporation Loss Sources), Unit 4.3 (Waste Water Collection, Treatment and Storage), the emissions rates of H₂S for each STP's units were estimated. More details can be verified in Miranda (2017).

FINDINGS AND ARGUMENT

The H₂S concentration on liquid and gaseous phases and the estimated emission rate for H₂S is presented on Table 1, for each of the analysed STP unit.

Table 1. Concentration of H₂S in liquid and gas phases and estimated emission rate for H₂S in different units of the studied STP

Unit	Concentration		Emission rate (g/s)
	Liquid phase (mg/L)	Gas phase (ppm)	
Point 1 - Inflow box	1.58	0.5	0.009
Point 2 - Post-screening	1.70	2.00	1.310
Point 3 - Flow distribution box for the UASB	1.63	0.05	0.941
Point 4 - UASB reactors	4.06	12.05	0.456
Point 5 - Post-UASB collection box	4.24	27.00	3.452
Point 6 - Flow distribution box for trickling filters 1-4	2.12	12.00	0.336
Point 7 - Flow distribution box for trickling filters 5-8	1.79	4.80	0.283
Point 8 - Trickling filters 1-4	2.12	*	0.961
Point 9 - Trickling filters 5-8	1.79	*	0.811
Point 10 - Secondary Clarifiers	1.63	0.02	0.055

The highest concentration in liquid phase were observed for points 4 and 5 (4.06 and 4.24 mg/L, respectively), since they are units immediately after UASB reactors, where anaerobic process are carried out with sulfate reduction and H₂S formation (TALAIEKHOZANI *et al.*, 2016). The inflow box (point 1) was the unit with smallest concentration of H₂S in liquid phase.

The emission rate estimated for point 5 was the highest (3.45 g/s), what matches with the highest

concentration of H₂S in liquid and air phases (27 ppm in air) and with the high turbulence of the wastewater in this unit. Although post screening (point 2) did not present a high concentration of H₂S in liquid phase, the emission rate in this unit was the second highest, due to the system turbulence.

For the inflow box (point 1) the estimated emission rate was the smallest (0.009 g/s), followed secondary clarifiers (point 10 - 0.055g/s), since

they are quiescent surfaces and small concentration of H_2S in sewage were observed in this units.

At the evaluated day, the H_2S emission rate for the whole STP was 7.5 g/s. This data can be used as input for dispersion models, in order to estimate the influence of H_2S in the STP surrounding population.

CONCLUSIONS

The results obtained in this study showed that units located after anaerobic process tend to present higher concentration of H_2S in liquid phase, what, associated with higher turbulence of sewage, contributes to higher emission rates. Moreover, the study demonstrates the importance of evaluating H_2S emissions by of each unit and its influence on the total emission of the STP. It can support decision making in regards to emission control, besides subsidizing pollutant dispersion models.

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TECHNIQUES TO MITIGATE DIFFUSE CH₄ AND H₂S EMISSIONS IN UASB-BASED SEWAGE TREATMENT PLANTS

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Abstract: In the last three decades UASB reactors have become a mature technology for the treatment of sewage in many tropical countries. Despite of the many advantages of this technology, there are some drawbacks that require further research, such as the elevated concentrations of dissolved H₂S and CH₄ in its effluent. Both dissolved gases can be released into the atmosphere downstream the anaerobic reactor, producing odors and corrosion in the case of H₂S and increasing the greenhouse gas emissions with a significant loss of energy in the case of CH₄. Different technologies have been recently proposed in the literature for i) Removing these dissolved gases from the anaerobic effluent by stripping them into a waste gas stream that would need a further treatment, and ii) Recovering the dissolved CH₄ for energy production purposes (heat and/or electricity). This study aims at reviewing the available technologies for dissolved H₂S and CH₄ stripping from the effluent of UASB reactors by proposing possible process flow diagrams to achieve their simultaneous removal from the anaerobic effluent and for recovering the CH₄ for energy production purposes. Whether the recovery of CH₄ in a single stage is not feasible, H₂S and CH₄ can be simultaneously stripped by using technologies such as diffused aeration, simplified desorption chamber or packed desorption chamber. The abatement of these gases can also be directly achieved in the biological aerobic posttreatment, by using DHS reactors. If the goal is CH₄ recovery with an abatement of dissolved H₂S, two in-series technologies might be necessary. The first stage would strip the CH₄ into a concentrated gas stream and the second one would abate the remaining dissolved gases. Processes such as vacuum chambers, membrane contactors and enclosed DHS reactors have been tested for the CH₄ recovery.

Keywords: Dissolved gas, stripping, odor, greenhouse gas, anaerobic reactor

INTRODUCTION

In the last three decades, the application of anaerobic-based technologies in sewage treatment plants (STP) has become a common practice in many tropical countries around the world, being the Upflow Anaerobic Sludge Blanket (UASB) reactor the technology mostly used. When compared to traditional aerobic technologies such as activated sludge, the UASB reactors present the following main advantages (Chernicharo, van Lier, Noyola, & Bressani Ribeiro, 2015): lower CAPEX/OPEX, lower sludge production, no energy consumption, and biogas production (of potential use for energy recovery). However, in spite of these advantages, anaerobic-based technologies for sewage treatment are characterized by producing a liquid effluent with high concentrations of dissolved H₂S (7 - 11 mgS·L⁻¹) and CH₄ (18 - 22 mg·L⁻¹) (Souza, Chernicharo, & Melo, 2012). Because of turbulent hydraulic conditions downstream the anaerobic reactor, these gases are released into the atmosphere, eventually posing significant odor and greenhouse gas (GHG) emissions. Additionally, the liquid effluent of UASB reactors usually presents high concentrations of suspended solids (50 - 100 mg·L⁻¹) (Von Sperling, 2014), therefore implying in clogging risks of many of the traditional gas stripping technologies.

For the H₂S, the most used control techniques are based on gas stripping from the liquid phase, resulting in the generation of a waste gas that needs further abatement. For CH₄, depending on the specific conditions of the STP, recovery for further energy production (electricity and/or heat) is preferable than just stripping or flaring it.

This study aims to review the available technologies for H₂S and CH₄ abatement/recovery from the effluent of UASB reactors. Different process flow diagrams (PFD) were proposed in regards to this treatment objective.

METHODS

The different technologies for the H₂S and CH₄ stripping from the UASB reactors effluent considered in this paper were determined from a literature review. The review presented in Heile et al. (2017) was used as a first approach to this subject, complementing it with the most recent information related with the UASB reactors. Depending on the treatment goals these technologies could be used individually or by combining at least two of them.

Table 1 shows the technologies that were considered in this paper and its main references. All of these technologies have been tested in laboratory or pilot scale, and the performances the authors reported for H₂S and CH₄ abatement are shown in Table 1. Some information, such as the removal of H₂S in membrane contactors, is still not available in literature and was not considered in this article.

From the information presented in Table 1 and considering the conditions described by the authors for the operation of each technology, different PFD were established for i) The abatement of H₂S and CH₄ dissolved in the anaerobic effluent by producing a waste gas that would be sent to a further treatment and ii) The recovery of a CH₄-rich gas stream for energy reuse purposes in a first stage, and stripping of the remaining H₂S and CH₄ into a waste gas that would require a further treatment in a second stage.

Table 1. Technologies for the H₂S and CH₄ stripping from the effluent of UASB reactors

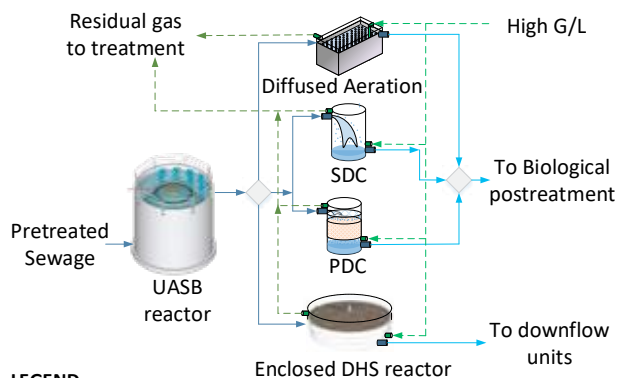
Technology	Principle	Reported abatement	References
Diffused Aeration	Compressed air is sparged at the bottom of a deep tank receiving the anaerobic effluent, stripping the dissolved gases to a waste gas. High air/water ratios are normally used in combination with a high hydraulic retention time.	99% for CH ₄ abatement 71 to 77% for H ₂ S abatement	Khan et al. (2011)
Simplified Desorption Chamber (SDC)	A free-fall of liquid phase is produced in a closed tower, and an air flow at high air/water ratios is introduced in the bottom of the system. The air/water interphase is big enough to produce the H ₂ S and CH ₄ stripping to a residual gas.	50% to 70% for CH ₄ abatement 40% to 70% for H ₂ S abatement	Brandt et al., (2018) Glória et al. (2016)
Packed Desorption Chamber (PDC)	A packing material is added to the above-mentioned system, increasing the air/water exchanging surface.	70 to 90% for CH ₄ abatement 65 to 85% for H ₂ S abatement	Brandt et al. (2018) Santo (2017)
Downflow Hanging Sponge (DHS) reactor	By using sponge packing media, oxidizing biomass can be supported in the system, converting the dissolved H ₂ S and CH ₄ . Both, gas stripping and biological oxidation are responsible for H ₂ S and CH ₄ removal. The authors propose a two in-series configuration: the first unit for recovering the CH ₄ and the second one for oxidizing the remaining CH ₄ and H ₂ S. Aerobic posttreatment of the UASB effluent occurs when high G/L are used (in the second DHS reactor).	Up to 76% for CH ₄ recovery. Up to 99% abatement for CH ₄ .	Matsuura et al. (2015)
Membrane Contactors (MC)	High interphase areas between liquid/gas phases are provided in a very compact unit. Pre-treatment is necessary to avoid clogging, and it can be operated with stripping-gas or with vacuum.	71 to 99% for CH ₄ . Recovered gas with CH ₄ content up to 30%.	Cookney et al. (2016)
Vacuum Assisted Chamber	The liquid effluent passes between two concentric cylinders. An air/water interphase is produced at the top of the unit, where a vacuum pressure is provided, creating the driving force required for the stripping process.	75% recovery of CH ₄ 50% abatement of H ₂ S	Possetti et al. (2018)

RESULTS AND DISCUSSION

PFD proposed for the H₂S and CH₄ stripping (without CH₄ recovery) are shown in the first section, meanwhile PFD for the CH₄ recovery and H₂S stripping are presented in the second section.

1. Process flow diagrams aiming at the CH₄ and H₂S abatement from the effluent of UASB reactors

Figure 1 shows the processes proposed for the CH₄ and H₂S abatement without energy recovery.



LEGEND

UASB: upflow anaerobic sludge blanket PDC: packed desorption chamber
SDC: simplified desorption chamber DHS: downflow hanging sponge

Figure 1. PFD for CH₄ and H₂S removal from the anaerobic effluent of UASB reactors

As seen in Figure 1, different technologies can be used for the simultaneous stripping of H₂S and CH₄ from anaerobic effluents. For all these cases, a removal performance greater than 60% for both dissolved gases can be expected, as presented in

Table 1. For all these technologies, gas to liquid ratios (G/L) greater than 2.0 would be expected, since the dilution of the residual gas is not a concern.

The simplified desorption chamber (SDC) and the packed desorption chamber (PDC) would be very compact systems, with hydraulic retention times (HRT) in the order of 5 to 15 min, although the SDC would have the worse efficiency of the proposed processes (50 to 70% and 40 to 70 % for CH₄ and H₂S, respectively). The diffused aeration system requires more than 30 min of HRT and would have a greater energy consumption because of the continuous air sparging in the system. For these units, a biological posttreatment would be required downstream.

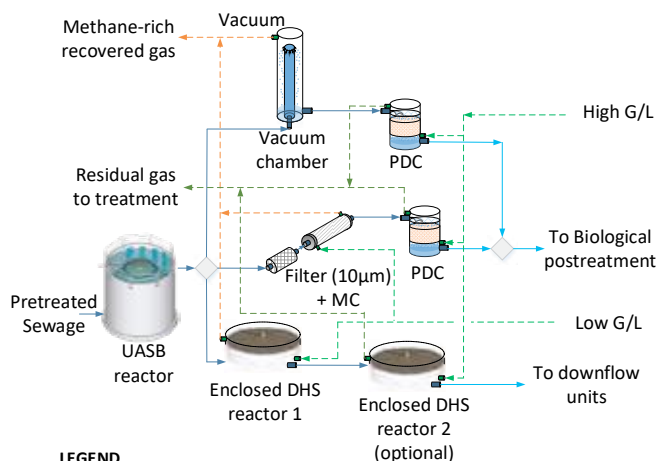
In the case of the enclosed DHS reactor, a larger HRT is required (around 2h) for both, organic matter/suspended solids removal from the anaerobic effluent dissolved H₂S and CH₄ abatement in a single unit.

2. Process flow diagrams aiming at the CH₄ recovery and H₂S abatement from the effluent of UASB reactors

Processes suitable for the CH₄ recovery and the stripping of the remaining dissolved gases can be seen in Figure 2.

In this case, when abatement efficiencies greater than 60% for both dissolved gases are expected, it seems that the combination of two-in-series technologies would be necessary: (i) a first process stage aiming at CH₄ recovery at high concentrations (CH₄ content greater than 20% v/v for heating

production and greater than 30% v/v for electricity generation). In this case, a gas to liquid ratio (G/L) lower than 0,10 or vacuum application would be necessary for avoiding the dilution of the recovered CH₄. (ii) in a second process, the remaining dissolved CH₄ and H₂S would be stripped by using high G/L and sent to a further treatment.



LEGEND

UASB: upflow anaerobic sludge blanket PDC: packed desorption chamber
MC: membrane contactor DHS: downflow hanging sponge

Figure 2. PFD for CH₄ recovery and H₂S removal from the anaerobic effluent of UASB reactors

The vacuum chamber unit would have a CH₄ recovery efficiency lower than the membrane contactor (MC) and the first DHS reactor, although it would be simpler than the MC and more compact than the DHS reactor. Because of the suspended solids in the UASB reactor effluent, the MC requires a pretreatment (10 µm) to avoid clogging, however a very compact unit (HRT of approximately 15s) and high CH₄ recovery rates would be expected. Finally, the first DHS reactor with an HRT of 2,0 h would recover an important part of the dissolved CH₄ and provide a first posttreatment for the anaerobic effluent that could achieve the less stringent discharge limits (BOD of 39 ± 12 mg·L⁻¹, COD of 89 ± 24 mg·L⁻¹ and SS of 32 ± 27 mg·L⁻¹, according to Maatsura et al., 2015). If a better quality of the effluent in terms of dissolved gases and organic matter is required, a second DHS reactor (HRT of 2 h) could be considered.

CONCLUSIONS

The main available processes for H₂S and CH₄ stripping from the UASB reactor effluent are: diffused aeration, simplified desorption chamber, packed desorption chamber, DHS reactor, vacuum chamber and membrane contactor. When operated at low airflow rates or with vacuum, some of these technologies would allow the recovery of CH₄ for energy production (heat or electricity), and CH₄ recovery with the simultaneous stripping of the remaining H₂S would be possible by combining at least two of these processes.

Case by case analysis would be necessary when selecting the most appropriate stripping technology in a UASB-based sewage treatment plant, by considering at least the following factors: CH₄ recovery and energy production feasibility, energy

balance, carbon footprint, available space, CAPEX, OPEX and operating simplicity.

Finally, most of these technologies have been tested in a laboratory and pilot scale, and full-scale testing are still necessary.

ACKNOWLEDGEMENT

The authors wish to acknowledge the support obtained from the following institutions: Instituto Nacional de Ciência e Tecnologia de ETEs Sustentáveis - INCT ETEs Sustentáveis; Fundação de Amparo à Pesquisa do Estado de Minas Gerais - FAPEMIG; Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq; Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - CAPES.

E. Centeno acknowledges the University of Costa Rica and the Program Estudantes-Convênio de Pós-Graduação - PEC-PG, from CAPES/CNPq/MRE-Brasil for supporting his PhD with a scholarship.

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EVALUATION OF METHANE EMISSION FROM A HIPOTETIC FOOD WASTE ANAEROBIC BIODIGESTER AT A UNIVERSITY RESTAURANT

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Abstract: The research aimed to acquire data of food waste generation from the restaurant of a Federal University in Brazil and to verify its potential for biogas production. Two different methodologies were used to quantify the theoretical potential of methane generation in anaerobic treatment: estimation from volatile solids (degradability content) of the substrate; and the Guidelines for National Greenhouse Gas Inventories established by the Intergovernmental Panel on Climate Change (IPCC). The restaurant produces a daily average mass of 112 kg of food waste. Considering that the fraction of volatile solids, it was estimated a mean methane gas production of 10.4 m³/day. Calculations with Tier 1 of the IPCC methodology estimated a daily methane gas production of 0.13 m³. This difference observed between the obtained results suggests attention to using the Tier 1 methodology. A standard value of the emission factor as input data assumed in different regions can lead to a quantification of gas generation different to the actual value since the local temperature and waste composition determine the factors for the kinetic degradation of anaerobic digestion.

Keywords: Biogas, Anaerobic Digestion, Greenhouse Gases, Food Waste.

INTRODUCTION

Population growth has contributed to increasing waste production and the need for appropriated waste disposal areas, impacting the environment. Organic solid wastes, when in pristine environments, are spontaneously degraded by recycling of the nutrients in the biogeochemical cycles. When in large volume and inappropriately arranged, they can represent a serious environmental risk due to the generation of leachate that is responsible for the contamination of aquatic bodies and soil, the proliferation of vectors and the emission of greenhouse gases (GHG) into the atmosphere. For these reasons, the use of adequate methods of management and treatment of these wastes are essential for the correct stabilization of organic matter (BRAZIL, 2016).

Organic waste represents 51.4% of the total urban waste generated in Brazil (IPEA, 2012). They are usually composed of putrescible materials mainly originated from food debris. Every year around a third of all food produced in the world is wasted, which is equivalent to about 1.3 billion tons of food. In 2007, greenhouse gas emissions from food wastes were approximately 3.3 billion tonnes of CO₂ equivalent, being the third largest global source of GHG, preceded by emissions from the United States and China (FAO, 2013).

In developed countries, the treatment processes currently used for the organic fraction of municipal solid waste are composting and anaerobic digestion. The latter one being a more attractive and sustainable alternative for the treatment of this type of waste, due to the formation of biogas (a natural gas fuel with high energy potential),

lower energy consumption, lower production of sludge and a smaller area for implantation (Gomez, 2006; Silva, 2009).

The objective of this research was to verify the potential for biogas production from food waste generated in a restaurant of a Federal University of Brazil.

METHODS

The quantification of food waste data produced at the University Restaurant (UR) of the Federal University of Juiz de Fora (UFJF) was provided by *Trigoleve Refeições Coletivas* company, which manages the restaurant. On average, 8,300 meals are served daily, including breakfast, lunch, and dinner. Food waste is collected in the restaurant separately, not mixed with other materials such as plastic, for example.

The methodology used to evaluate the biogas generation potential in the biodigester and its energy use was based on the following three steps presented below.

1. Estimation of the amount of methane gas (CH₄) produced from the degradability content of the substrate according to literature data. Table 1 shows the percentage of volatile solids of food waste presented by different studies. Ferreira (2015) studied the performance of a real methanization system with energy recovery through biogas and found an average production value of CH₄ in the order of 400 m³ per ton of volatile solids.

Table 1. Percentage of volatile solids (VS) of food waste

Author	VS (%)
Zhang <i>et al</i> (2007)	26.4
Li <i>et al</i> (2011)	22.6
Zhang <i>et al</i> (2011)	17.1
Browne <i>et al</i> (2012)	27.6
Zhang <i>et al</i> (2013)	21.0
Mean value	23.0

2. Estimation of methane gas amount produced from a certain amount of the substrate, according to the methodology indicated by the Intergovernmental Panel of Climate Change (IPCC, 2006) for Biological Treatment of Solid Waste. Tier 1 of this methodology is the most general method and should be used only when there is no local data available, either in the literature or from situ measurements. Level 2 suggests the use of emission factors obtained from measurements made previously by other studies. Level 3 is the most complete and accurate method, with the use of emission factors obtained by the biogas plants already in operation and being tested at pilot scales. Unfortunately, these data are not yet available in Brazil.

The emissions of CH₄ were estimated with equation 1:

$$CH_4 \text{ emissions} = \sum (M_i \times EF_i) \times 10^{-3} \quad (1)$$

Where:

CH₄ emissions- methane emissions (kg CH₄);

M_i- mass of organic waste type i biologically treated (kg);

EF_i- emission factor for treatment i (g CH₄/kg treated residue).

The emission factor for the anaerobic treatment of municipal solid waste varies from 0 to 8 g CH₄/kg of treated waste, depending on factors such as type, quantity and consistency of the residue, process temperature, among others. If it is not possible to determine the emission factor of the sample, it is recommended to use the emission factor of 0.8 (IPCC, 2006). These values were obtained by considering as organic matter waste composed of municipal solid waste in general, such as food waste, pruning and sweeping services, among others.

3. Estimation of the energy potential produced by methane gas. According to Coldebella *et al.* (2006), methane under normal conditions of temperature and pressure (NCTP) has a lower calorific value (LCV) of 9.9 kWh/m³, while biogas has a LCV between 4.95 and 7.92 kWh/m³, if its methane content is between 50% and 80%. Considering the efficiency of the conversion of biogas into electricity with generator sets (Otto cycle motors) to be approximately 25%, according to CCE (2000), it was possible to estimate the electricity generated in the scenario studied.

FINDINGS AND ARGUMENT

Considering the mean value of organic waste generated by the restaurant during the study period (January-2015 to May-2016), the proposed biodigester should be designed to treat 112 kg/day of waste (or 2,235 kg/month), considering that the restaurant opens Monday through Friday.

The estimated volatile solids (degradability content) of the substrate, considering the average of 23.0% of VS on food waste, presented a value of 25.76 kg VS/day, with the daily methane production being 10.4 m³.

Calculations with Tier 1 (default values) of the IPCC methodology, where the recommended emission factor is 0.8 g CH₄/kg of treated waste, estimated a value of 0.0896 kg de CH₄ produced. Knowing the density of methane gas (0.656 kg/m³), the production found was 0.13 m³/day.

In addition to the recommended value, IPCC (Tier 1) presents a range of possible emission factors varying from 0 to 8. Repeating the calculation with the emission factors within this range, the following values were obtained (Table 2):

Table 2. Production of CH₄ considering different emission factors

Emission Factor (g CH ₄ /kg)	CH ₄ Production (kg/day)	CH ₄ Production (m ³ /day)
0.2	0.0224	0.0341
0.4	0.0448	0.0683
2.4	0.2688	0.4098
4	0.4480	0.6829
5.6	0.6272	0.9561
8	0.8960	1.3658

These emission factors suggested in the IPCC methodology were obtained based on the local reality of the study, that is, in the United States (USA). The composition of urban solid waste generated in the United States differs from the Brazilian reality. The amount of food waste in the USA represents about 14.6% of the total waste generated. The composition of American waste still has 13.5% of the pruning and cleaning of gardens and 6.2% of wood, plant components that have cellulose and are more difficult to be degraded than food waste (EPA, 2013). For this reason, the values found using Tier 1 were so far from those obtained by the volatile solids.

The emission factor estimated from volatile solids data from literature and equation 1 is shown in Table 3. Table 4 shows the energy potential of methane gas produced per day and per month, assuming this emission factor.

Table 3. Calculated emission factor (EF)

CH ₄ production (1 ton of SV)	SV content in the sample	CH ₄ sample production	Mass to be treated	EF
400 m ³	25.76 Kg	10.304 m ³ = 6.759 kg*	112 kg	60 g CH ₄ /kg treated food waste

*knowing that the methane gas has a density equal to 0.656 kg/m³, under normal conditions of temperature and pressure (NCTP).

Table 4. Energy potential of methane gas produced

Production per day	Actual production per day (conversion efficiency)	Estimated production per month*	Equivalent house demand**
102.00 kWh	25.50 kWh	510 kWh	3 houses

*Considering production from Monday to Friday.

** The mean monthly residential consumption of energy per consumer unit in the period from December 2014 to December 2015 was 161.8 kWh (EPE, 2016).

Considering the use of biogas for direct burning, the gas volume generated assuming the emission factor of 60 g CH₄/kg, can maintain a double burner on for about 23 h/day, according to information provided in the company manual 'BGS Equipment for biogas' (a double burner biogas cooker with a consumption rate of 0.45 m³/h of biogas per burner).

The volume required by the anaerobic digestion system is around 15 m³, totally compatible with the available area around the restaurant in the UFJF campus. Figure 1 shows a top view of the University Restaurant. It is possible to observe the existence of areas in the surroundings of the restaurant where it would be possible to install and operate the system.



Figure 1. Top view of the University Restaurant

CONCLUSIONS

The difference in the order of magnitude of the results suggests attention when using Tier 1 of the IPCC methodology for sites with different waste composition. Utilization of a default emission factor for different regions may underestimate or overestimate gas generation since the kinetic

degradation of anaerobic digestion is highly dependent on temperature and waste composition.

It is recommended that default values should be replaced by values compatible with local reality, as suggested by Tier 2 and 3, avoiding large differences between measured and calculated CH₄ emissions. This fact requires attention and indicates the need for future studies aiming to obtain local emission factors.

The treatment of urban organic waste with the generation of biogas offers social, environmental and economic advantages, since the volume of waste that would be destined to landfills decreases. Thus, there would be a reduction in the emission of greenhouse gases from the uncontrolled degradation of organic waste, as well as the possibility of generating energy through the use of biogas generated, contributing to the diversification of the energy matrix.

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ESTIMATION AND IMPACT OF METHANE EMISSIONS IN BRAZILIAN ANAEROBIC-BASED SEWAGE TREATMENT PLANTS

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Anaerobic technologies have been effectively contributing to expand the Brazilian sewage treatment index, particularly by the use of the UASB (Upflow Anaerobic Sludge Blanket) reactors along the country. However, the CH₄ emissions from the generated biogas and diffusive emissions are still concerns. Therefore, the objective of this study is to present an estimation of methane emissions in Brazilian anaerobic-based STPs and its relative impact in terms of carbon footprint, when compared to other sectors (energy, industrial processes, agriculture, change of land use, and waste treatment). The UASB-based STPs carbon footprint was estimated by using a tool that considers different scenarios for biogas and diffusive emissions (Chernicharo *et al.*, 2017) and compared with the greenhouse gases (GHG) emission amount from the sectors considered in this study in 2015 (Brasil, 2017b). The results show that the waste treatment sector has the lowest annual equivalent CO₂ emissions, approximately 5%. Therefore, sewage treatment, that represents 22% of the waste treatment sector, would have a very low impact among the Brazilian total carbon footprint (Brasil, 2017b). In addition, depending on the adopted strategies for the integrated management of sludge, biogas and diffusive emissions, the GHG emissions from anaerobic-based STPs can be neutralized or even contribute to reduce the carbon footprint of the sewage treatment plants if the biogas is used to replace fossil fuels, such as liquefied petroleum gas for cooking.

Keywords: methane production, carbon footprint, sewage treatment, biogas.

INTRODUCTION

There is still a long journey ahead to achieve the universalization of sanitation in Brazil, as only 46% of the total generated sewage is currently treated. However, anaerobic technologies have been effectively contributing to expand the sewage treatment index, particularly by the use of the UASB (Upflow Anaerobic Sludge Blanket) reactors along the country. Some of the reasons that explain the preference of UASB reactor are: operational simplicity, low sludge production, low operational costs, and generation of biogas, associated with the possibility of energy recovery.

The biogas produced in UASB reactors comprises mainly methane (60-80% v/v), nitrogen, and carbon dioxide, whereas hydrogen sulphide, oxygen, hydrogen, carbon monoxide, ammonia, siloxanes, water and particulate matter are present in smaller proportions (Noyola *et al.*, 2006).

Methane (CH₄) has a high calorific value and its concentration defines the potential of recovering energy from biogas. In addition, CH₄ is considered one of the most important greenhouse gases (GHG), because it has a global warming potential 28 times higher than that of carbon dioxide (IPCC, 2014).

Generally, when the energy is not recovered from biogas, it is burned in open flares (typically applied in Brazilian Sewage Treatment Plants - STPs) to avoid the CH₄ emission into the atmosphere. However, there is still equivalent CO₂ emission from the inefficient burning of biogas.

Therefore, the objective of this study is to present an estimation of methane emissions in Brazilian

anaerobic-based STPs and its relative impact in terms of carbon footprint, when compared to other sectors (energy, industrial processes, agriculture, change of land use, and waste treatment).

METHODS

The carbon footprint was estimated by using a tool that calculates the corresponding amounts of methane emission in three different compartments: internal surface of the gas-liquid-solid (GSL) separator; open settler compartment; effluent (dissolved methane) and inefficient burning in open flares (Figure 1).

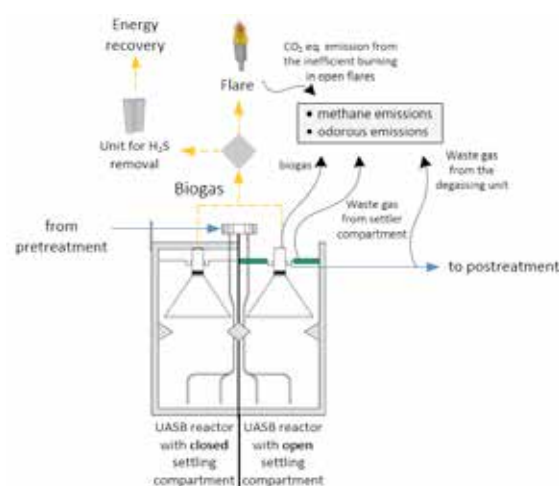


Figure 1. Main points of methane emissions in UASB reactors

The estimation of equivalent CO₂ emission was based on the input of the total population equivalent served by a UASB-based STP

(21,437,100 inhabitants) in Brazil (Chernicharo *et al.*, 2017; Brasil, 2017a).

The parameter of comparison was the greenhouse gases (GHG) emission amount from the sectors considered in this study in 2015, obtained from Brasil (2017b).

FINDINGS AND ARGUMENT

The results show that the waste treatment sector has the lowest annual equivalent CO₂ emissions compared to other sectors (energy, industrial processes, agriculture and change of land use), 63 MtCO₂eq., approximately 5% of the total GHG emissions in 2015 (1,368 MtCO₂eq.), as depicted in Figure 2. Consequently, domestic sewage treatment, that represents 22% of the waste treatment sector (Figure 3), has a very low impact on the Brazilian GHG emission index (Brasil, 2017b).

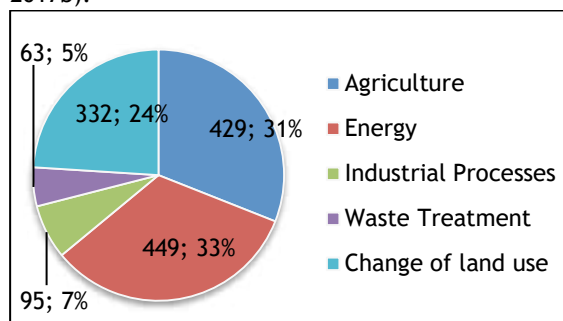


Figure 2. Greenhouse gases emissions by sector in Brazil (MtCO₂eq.) (Brasil, 2017b).

According to data published by the Agência Nacional de Águas (ANA) in 2017, UASB reactors are installed in 39% of the 2,657 sewage treatment plants (STP) surveyed in Brazil, serving a population of approximately 21.5 million inhabitants, which is approximately 30% of the total estimated population with sewage treatment in the country (71.7 million inhabitants) (Brasil, 2017a). Considering the total population equivalent served by a UASB-based STP (21,437,100 inhabitants) in Brazil, the equivalent CO₂ emission is 1.2 MtCO₂eq.. Therefore, it represents an even smaller impact on the Brazilian carbon footprint.

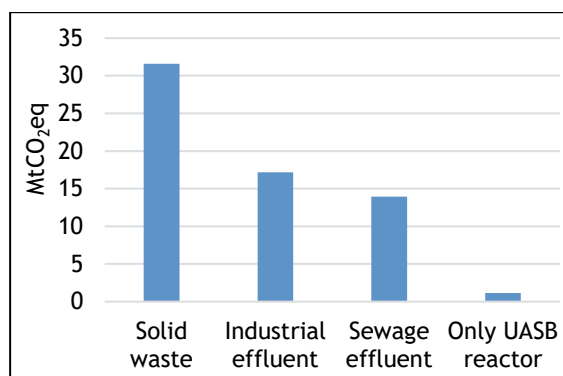


Figure 3. Greenhouse gases emissions by waste treatment sector and by UASB-based STP (Brasil, 2017a; Brasil, 2017b; Chernicharo *et al.*, 2017).

CONCLUSIONS

Depending on the adopted strategies for the integrated management of sludge, biogas and diffusive emissions, the GHG emissions from anaerobic-based STPs can be neutralized or even contribute to reduce the carbon footprint of the sewage treatment plants if the biogas is used to replace fossil fuels, such as liquefied petroleum gas for cooking.

Therefore, the design of UASB reactors must consider the aspects related to capture/treatment of biogas and waste gas, aiming to reduce the carbon footprint of the STP and to potentialize energy recovery from biogas.

ACKNOWLEDGEMENT

The authors wish to acknowledge the support obtained from the following institutions: Instituto Nacional de Ciência e Tecnologia de ETEs Sustentáveis - INCT ETEs Sustentáveis; Fundação de Amparo à Pesquisa do Estado de Minas Gerais - FAPEMIG; Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq; Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - CAPES.

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STRATEGIES FOR THE CONTROL OF CH₄ AND H₂S EMISSIONS FROM BIOGAS IN ANAEROBIC-BASED SEWAGE TREATMENT PLANTS

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Anaerobic sewage treatment technology, mainly UASB reactors, has been widely applied around the world in recent decades. However, the H₂S removal from the generated biogas, and the increase of energy recovery from CH₄ are still concerns. Therefore, this study aims to present an analysis of the most common applied techniques for biogas treatment and use concerning CH₄ and H₂S emissions control and its energy recovery. In this instance, the potential of CH₄ and H₂S emissions mitigation from anaerobic-based sewage treatment plants (STPs) was analysed through the simulation of different technological scenarios for biogas treatment and energy recovery according to STP size (small $\leq 10,000$; 10,000 < medium < 100,000; and large-scale $\geq 100,000$ inhabitants). The carbon footprint of each scenario was estimated by using a simulation tool that considers different techniques for biogas use, namely: sludge sanitization, cooking, water heating, thermal dryers, boilers (for steam generation), combined heat and power engines, and direct biogas flaring without energy recovery. For small-scale STPs, the simulations showed that the use of biogas for cooking is the best option compared to the other technological scenarios considered, as it not only neutralizes the STP emissions but also prevent the emission of 1,775 kgCO₂eq.year⁻¹.inhabitants⁻¹. For medium and large-scale STPs, the use of biogas on boilers was the best scenario, avoiding the emission of 1,775 kgCO₂eq.year⁻¹.inhabitants⁻¹. The results can be important for decision makers choosing the best gaseous emissions management practices in UASB-based STPs.

Keywords: anaerobic reactors, energy recovery, greenhouse gas, hydrogen sulphide, methane.

INTRODUCTION

The use of anaerobic technology in sewage treatment plants (STPs), mostly UASB reactors, has grown significantly in the last decades and are now considered a consolidated technology in Latin America. However, even with its recognized advantages and wide use, UASB reactors still have constraints that must be properly managed.

The presence of methane (CH₄) and hydrogen sulphide (H₂S) in the biogas is one of the main concerns, which has guided several scientific studies not only to remove H₂S from biogas, but also to increase the potential of energy recovery from CH₄. The H₂S is a toxic gas and may be a risk to human health, even at low concentrations (WEF, 2004). H₂S is also responsible for the characteristic odour of anaerobic processes, since it has a human detection threshold ranging from 0.47 to 100 ppbv (Metcalf and Eddy, 2016). Moreover, the presence of H₂S in biogas (between 200 and 5,000 ppmv - Possetti *et al.*, 2019) can hindered its energy recovery, because it can cause corrosion of components of energy recovering facilities. According to the intended use of biogas and required technology, there is a need to reduce the concentration of H₂S to 0.5 to 200 ppm (DWA-M 361, 2011; Monteleone *et al.*, 2011). Therefore, energy recovery from biogas is mainly dependent on the efficiency and related costs of the H₂S abatement process.

Regarding CH₄, it is the main constituent of the biogas produced in anaerobic-based STPs and its high calorific value (35.9 MJ.Nm⁻³) is responsible for the biogas energy potential. In addition, CH₄ is considered one of the most important greenhouse gas, since it has a global warming potential 28 times higher than that of carbon dioxide over a 100-year

horizon. CH₄ emissions can be ascribed to inefficient flares for biogas burning or when there are leaks in the gas lines, which can lead to an increase of the carbon footprint of the STP. Therefore, this study aims to present an analysis of the most common applied techniques for biogas treatment and use regarding CH₄ and H₂S emissions control and its energy recovery.

METHODS

The analysis of the main H₂S removal techniques found in the literature was carried out evaluating the feasibility of applying these techniques in small, medium and large scale STPs.

For small-scale STPs, simple alternatives for the use of biogas were considered, such as excess sludge sanitization, cooking and water heating. For medium and large-scale STPs, the considered alternatives for biogas use were thermal dryers, boilers (steam) and combined heat and power (CHP) generation. Additionally, vehicular fuel production was also considered for large-scale STPs. The emissions avoided by the considered technologies were compared with the CO₂ equivalent emission by the inefficient burning in open flares (typically applied in Brazilian STPs).

The carbon footprint of each scenario was estimated by using a tool called “Carbon Emission Avoidance and Energy Recovery in STPs” developed in a spreadsheet of Microsoft Excel®. This tool uses a database of around 50 coefficients and default parameters to estimate the total amount of CO₂ equivalent supposed to be emitted into the atmosphere considering different technological scenarios for energy recovery from biogas, according to STP size (small $\leq 10,000$; 10,000 < medium < 100,000; and large-scale $\geq 100,000$

inhabitants) (Chernicharo *et al.*, 2017). For the estimates of each scenario presented in this study, the following population equivalents were used: (i) small scale = 10,000 inhabitants; (ii) medium scale = 55,000 inhabitants; (iii) large scale = 100,000 inhabitants.

FINDINGS AND ARGUMENT

H₂S emissions control

Several studies on removal of H₂S from biogas have evaluated different techniques and methods, such as: adsorption, absorption (chemical scrubber, catalytic oxidation), thermal oxidation (direct combustion), chemical inhibition, membrane separation, microaeration, biofilter, biotrickling filter and bioscrubber (Chernicharo *et al.*, 2010).

However, many of these technologies are sophisticated, costly to deploy and operate and are generally not suitable for the treatment of biogas in anaerobic-based STPs. Thereby, this study analyses only the alternatives that bring together the greatest set of advantages for biogas treatment aiming its further use by considering the sustainability, simplicity and low implementation

and operating costs. The analysis of the main characteristics of each considered technique (Table 1) allows to infer that since the biofiltration and microaeration promote the dilution of biogas with N₂ and O₂, reducing its calorific power and consequently the electric potential recovery, they are the best options if heat recovery from biogas is the goal of the treatment. As a result, the applicability of these techniques are more feasible in small and medium-sized STPs. For biogas from UASB reactors treating sewage, the CH₄ concentration is typically around 75%, however its yield is usually low (0.21 Nm³biogas.kgCOD_{remov}⁻¹). Therefore, a clear economic viability for electricity generation from biogas is only made for large-scale STPs (> 100,000 inhabitants) (Possetti *et al.*, 2019).

Among the analysed techniques for biogas treatment, the best technology regarding electricity generation is adsorption in a solid media, because it allows the selective removal of H₂S, is mechanically simple and has a high and reliable performance (Table 1). Nevertheless, the use of alternatives adsorbents must be considered, because the cost of the adsorbent most commonly applied (activated carbon) often makes biogas treatment very expensive.

Table 1. Technologies for H₂S removal from biogas in anaerobic-based STPs.

Technology	Principle	Advantages	Disadvantages
Adsorption	Molecules come in contact with the surface of a solid adsorbent and bind via weak molecular forces.	– Moderate capital costs – Mechanically simple – Small area demand – High and reliable performance – Selective removal of H₂S	– Generation of a waste containing the adsorbed pollutants – Very high operating costs – Applicable to low H₂S loads if activated carbon is considered
Biofiltration	The biodegradable compounds are absorbed by the packing media and biofilm, being biologically oxidized	– Low capital costs – Low operating costs – Applicable for large flows	– Applicable for low/medium H₂S concentrations – High footprint – Sensitive to variations in influent H₂S concentrations – Compaction of the packing media and increase of the head loss – Dilution of biogas with N₂ and O₂
Microaeration	Injection of atmospheric air into the three-phase separator of the reactor	– Low capital costs – It does not require the use of chemicals – Low maintenance – Possibility of sulphur recovery	– Corrosion in the reactor – Accumulation of sulphur inside the reactor – Dilution of biogas with N₂

Reference: Adapted from Chernicharo *et al.*, 2010.

CH₄ emissions control

For small-scale STPs, the simulations carried out showed that the use of biogas for excess sludge sanitization can totally prevent the small-STPs carbon footprint. This scenario considered that the CO₂eq reduction is associated with the elimination of biogas flaring and the avoided emissions due to sludge transport to final disposal.

On the other hand, the use of biogas for cooking and water heating not only neutralize the STP emissions but also prevent the emission of 1,775 and 201 kgCO₂eq.year⁻¹.inhabitants⁻¹ respectively (Figure 1). The use of biogas for cooking considered the CO₂eq. reduction related to the replacement of LPG by biogas, while the use of biogas for heating water in households considered that the CO₂eq. reduction is

associated with the replacement of electric energy by biogas, taking into account the emission factor of the Brazilian electric matrix and the energy consumption of a shower.

For medium-scale STPs, it was observed that all of the recovery scenarios (biogas for sludge drying, steam or combined heat and power generation) are able to neutralize STP emissions and further prevent approximately 6.05 kgCO₂eq.year⁻¹.inhabitants⁻¹ (Figure 2), that would be emitted if flaring was applied. The best alternative seems to be the use of biogas on boilers to produce steam for, e.g., sludge drying and sanitization. This alternative, due to replacement of LPG by biogas, can avoid the emission of 1,775 kgCO₂eq.year⁻¹.inhabitants⁻¹, approximately 1300 times more than the considered option of using CHP engines (1.40 kgCO₂eq.year⁻¹

¹.inhabitants⁻¹). Biogas usage in CHP engines considered the savings of electric energy. The carbon emission avoided was estimated taking into account the Brazilian electrical matrix. The steam produced in the boiler can be used, e.g., to sludge drying and sanitization, reducing emissions related to the transport of sludge to final disposal, due to the volume reduction after thermal drying.



Figure 1. Schematic representation of the proposed different biogas usages in small-scale STPs.



Figure 2. Schematic representation of the proposed different biogas usages in medium-scale STPs.

As for medium-scale STPs, the simulations for large-scale STPs showed that the best alternative in terms of CH₄ emissions mitigation was the use of biogas on boilers (Figure 3). The alternative of using biogas as vehicular fuel also appears as an important option, since it can avoid 7.46 kgCO₂eq.year⁻¹.inhabitants⁻¹, approximately 5 times more than the use of biogas on CHP engines (1.40 kgCO₂eq.year⁻¹.inhabitants⁻¹).



Figure 3. Schematic representation of the proposed different biogas usages in large-scale STPs.

CONCLUSIONS

The energy recovery from biogas for more noble purposes (electric power generation) requires the use of a method to selectively remove the H₂S, for which adsorption is recommended. However, for heat recovery, biofiltration and microaeration techniques should be preferably applied.

The biogas recovery for cooking in small-scale STPs and for produce steam in boilers for, e.g., sludge drying and sanitization in medium and large-scale STPs are able to neutralize or even create a positive carbon footprint.

ACKNOWLEDGEMENT

The authors wish to acknowledge the support obtained from the following institutions: Instituto Nacional de Ciência e Tecnologia de ETEs Sustentáveis - INCT ETEs Sustentáveis; Fundação de Amparo à Pesquisa do Estado de Minas Gerais - FAPEMIG; Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq; Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - CAPES.

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EVALUATION OF THE H₂S, NH₃ AND VOLATILE ORGANIC COMPOUNDS EMISSIONS IN THE WWTP EL SALITRE THROUGH BOGOTÁ CLIMATE REGIMEN

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Abstract: Offensive odours are a social problem because they affect the health and quality of life of the population that lives near to the emission sites. Given this situation, in Colombia regulatory standards have been established for the control and management of gas emissions in industries. Thus, it is important to quantify emissions in areas nearby urban populations to establish possible control systems and fulfil legislation. In this work, gases emitted in the wastewater pre-treatment area of the *El Salitre* Wastewater Treatment Plant (WWTP) in Bogotá, Colombia, were quantified during the dry and rainy seasons. H₂S, NH₃ and volatile organic compounds (VOCs) were measured using a portable gas detector. In addition, VOCs were identified by gas chromatography/mass spectrometry. It was observed that gas emissions are directly related to the daily rainfall. The dry season showed the highest concentrations of the three evaluated gases: H₂S concentration rose up to 350 ppm, VOCs to 120 ppm and NH₃ to 34 ppm. In both seasons, a daily variation was observed in their concentration, where a higher gas concentration was detected at night. Regarding the identification of VOCs, in both seasons the same VOCs were found, but only 15 had a relative abundance higher to 1%: N,N-dimethylacetamide was the most abundant VOC (15-23%), followed by phenol (9-13%), toluene (3-8%) and xylene (3-4%). Among these VOCs, only N,N-dimethylacetamide and toluene showed a variation in abundance depending on the season and day period. Sulfur VOCs, represent 1-2% of the abundance. The high relative abundance of these compounds may represent a risk for exposed people, due to their toxicity at low concentrations. These results indicate that the implementation of mitigation measures is required, mainly in the dry season, and they will allow formulating adapted strategies to control and eliminate these gases at the WWTP.

Keywords: WWTP, hydrogen sulfide, ammonia, VOCs, offensive odours

INTRODUCTION

Offensive odors are a form of air pollution because they cause discomfort to the population and damage to health or the environment (SEPA, 2010). Odors are generally due to the emission of a mixture of volatile compounds with low detection threshold, such as hydrogen sulfide (H₂S), ammonia (NH₃) and volatile organic compounds (VOCs). These compounds are generated in industrial processes, such as the food processing, paint, paper and refineries industries; and naturally, in the livestock, composting and wastewater treatment (Revah & Morgan-Sagastume, 2005). The offensive odors in Wastewater Treatment Plants (WWTPs) are caused by the management of wastewater, the degradation of organic matter within the plant, as well as the generation and final disposal of solid waste, such as activated sludge. The main compounds that contribute to the odor are H₂S, dimethyl sulfide, mercaptans and NH₃, although alcohols, volatile fatty acids, aldehydes, ketones and amines have also been detected. These compounds are usually in trace levels (µg/m³), where they are toxicologically safe. However, even at these

concentrations, they could generate an occupational risk in closed spaces within the WWTP, such as in the sludge management area (Iranpour, Cox, Deshusses, & Schroeder, 2005). Of these compounds, H₂S has a high impact when is released in high quantities, which could cause corrosion in equipment and pipes in the plant (Talaiekhosani, Bagheri, Goli, & Talaei Khoozani, 2016).

WWTP El Salitre achieves the chemically assisted primary treatment of wastewater produced by approx. 4 million inhabitants of Bogotá. In addition, the sludge from primary stage is treated through mesophilic anaerobic digestion. Under the El Salitre conditions, the wastewater volume treated and proximity to residential areas, the odor management system consists mainly of the constant monitoring of the efficiency of sludge digestion, the use of tree barriers and the quarterly odor monitoring (EAAB). According to the management reports of the plant, these actions avoid the affectation by odors generated by the plant in the neighborhoods, but these are perceptible inside the plant. A study carried out in 2010 (Air Clean System, 2010),

identified the water inlet and pre-treatment area as the one with the highest H_2S concentration and determined that the highest emission of H_2S occurs in dry weather when there are high solar radiation and low wind speeds and, since they are not maintained throughout the year, are considered as critical conditions for generation of offensive odors. However, this study did not consider the other gases that can be found in the emissions of a WWTP and that also causes offensive odors. Therefore, the objective of this work was to establish the characteristics and conditions of gas emissions that generate offensive odors in the WWTP, which could serve as a model to propose an odor control system.

METHODS

The monitoring of the emission was carried out in a confined zone of the pretreatment area of WWTP El Salitre. This area was chosen because it presents the highest emission of H_2S (ACS 2010). In addition, the staff of the plant reports a high intensity of the smell of this compound. The detector MultiRAE gas (RAE) was used for the measuring of H_2S , NH_3 and VOCs. The frequency of data collection was 5 minutes. Readings higher than 100 ppm of H_2S were measured with the detector Biogas 5000(Landtec). The monitoring was carried out from February 15 to May 28, 2018, a period that covered the dry and rainy season of Bogotá. The data obtained with the MultiRAE detector were downloaded to a portable computer using the Pro-RAE Studio II program and processed using Excel and RStudio. WWTP El Salitre provided the precipitation data for the monitored months.

The identification of volatile organic compounds in one day of both seasons was also carried out by means of gas chromatography coupled to mass spectrometer (method ASTM 6520-06 / EPA 8260B)

RESULTS AND DISCUSSION

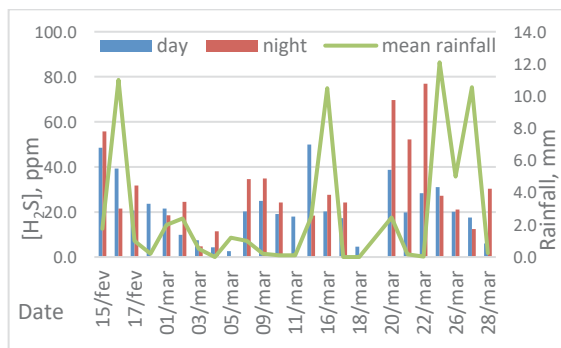


Figure 1. H_2S emission during dry season (February 15th to March 28th)

It was observed that in general, the gas emissions are related to the daily rainfall. Therefore, the concentrations of the gases were higher in the dry

season, and then decreased in the rainy season. Figure 1 show this trend for H_2S emissions, and the same behavior was observed for VOCs and NH_3 emissions. During the dry season, the average concentration of VOCs was between 3 and 30 ppm, and it was between 1 and 7 ppm for ammonia.

In the rainy season (Fig 2), the emission of gases diminished drastically, with the days of the highest precipitation (3-4 April, 8 May) the concentration of H_2S was close to 1 ppm, and 2 ppm for VOCs. In the case of ammonia, during the season, the average concentration was lower than the detection limit (<1 ppm) and the maximum concentration was 2 ppm.

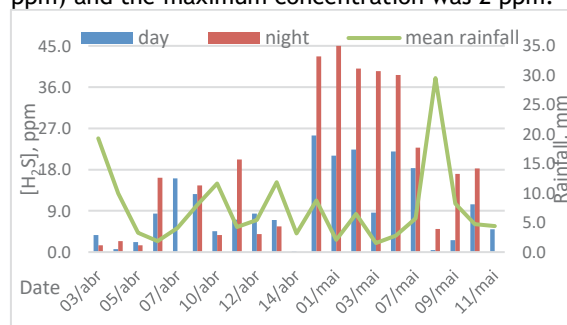


Figure 2. H_2S emission during rainy season (April 03 to May)

It was also observed that in most days of the dry season, the gases concentrations were highest at night time. In the case of H_2S , the difference between the average emissions at day time and night time was up to 40 ppm. This is because in the night hours, the wind speed and temperature decrease, which favors the gas accumulation in the sampling area. On the contrary, in the morning and afternoon, the increase of temperature and the wind speed allows the dispersion of emitted gases in the air. This monitoring shows the high variability in the gas emissions, especially in the dry season, so that, this behavior must be taken into account for the formulation of odor control strategies and schedules for the maintenance of the structures that are affected by the high emission of H_2S .

Regarding the identification of VOCs, in the rainy season, 77 and 69 VOCs were identified at the day and night, respectively, while in the dry season 65 and 54 VOCs were identified. In both seasons the number of compounds at daytime was higher than at night, which could be due to a higher industrial activity, therefore, the wastewater would have a high type of pollutants at this time.

In table 1 is shown the compounds with a relative abundance higher than 1%, which only corresponds to 17 of the totals VOC's identified. This shows the high complexity of the WWTP emissions.

Table 1. Relative abundance (in percentage) of VOCs presents in the emissions of the WWTP El Salitre

Compound	November		March	
	Day time	Night time	Day time	Night time
N, N-dimethylacetamide	22,48	23,32	14,80	25,90
Phenol	10,2	10,21	9,57	13,50
Tetrachloroethylene	1,43	3,84	1,05	2,14
Toluene	4,09	3,20	8,35	2,90
m/p-xylene	2,92	2,97	3,45	3,99
2-buthyl-1-octane	2,35	N.D.	N.D.	N.D.
Nonane	2,54	1,97	2,92	2,38
SO ₂	0,856	1,40	0,56	0,68
D-limonene	2,02	1,35	3,35	1,7
2,6-dimethyloctane or 3,6-dimethyloctane	1,35	1,22	1,22	1,01
1,2,3-trimethylbenzene 1,2,4-trimethylbenzene or 1,2,5-trimethylbenzene	1,38	1,16	N.D.	N.D.
1-ethyl-2-methylbenzene 1-ethyl-3-methylbenzene	1,23	1,13	0,98	1,05
Propyl cyclohexane	1,14	1,12	1,24	1,09
o-xylene	0,95	0,95	1,20	1,31
Undecane	0,95	N.D.	1,38	0,87
cis-1,4-dimethylcyclohexane	N. D.	0,94	1,11	0,98
2-methyloctane	0,87	0,84	1,22	N.D.
[COV], ppm	16,3	3,8	2,5	0,4

*N.D. Not detected

N,N-dimethylacetamide has been reported as the main pollutant of wastewater from acrylic production and used for industrial coatings, films, paint strippers and other applications (Chen *et al* 2017). Tetrachloroethylene is widely used for dry cleaning.

The presence of compounds such as phenol and toluene, of known toxicity (US-EPA 2017), in the emissions of the pretreatment zone, indicate that more in-depth studies should be carried out to verify the risk that the long-term exposure of these gases in the WWTP.

CONCLUSIONS

According to the results found during the monitoring of gases carried out in the pretreatment area of the WWTP, the H₂S is the compound with the highest emission, therefore, the implementation of mitigation actions is required, mainly in the dry season.

The emissions of NH₃ and VOCs are in similar concentrations, but the complexity of the mixture of VOCs indicates that their elimination from the gas

stream represents a challenge for existing technologies.

The monitoring also allowed establishing the concentrations and type of transitory conditions that should be taken into account when designing mitigation strategies and elimination of the gases that generate offensive odors.

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**AIR POLLUTION
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Session 11

Air Pollution Control

A Visual Analysis Tool for Health Indexes and PM₁₀ from São Carlos, São Paulo State, Brazil

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Abstract: Particulate matter with an aerodynamic diameter smaller than 10 μm (PM₁₀) is considered air pollutants associated with many health problems. PM₁₀ penetrates in the upper respiratory tract, causing respiratory problems such as pneumonia and asthma. The objective of this study was to apply an interactive visualization tool developed mainly in JavaScript programming language and D3 library. The tool is portable and can be used in all modern browsers, requiring no software installation. Air samplings were collected daily in a first stage (2014-2015) and in a second stage (2015-2017) the air samplings were performed on alternate days during the week, both comprising periods of 23h and 30 minutes. The equipment used for PM₁₀ sampling was the large volume sampler (Hi-vol). The visualization tool helped to observe that PM₁₀ concentrations in the city of São Carlos-SP decreased significantly and, as can be seen, there was a reduction in medical cases related to the respiratory system diseases, in comparison with historical data collected years ago in the same city.

Keywords: Particulate matter (PM₁₀), Information visualization, Time series.

INTRODUCTION

Particulate matter with diameter into the range of 0.1 to 10 μm are reported in the literature as those that may be retained in the upper respiratory tract or even penetrate deeper into the pulmonary alveoli, causing diseases in the respiratory and cardiovascular systems (Carugno et al., 2018; Santurtún et al., 2017; Feng et al., 2019).

The acquisition and analysis of environmental data are of central importance to the identification of the precursors to pollution, in local and global terms. Creating tools to understand the origin and seasonal movement of pollutants is critical as public management agencies can rely on when making decisions to reduce the impact of air pollution on human health. However, there is a considerable gap between the devices' ability to collect and store data and the ability of the available tools to organize and display these data as useful information. Exploring air quality monitoring data is necessary because it helps in identifying patterns and characteristics that can guide future research. (McLachlan et al., 2008).

1. Area of study

The city of São Carlos is a medium-sized city (Figure 1). According to IBGE data, São Carlos has 249,415

inhabitants (IBGE, 2019). São Carlos is also among the medium-sized Brazilian cities due to its academic, technological and industrial vigor. The agribusiness sectors are well developed, both in livestock, sugar-alcohol and sugar cane. With all these qualities, the city presents itself as important for the monitoring of atmospheric air quality (Marques, 2000). The PM₁₀ monitoring site in the central area of the city was placed in "Dos Voluntários" public square (latitude 22°1'12''S; longitude 47°53'24''W), which was considered appropriate, due to the high daily flows of people, services, and vehicles in the vicinity. Figure 1 shows the map of the state of São Paulo, city of São Carlos, study site and sampling point.

METHODS

1. Sampling

PM₁₀ measurements were taken daily from April 2014 to March 2015 (Monday to Monday) and from May 2015 to November 2017 (alternate days). For the collection of the particulate matter (PM₁₀), the equipment used was the high volume sampler (Figure 2).

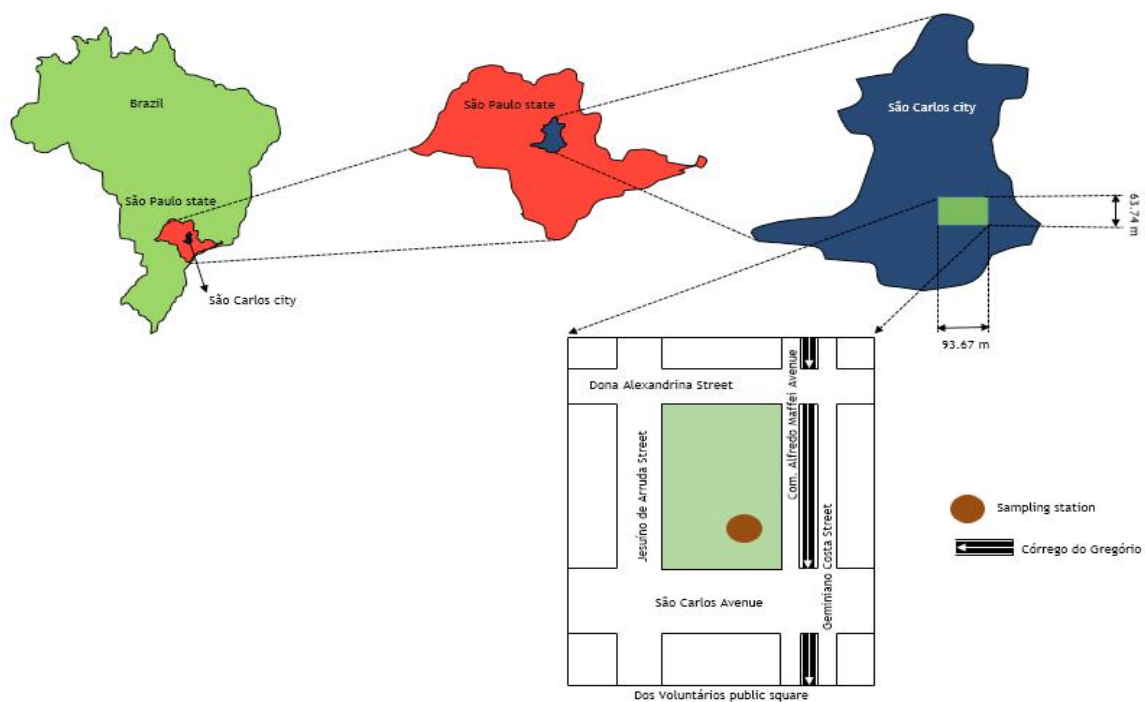


Figure 1. Map indicates the location of São Carlos and the sampling site

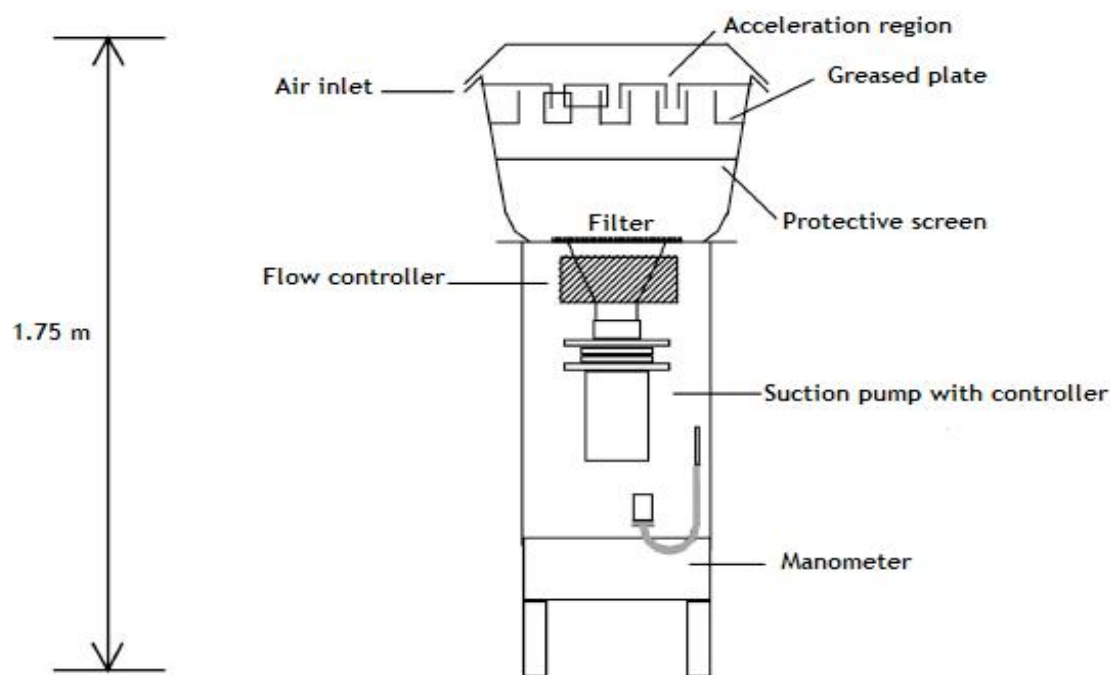


Figure 2. High Volume Sampler (Marques et al.,2001)

Figure 3 shows the schematic diagram of the PM₁₀ sampling methodology.

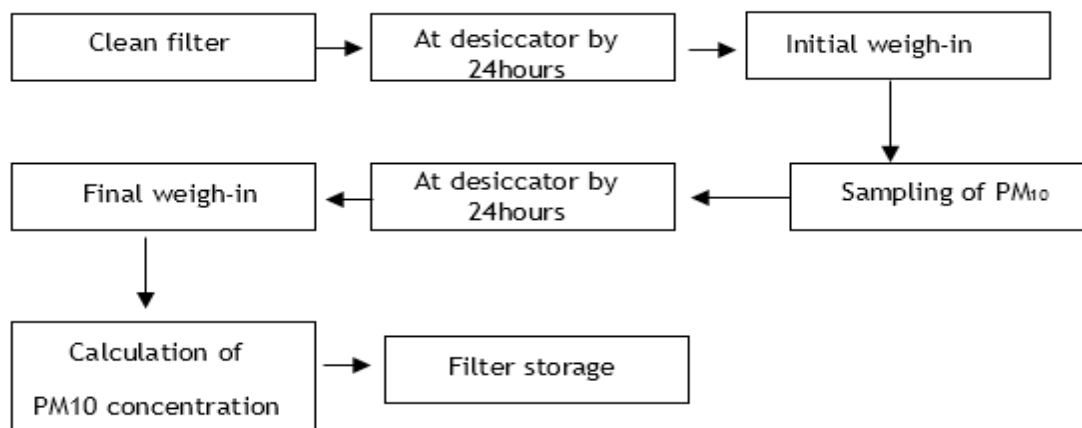


Figure 3. Schematic diagram of the PM₁₀ sampling methodology

The equation used to calculate the concentration:

$$\text{PM}_{10} \text{ is: } C = 10^6 \frac{M_t}{V_r} \text{ } [\mu\text{g}/\text{m}^3],$$

where: M_t is difference between final weigh-in and initial weigh-in, and V_r is real volume to sample.

2. Visualization system

An efficient information visualization tool should be designed aiming at reduce the cognitive effort

involved in the data analysis process (Goethem et al., 2016). Figure 4 shows a schematic diagram of the interactive information visualization methodology. Thus, to provide support to the visual analysis of acquired data, an interactive web-based visualization interface was built, which is available online with free access at <https://evortigosa.github.io/health2/>.

The interface was developed mainly in the JavaScript programming language with D3.js graphics library (Bostock et al., 2011).

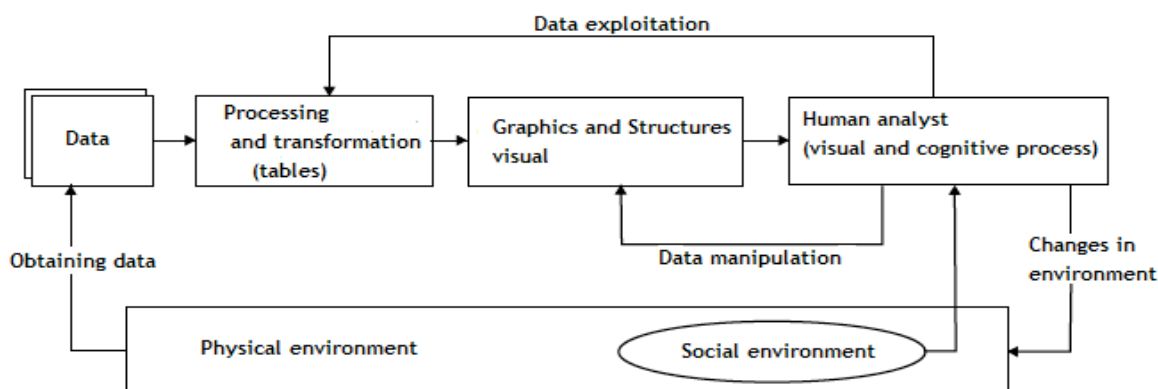


Figure 4. Schematic diagram of interactive information visualization (Ware, 2004)

3. Respiratory System Diseases

The datasets consist of time-variant data, or time series, containing medical registers of diseases

related to the human respiratory system and were obtained from the Hospital Information System from SUS (Sistema Único de Saúde), which is maintained by the Ministry of Health. The SUS collects dozens of variables related to hospital admissions in public

and private institutions, throughout the whole Brazilian territory, generating an extensive database that provides a big picture of health in Brazil. These data are compiled and made available according to the month and year of occurrence and can be accessed at <http://www2.datasus.gov.br/DATASUS/>.

For the visual analysis, the following variables were selected: laryngitis, pneumonia, bronchitis, tonsillitis, asthma and other diseases. The temporal evolution of each selected disease was grouped according to the patients' age, within 8 age ranges: under 5 years, 5 to 9 years, 10 to 19 years, 20 to 29 years, 30 to 39 years, 40 to 49 years, 50 to 59 years and 60 years or more.

FINDINGS AND ARGUMENT

To contrast with the before mentioned SUS data, three PM10 datasets were considered: the first set was acquired daily (April 2014 to April 2015); the second on alternate days (May 2015 to November 2017); and the third are historical data from 1997 to 2006 (twice a week acquisition). Note there was a time gap between 2006 and 2014 when there was no air quality monitoring program in São Carlos.

Figure 5 and Figure 6 show examples of visual analysis regarding two respiratory diseases: Figure 5 presents the behavior of PM10 concentration versus Pneumonia evolution; Figure 6 contrasts PM10 with Asthma. The interface present information from 2004 and 2014 in both scenarios. As can be observed through the years, an increase in the PM10 concentration in the atmospheric air is followed by an increase in medical records of human respiratory system diseases.

In Figures 5 and 6 it is possible to observe on the right side of both Figures five general profiles of time series devoted to present an overview of the other analyzed diseases. In other words, the red colored area charts present the general behavior of the other diseases related to the same PM10 period, covering all the acquired information on the same screen's space.

The colors of each bar represent the age ranges under analysis and presents a piece of important

information: the more sensible age groups to respiratory diseases are concentrated in two ranges, people under 5 years and those with 60 years or more.

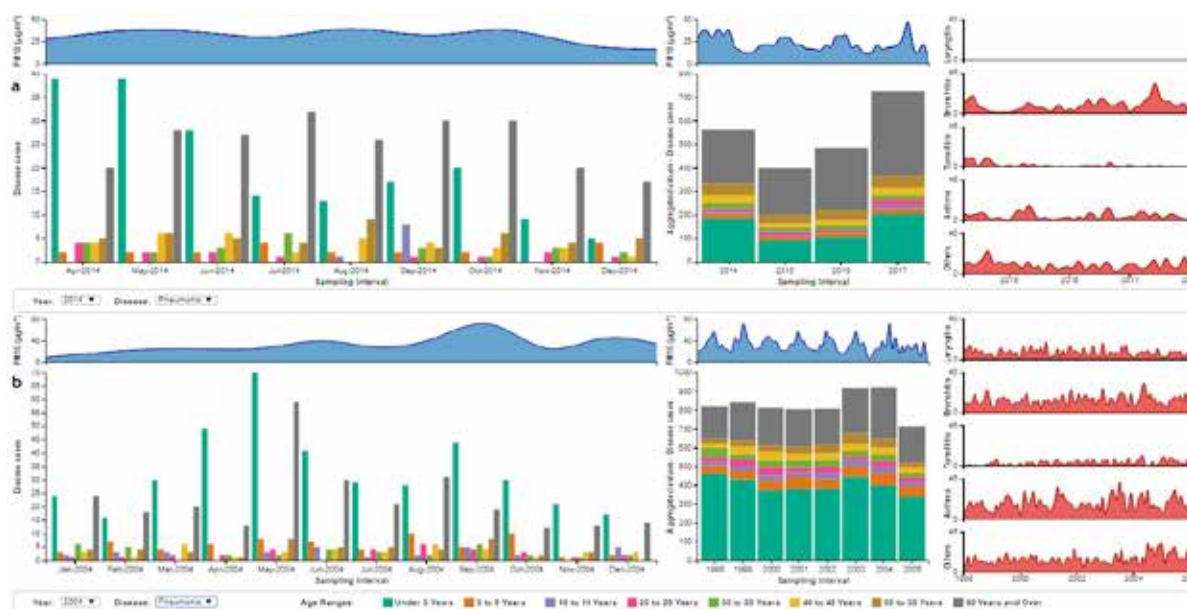


Figure 5. Annual evolution of the age groups diagnosed with Pneumonia, under the mean values of PM10 for the year 2014 (area chart above) and 2004 (area chart below-b)

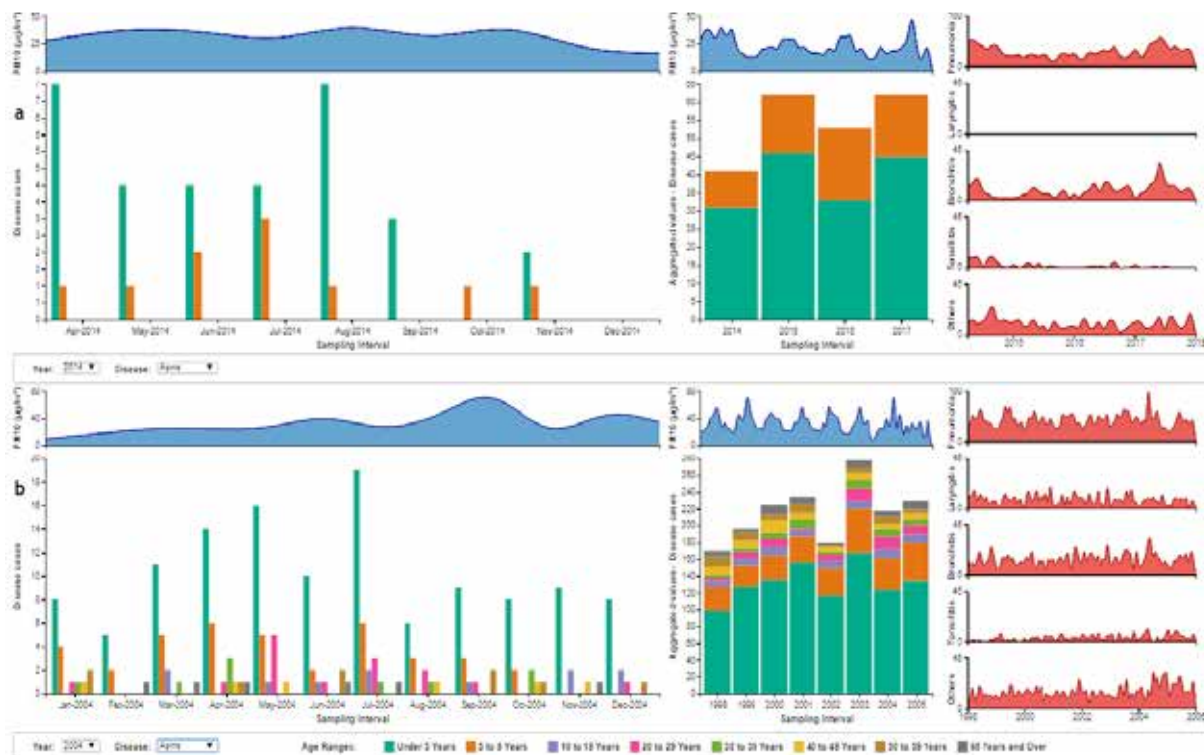


Figure 6. Annual evolution of the age groups diagnosed with Asthma, under the mean values of PM10 for the year 2014 (area chart above) and 2004 (area chart below-b)

CONCLUSIONS

Particulate matter and respiratory tract diseases visual analysis revealed that in the last decades there was an improvement in the air quality in São Carlos-SP, mainly due to new practices and regulations in pollution sources, and as observed, there was a significant reduction in cases of people with diseases affecting their respiratory system.

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CA/CPB ELECTROSPUN NANOFIBER AND THEIR POTENTIAL APPLICATION FOR RETENTION OF FINE ATMOSPHERIC PARTICLES

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Abstract: Control the atmospheric particles emission is very important for environment and human's health. Actually, several equipment and systems are available in the market to control atmospheric emissions, those from industries uses. Among these, we can mention filters, which may have composition and varied models according to the gaseous effluent to be treated. Therefore, biodegradable filters of cellulose acetate/cationic cetylpyridinium bromide (CPB) nanofibers were prepared by electrospinning, in order to apply it on retention of fine atmospheric particulate matter. Thus, this work aims to compare its fiber diameter and morphology with the glass fiber HEPA (High Efficiency Particulate Air) commercial filter. The fiber diameter of the developed nanofiber was about 200 nm, and for the HEPA filter it was about 600 nm. In addition, based in this size and morphology is expecting to retain smaller particles size when compared to HEPA. For this, are necessary several tests, in order to know its permeability and efficiency, and then propose an application of this new nanofiber as a tertiary treatment for air cleaning.

Keywords: Air pollution control, nanofiltration, particulate matter, efficiency.

INTRODUCTION

Actually, several equipment and systems are in the market to control atmospheric emissions, especially those from industries. Among these, we can mention the filters, which may have composition and models varied according to the gaseous effluent to be treated (Nevers 2010; Theodore and Buonicore 1976).

Research on materials applied to the control of air pollution is gaining notoriety, such as those involving the development of new polymers (Liu et al. 2015) and biomaterials (Leson and Winer 2012), as well as the process of adsorption by plasma (Urashima and Chang 2000). The electrospinning technique is widely used in the production of nanofibers, since its products have a uniform appearance, besides allowing the use of several polymer solutions (Ramakrishna et al. 2006; Schiffman and Schauer 2008). Cellulose acetate (CA) is a biodegradable semi-synthetic polymer, and its natural source is cellulose, a polymer found in greater abundance on the planet (Goetz et al. 2016). When surfactants are added to polymer solutions, they confer structural stability to these materials (Kvítek et al. 2008), as well as in the case of nanofibers reducing their diameters and the formation of beads (Zheng et al. 2014).

Thus, this work aims to compare the CA/CPB nanofiber, specially its fiber diameter and morphology, to the glass fiber HEPA (High Efficiency Particulate Air) commercial filter, using Scanning electron microscopy (SEM) images.

METHODS

The diameter and morphology of the CA/CPB electrospun nanofibers were evaluated by SEM, using a Quanta 250 (Philip-FEI) microscope equipped with dispersive energy spectroscopy (EDS). For analysis, the samples were dispersed in double-sided tape coated with a thin layer of gold (30 nm). From the images obtained in the SEM, the average diameter was calculated using the Software Size Meter 1.1. For the glass fiber HEPA, the data were obtained in the research of Bortolassi et. al. (2017).

FINDINGS AND ARGUMENT

For the two fiber types, the obtained SEM images are shown in Figure 1. The electrospun nanofiber (a) is bead-free, and has small and homogeneous diameter distribution (Table 1). Zuo et al., (2005) and Lin et al., (2012) affirm that cationic surfactants prevented the formation of beads, when added to polymer solutions. The use of a non-ionic surfactant no longer completely prevented the

formation of granules, so it was hypothesized that the charged surfactants increased the solution conductivity, and the net charge density, causing an increase in instability, producing more uniform fibers (Zheng et al. 2014).

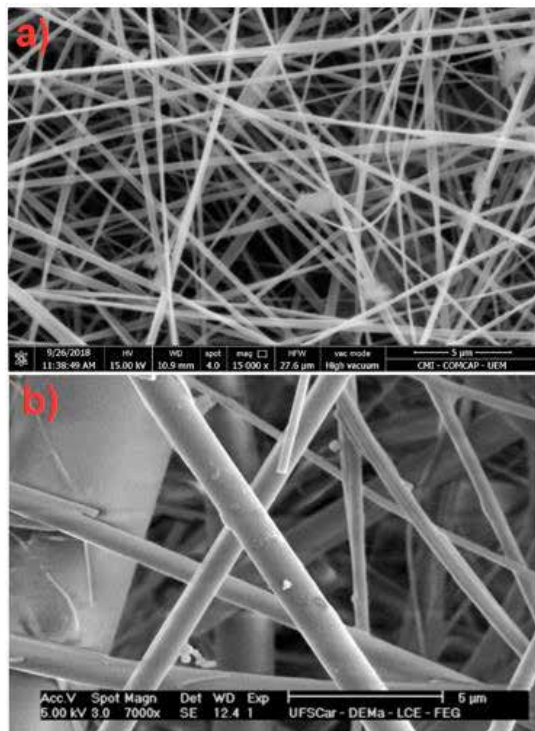


Figure 1. Scanning Electron Microscopy image of CA/CPB nanofiber (a) and glass fiber HEPA filter (b).

The average diameter of the HEPA filter is about 600 nm (Bortolassi et. al. (2017), much bigger than the CA/CPB. Based on this and in its morphological aspect is possible to affirm that the developed nanofiber could be used as an air filter too. Besides that, is important perform other tests in order to know its behavior in contact with an air flow containing particles.

Table 1. Header

Material	Average Diameter (nm)
CA/CPB nanofiber	227 ±0.32
Glass Fiber HEPA	590

CONCLUSIONS

Based on this exploratory research, it is concluded that is possible to use the CA/CPB electrospun nanofiber as an air filter, hence this type of material is been largely used actually. When compared to the glass fiber HEPA, it shows small fiber diameters and homogeneous distribution. To affirm assertively this

are necessary tests to analyse the feasibility of this application (e.g., permeability, efficiency on particle retention and pressure drop tests).

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EVALUATION OF FILTER MEDIA FOR BAGHOUSE FILTERS IN A STEEL INDUSTRY

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Abstract: Nowadays, in addition to complying with the emission limits determined by the laws, some companies seek to minimize their operating costs. In order to achieve this, they should choose a material suitable for the filter media, considering gas characteristics (mass flow, temperature and corrosivity) and particulate matter (hygroscopy, abrasiveness and size). It is also necessary that the filter has extended span life and operate with low pressure drop and high collection efficiency for fine particles. Thus, this study aims to compare the performance of two filter media, polyester and polyester with PTFE membrane from two manufacturers (A and B), generally employed in the secondary dust removal system of a steel mill, using pulse jet cleaning. In this way, were analysed the collection efficiency of filter media for micrometrics particles and the filtration tests on a filter equipment based on VDI 3926 standard that simulates a reverse air pulse jet bag filter. Experimental results from the first filtration cycle show that the fabrics of manufacturer A had less total filtration time and higher efficiency than the B filter media.

Keywords: Baghouse filter, filter media, filtration, pulse jet, steel mill

INTRODUCTION

Bags are filter media that can be made of different materials and receive various treatments. One of the materials most used in industrial bag filters is polyester, since it supports relatively high temperatures (130 °C) and has a low relative cost compared to other materials. It can be coated with PTFE (polytetrafluoroethylene) to reduce the emission of particulate matter, to protect the filter media against particle penetration, to reduce adhesion between the cake and the fibers, making cleaning easier. Since manufacturers may have different production and quality control processes, filter media may differ in efficiency of collection, pressure drop, life, and other characteristics (Aleksandrov et al, 2010).

Therefore, it is extremely important to choose a filter media for each industrial process. It should reconcile high life, low pressure drop, high particle collection efficiency. It should be constituted of a material that supports the gas properties (temperature and corrosivity) and the particulate material (hygroscopy, abrasiveness and size) (Turner et al., 1998). Since a bag filter can have thousands of square meters of filtration area and an industry can rely on dozens of such equipment, the application of a misplaced filter medium can result in the early exchange of the bags, excessive energy expenditure in the ventilation system, emission of particles above legal limits and damage to the

health of the population, resulting in a significant financial loss for the industry.

Sherman, Leith and Symons (1990) evaluated through 24 experimental conditions the penetration of particles in different filter media, using a pilot scale cleaning filter with pilot scale jet and limestone powder and fly ash. They observed lower emission of particles for PTFE treated sleeves in all experimental conditions. Schiller and Schmid (2014) performed filtration tests with the objective of determining the best combination of 3 precoating materials and 11 types of filter media in the capture of ultrafine particles (<370 nm) present in the gases of a wood pellet heater.

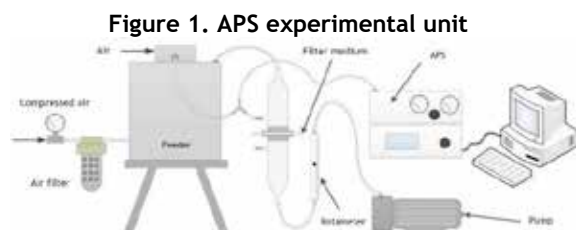
Thus, in this work, polyester filter media with and without PTFE membrane from two manufacturers were evaluated. Characterization of the particulate material collected in the bag filter of the process under study and of the filter media, evaluation of the efficiency of collection of fine particles (PM_{2.5}), ultrafine (PM_{1.0}) and nanometrics (10 to 300 nm) and tests based on the VDI 3926 standard.

METHODS

Efficiency collection of Micrometrics Particles

For the polyester (PE) filter media, with and without the PTFE membrane of the two suppliers (A and B), filtration tests with steelworks powder were performed in the experimental unit shown in Figure

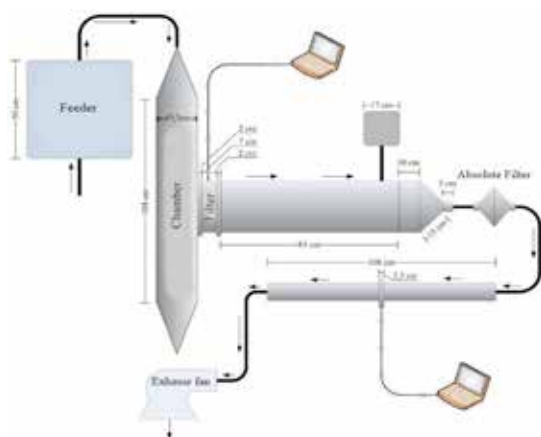
1. This unit is composed of a TSI model 3433 aerosol generator, a TSI 3302A aerosol thinner, an Aerodynamic Particle Sizer 3320 (APS) spectrometer, also from TSI, filtration unit with a rotameter and a vacuum pump. The filtration area of the filter medium was 17.57 cm² (diameter 4.73 cm), and the air-cloth ratio used was 2 m/min, the same as that of VDI 3926.



Filtration cycles

The filter media were subjected to filtration tests with air and steelworks powder til the pressure drop limit of 100 mmH₂O when was cleaned by pulse jet of 5 bar. The filtration equipment used was based on the test rig of VDI 3926 standard. The particulate matter used was the dust collected from the secondary dedusting bag filter of the steelworks. The filter medium and the absolute filter were weighed before and after the experiment to calculate the efficiency of collected. The tests were done in triplicate. The objective of these experiments was to compare the performance of the filter media in cycle duration, collection efficiency and collected mass in the filter media.

Figure 2. Filter equipment



The collection efficiency was calculated according to Equation 1, which represents the fraction of the particles retained by the filter medium. C_i and C_f are, respectively, the concentration of particles before and after the filter (Cirqueira et al, 2017).

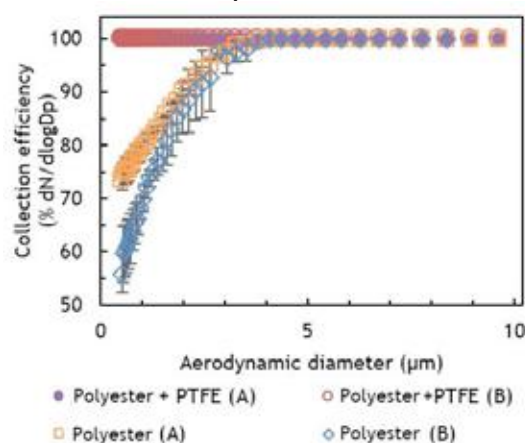
$$E = \frac{C_i - C_f}{C_i} \times 100\% \quad \text{Eq. (1)}$$

FINDINGS AND ARGUMENT

Efficiency collection of Micrometrics Particles

Filtration tests for micrometrics particles (0.523 to 10 µm) were performed in the APS unit (see Fig. 1). The collection efficiency of polyester filter medium from manufacturer A was 100% for PM₁₀, 94% for PM_{2.5} and 79% for PM_{1.0}, while for manufacturer B was 100% for PM₁₀, 95% for PM_{2.5} and 66% for PM₁. On the other hand, the filter media PE with PTFE membrane demonstrated an efficiency higher than 99% for the entire diameter range analyzed, with no great differences between the manufacturers.

Figure 3. Efficiency collection of micrometrics particles

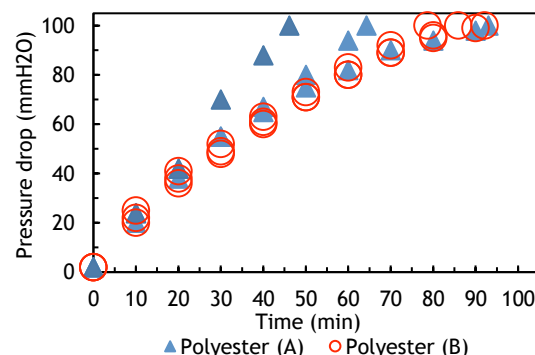


Filtration cycles

For analyze cycles duration and efficiency collection were done filtration tests in filtration unit based on the standard VDI 3926 (see Fig. 2) for polyester filters (PE and PE with PTFE) from both manufacturers.

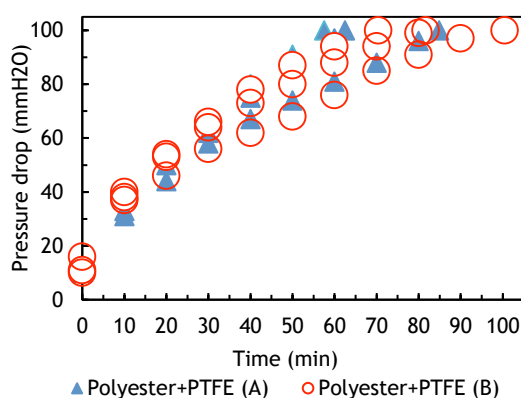
Figure 4 shows the triplicates pressure drop curves measured on the filter as a function of filtration time, for the polyester filter media from manufacturers A and B.

Figure 4. Pressure drop curves for polyester filter media



The filter of polyester from manufacturer B showed lower deviations from cycle duration (8%) than manufacturer A (38%). However, this was not observed for PTFE membrane polyester from manufacturer B (see Fig. 5), which showed a deviation of 18% over the cycle duration, but still lower than the observed for the manufacturer A. The initial pressure drop of PTFE-membrane filter media is greater than those without such membrane. This occurs because the PTFE membrane acts as an additional filter media, causing the increase in total pressure drop.

Figure 5. Pressure drop curves for polyester with PTFE membrane filter media



The collection efficiency of the polyester of manufacturer A was 99.95 ± 0.02 while for manufacturer B, was 99.96 ± 0.03 . For PTFE membrane filter media, manufacturer A was 99.98 ± 0.01 and 99.97 ± 0.02 for manufacturer B. Filters from manufacturer B collected more particulates over a longer filtration time than filters from manufacturer A.

The mass collected by the polyester filter medium of manufacturer A was $15.0 \pm 31\%$ while that of manufacturer B was $16.8 \pm 11\%$. For PTFE membrane filter media, manufacturer A retained $15.8 \pm 14\%$ and manufacturer B, $18.2 \pm 9\%$. It is also noted that the deviations presented for manufacturer B were 11% in relation to the collected mass and 8% in relation to the filtration time, being smaller than those of the manufacturer A (31% for the mass and 35% for the filtration time).

Regarding the collection efficiency, the values obtained were similar for all media analyzed, regardless of the supplier and the presence of the PTFE membrane, varying from 99.95% to 99.98% with deviations of 0.01 to 0.03%. This observed high efficiency can be related to the clogging point that was smaller for these filter media, forming in a short time the cake that acts as a new barrier for the particles.

A longer cycle duration to achieve the maximum pressure drop during gas filtration is a desirable for

the filter media used in pulsed jet cleaning bag filter, since is necessary a lower pulse frequency of air for cleaning resulting in longer lifespan for the bags. Therefore, it reduces the energy expenditure with the cleaning system. In view of that, filter media of manufacturer B obtained better results during the first filtration cycle, since they had a higher amount of mass retained in a longer filtration time.

CONCLUSIONS

From 0.523 to 10 μm , the polyester from manufacturer A obtained higher efficiencies over most of the diameter range.

In relation to the filtration tests performed on the equipment based on the VDI 3926 standard, the filter media of the manufacturer B obtained a longer average time in the first cycle without cleaning, retaining more mass.

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INFLUENCE OF OPERATING CONDITIONS ON THE ELECTROSTATIC PRECIPITATION OF NANOPARTICLES

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Abstract: Electrostatic precipitator is an industrial equipment used to collect particles from the air. Removal efficiency is affected by operating conditions and geometric parameters. Thus, this study evaluated the performance of a wire-plate ESP in the removal of NaCl nanoparticles from air. The experiments were performed with 2 and 4 discharge electrodes at different air velocities (1.03, 2.04 and 4.08 cm/s) and electric fields (3.08, 3.23 and 3.38 kV/cm). It can be concluded that the addition of discharge wires increases collection efficiency due to increase of current-voltage. The same behavior is obtained with the increase of electric fields. In contrast, the decrease in air velocity (1.03 m/s) caused a high collection efficiency, due to the increase in residence time.

Keywords: Electrostatic precipitator, particulate matter, geometry.

INTRODUCTION

Air pollution is mainly caused by the emission of particulate matter and long-term exposure can cause several health problems due to the deposition of these particles in the respiratory system. Industrial activities account for the majority of emissions, requiring the use of a control device to achieve the emissions levels allowed by the environmental legislation. In this context, electrostatic precipitators (ESPs) are widely used because they provide high collection efficiency and can be applied in processes with different operating conditions.

The main components of the ESPs are the collector plates and the discharge electrodes. In the wire-plate configuration, the wires are placed between the plates. The operating principle of the ESPs is to provide high voltage to the discharge electrodes, which will create an electrical field within the equipment, responsible for the air ionization. As the aerosol passes through the equipment, the particles are charged electrically and will be attracted to the collection electrodes, reducing the concentration in the outlet airflow.

The collection efficiency in the ESP depends significantly on operating conditions and geometric parameters, such as the number of discharge and collection electrodes, plate-to-plate and wire-to-wire spacing. Kasdi (2016) evaluated the influence of the number of wires, varying from 1 to 5, in a wire-plate ESP and concluded that the increase in the number of discharge electrodes improved the ESP performance. Oliveira and Guerra (2018) studied the effect of air velocity (1.7 - 19.9 cm/s) and electric field intensity (3.95 - 4.10 kV/cm). The collection efficiency presented a significant

variation, despite the small electric field increase, and higher velocities reduced this efficiency due to shorter residence times.

In this context, this study evaluated the influence of the number of discharge electrodes (wires) on the removal efficiency of an ESP operating at different air velocities and electric field.

METHODS

The experiments were performed on a wire-plate electrostatic precipitator consisting of two 6.5 cm spaced copper collector plates (30 x 10 cm) and stainless-steel discharge wires of 0.4 mm in diameter and spaced 6.5 cm apart. Figure 1 shows a schematic representation of the experimental apparatus.

In the experimental unit, there are purification filters that remove impurities from the inlet air. Nanoparticles of NaCl are generated by a TSI aerosol atomizer model 3079A and dispersed on inlet air. The aerosol is then passed through a TSI diffusion dryer model 3062 to retain the moisture excess. Before entering the ESP, the particles charges are neutralized by a Krypton-85 source. The ESP, connected to a high voltage SPELLMAN SL300, is responsible for air ionization, particle charging and collection. A TSI 3079 Scanning Mobility Particle Sizer (SMPS) was used to measure the efficiency of ESP in the collection of particles ranging from 5.83 to 228.8 nm. As the SMPS classifies the particles according to the electric mobility, before entering in the SMPS the aerosol was also neutralized by an Americium-241 source to prevent the measurements from being affected.

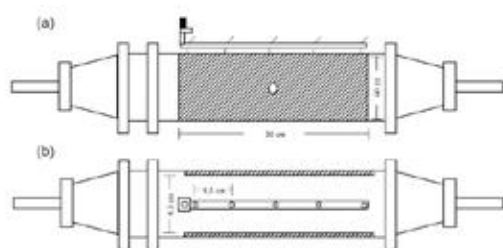


Figure 1. Schematic representation of the ESP:
(a) side view; (b) upper view

In this study, the concentration of NaCl in the atomizer was set at 0.1 g / L and the air velocity inside the ESP was 1.03, 2.04 and 4.08 cm/s. For each velocity, the influence of the electric field was evaluated to 3,08, 3,23 and 3,38 kV/cm. The ESP configuration was also studied, so the experiments described above were performed with the ESP configuration of 2 and 4 discharge wires, operating in negative polarity. All experiments were performed in triplicate.

The collection efficiency (η) was calculated by Equation 1, which relates the inlet (C_i) and outlet (C_o) aerosol concentration. It was used to determine which operational and geometric condition reached the highest particle removal. The influence of the residence time on particle removal was also evaluated; this parameter is calculated by the ratio of the ESP volume and the volumetric flow rate.

$$\eta = \frac{C_i - C_o}{C_i} \quad (1)$$

FINDINGS AND ARGUMENT

Figure 2 shows the current-voltage curves for each operational condition. Although the behavior of the curves obtained for 2 and 4 wires was almost the same, the current achieved for 2 wires was lower than 4 wires. As can be seen in Figure 2, the increase in current was greater with increasing voltage.

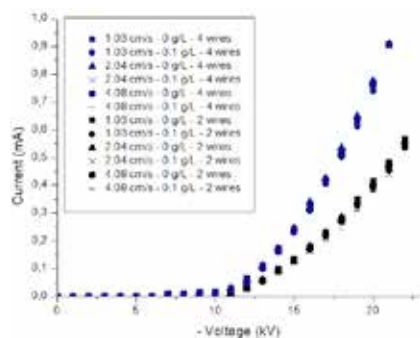


Figure 2. Current-voltage curves for 2 and 4 wires

Before analyzing the efficiency results, it is important to know the behavior of the inlet aerosol

particle size distribution. Figure 3 shows that most particles have a diameter on the range from 10 to 100 nm. Table 1 shows that the median diameter in the inlet flow was around 29 nm, with low values of geometric standard deviation (GSD), indicating a good data accuracy. According to Parker (1997), the main charging mechanism for particles with this size is the diffusional one.

As can be seen in Table 1 the increase of air velocity decreases the aerosol concentration.

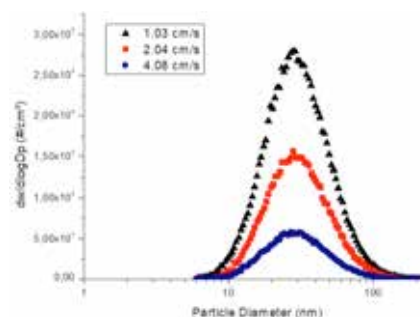


Figure 3. Inlet particle size distribution

Table 1. Median diameter (M.D), GSD and total inlet concentration (C_i)

	Wires	Velocity (cm/s)		
		1.03	2.04	4.08
M.D (nm)	2	28.97 ± 0.24	29.35 ± 0.11	29.26 ± 0.24
	4	29.11 ± 0.04	29.36 ± 0.54	30.03 ± 0.18
GSD	2	1.64 ± 0.02	1.64 ± 0.00	1.63 ± 0.01
	4	1.65 ± 0.01	1.66 ± 0.01	1.67 ± 0.00
Total C_i (µg/m³)	2	14.57 ± 2.33	7.41 ± 0.67	2.86 ± 0.27
	4	14.05 ± 1.19	9.40 ± 1.37	4.07 ± 0.29

The electric field effect is shown in Figure 4 for each velocity. As can be seen in Figure 4-a, the lowest velocity presented the highest collection efficiency, almost 100% for 3.23 and 3.38 kV/cm. However, for 3.08 kV/cm the removal was around 70% for 4 wires configuration and 50% for 2 wires. Increasing the air velocity to 2.04 cm/s (Figure 4-b) resulted in a reduction in the collection efficiency, which was more significant to 3.08 kV/cm. This effect was more pronounced for air velocity of 4.08 cm/s (Figure 4-c). Only the collection efficiency for 4 wires and 3.38 kV/cm remained around 97%. There was also an abrupt decrease for 2 wires and 3,23kV/cm, demonstrating the influence of the air velocity.

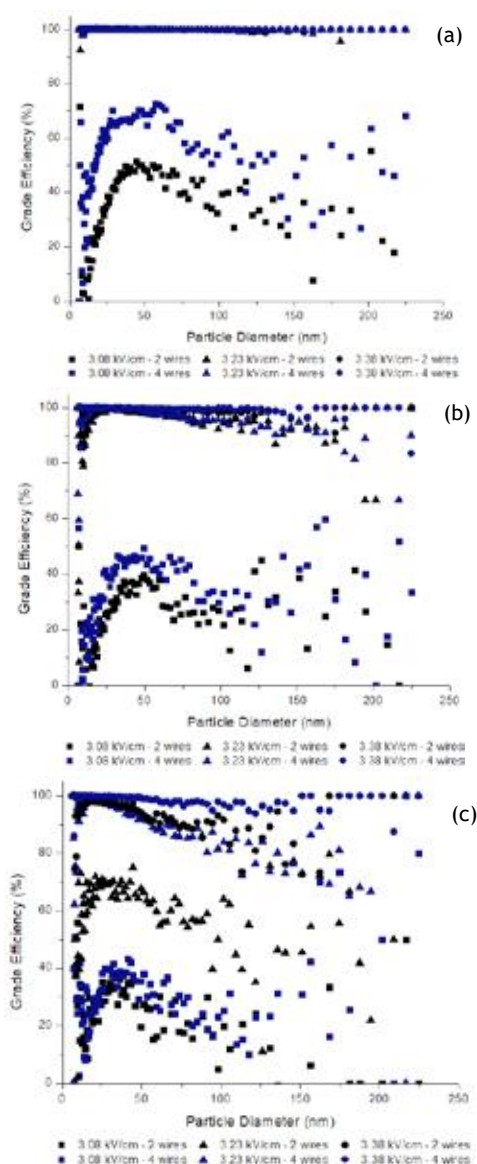


Figure 4. Grade efficiency to different electric field and number of wires for air velocities of (a) 1.03 cm/s, (b) 2.04 cm/s and (c) 4.08 cm/s

In order to have an overview of these results, the overall efficiency (Table 2) was calculated considering the inlet and outlet total concentration of the ESP. The results show that the increase in the air velocity reduced the overall efficiency in all experiments. The experiments with 4 wires achieved higher collection efficiency when compared with those for 2 wires, due to the higher electric field intensity and the current produced. This behavior was expected from the previous analysis of the current-voltage curves. Moreover, the overall efficiency increased with the electric field, this change was more significant from 3.08 to 3.23 kV/cm, where the maximum increase was 71% for 2 wires configuration and 2.04 cm/s air velocity.

Table 2. Overall Efficiency

Number of wires	Velocity (cm/s)	Electric Field (kV/cm)		
		3.08	3.23	3.38
2	1.03	41.57 ± 2.08	99.87 ± 0.06	99.92 ± 0.01
	2.04	28.87 ± 1.37	96.16 ± 0.51	99.20 ± 0.14
	4.08	21.59 ± 1.69	59.96 ± 1.33	91.79 ± 0.40
4	1.03	61.01 ± 7.39	99.88 ± 0.06	99.99 ± 0.01
	2.04	38.78 ± 1.80	96.40 ± 0.70	99.53 ± 0.08
	4.08	29.35 ± 0.18	86.92 ± 0.89	97.98 ± 0.09

In addition, the increase in air velocity reduced the overall efficiency, this difference is more relevant for 2 wires configuration. In this case, the electric field of 3.38 kV/cm achieved collection efficiency of 91% for 4.08 cm/s, an 8% reduction compared with the lower velocities. This behavior is related to the residence time, since the increase in air velocity reduces the duration of particle charging and collection. The residence time for the velocities of 1.03, 2.04 and 4.08 cm/s were 29.18, 14.72 and 7.36s, respectively. Then, the increase in air velocity from 1.03 to 4.08 cm/s reduced in 21s the residence time, which decreased the collection efficiency.

CONCLUSIONS

In this study, the influence of air velocity, electric field and number of discharge electrodes is evaluated in a wire-plate ESP. The analysis of the current-voltage and efficiency curves showed that a small increase in the electric field improved the ESP efficiency. However, increasing air velocity resulted in a lower collection efficiency, due to decreased residence time. The 4-wire configuration presented the most efficient collection, but particle collection for 2 wires were very similar to it under experimental conditions at low velocities and high electric field. Then, the ESP tested it is efficient and can operate under different conditions.

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ADVANCE AIR POLLUTION TREATMENT TECHNOLOGIES: APPLICATION OF SMART NANOMATERIALS

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Abstract: Environmental pollution is one of the current major global challenges faced by human beings. In the past two decades, the evolution of nanotechnology represents a revolution in the design, discovery, creation, and novel utilization of artificial nanoscale materials. To cope with environmental sustainability, nanomaterials have been employed in environmental sectors with several fashions. Nanotechnology provides novel treatment approaches and creates new technologies with superior advantages compare to the conventional techniques. The objective of this study is to present, the recent developments in air pollution treatment technologies due to smart nanomaterials. Several types of nanomaterial i.e., Carbon nanomaterials, Metallic Nanomaterials & Polymeric have been reviewed. Then their application as nano-adsorbents, nanofiber membranes, nanofiltration membrane & nanocatalysts for the removal of pollutants from air, have been discussed.

Keywords: Environmental pollution, nanotechnology, nanoscale materials, removal of pollutants, application of smart nanomaterials.

INTRODUCTION

The need for new technologies using existing materials was the beginning of a revolution through which nanoscience and nanotechnology emerged. Environmental pollution is one of the current major global challenges faced by human beings. In the past two decades, the evolution of nanotechnology represents a revolution in the design, discovery, creation, and novel utilization of artificial nanoscale materials. To cope with environmental sustainability, nanomaterials have been employed in environmental sectors with several fashions. Nanotechnology provides novel treatment approaches and creates new technologies with superior advantages compare to the conventional techniques. The objective of this study is to present, the recent developments in air

pollution treatment technologies due to smart nanomaterials.

METHODS

The work was carried out through research on articles related to the control of atmospheric pollution with the use of nanotechnology.

FINDINGS AND ARGUMENT

Different types of nanomaterials, such as carbon nanotubes, metals (oxides) and biological nanomarkers and are being discovered every day and, because more efficient, light, adequate and mainly low-cost final products are feasible. Several types of nanomaterial i.e., Carbon nanomaterials, Metallic Nanomaterials & Polymeric have been reviewed.

There are many products that have nanotechnology in their formulation and has grown by an average of 20% over the last few years according to the inventory of consumer products with nanotech components available on the world market (Project on emerging nanotechnologies 2018) and it can be used in the food industry, cosmetics, pesticides, clothing, digital cameras, automotive paints, among others. According to Startnano, the number of products with nanoparticles is 6059 in 825 companies in 47 countries, mainly in the cosmetics, construction and textile industries, with the United States being the country with the largest quantity and variety of products containing nanotechnology.

Moreover, there is the application of nanomaterials in the process of environmental decontamination, and this is due to the high chemical reactivity presented by these materials.

Graphite-based composite nanomaterials have properties that have recently been exploited for environmental decontamination (LIU; ZHOU; JIANG, 2014).

According Mukherjee (2016) the nanoparticles can present totally new characteristics due to their high relation surface/volume which make them more reactive than bulk forms of the same materials.

There are three major ways in which nanotechnology is being used to treat and reduce the different air pollutants; adsorption by nano-absorptive materials, degradation by nanocatalysis, and filtration/separation by nanofilters.

Nanotechnology assumes that many of today's problems, including air quality, can be solved or improved using nanoscale adsorbents, called nanoadsorbents. The carbon nanostructures have extremely physical properties, such as the average pore diameter, pore volume and surface area.

CONCLUSIONS

The rapid growth of nanotechnology has gained interest in the applications of nanomaterials potential in improved systems for monitoring.

Nanomaterials are excellent adsorbents, catalysts and sensors due to their large specific surface areas and high reactivities.

Air contaminants can be remediated and treated by various methods using nanomaterials as adsorbents.

Nano-adsorbents, nanofiber membranes, nanofiltration membrane & nanocatalysts for the removal of pollutants from air, have been discussed.

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EXPERIMENTAL AND NUMERICAL INVESTIGATION OF BUILDING EFFECTS ON WIND EROSION OF A GRANULAR MATERIAL STOCKPILE

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Abstract: In the present work, wind tunnel experiments and numerical simulations were carried out to evaluate the physical behaviour of the fluid flow surrounding an stockpile in the presence of an isolated cubic building upstream. Experimental results for the present cases were compared with those for the isolated stockpile configuration (without building). Observing the differences in the erosion patterns (non-erodible particle accumulation on the surface) and emission estimates (differential weighing) was possible to conclude that: (i) the emissions considerably increase due to the presence of the building, (ii) the higher the free stream velocity, due to the presence of the obstacle, the more efficient the dynamics of the pavement process is and (iii) the increase of the gap between the building and the pile does not generate expressive changes in the emitted mass measurements as the building orientation. These findings play an important role since it is possible to obtain an optimal industrial open yard configuration where fewer particles are emitted to the atmosphere.

Keywords: Air pollution, Wind erosion, Industrial site arrangement, Particulate matter, Emission control.

INTRODUCTION

Wind erosion process can lead to several environmental consequences as loss of material and increase of particulate concentrations to the atmosphere. The air pollution is of particular interest since it has a direct impact on human health, mainly in regions with high availability of diffuse sources such as ore and coal stored in piles on open yards of industrial units.

Wind erosion is dominated by the aerodynamic forces (drag and lift forces) that acts to remove the particle from the surface and by the gravity and cohesion forces that acts to restrain its movement. The aerodynamic forces is usually quantified by the friction velocity, $u_* = \sqrt{\tau/\rho}$, a variable that represent the conceptual value of shear stress, τ , on the surface. The gravity and cohesion forces are considered by the threshold friction velocity u_{*t} , which defines the minimum friction velocity in which particle movement is initiated (Shao, 2008). The balance between the friction velocity and the threshold friction velocity determines a criteria (Shao and Lu, 2000) that are used to know if particles will move or not. It is important to discuss that u_{*t} is related to surface properties, such as texture, moisture, density of the material and particle size distribution, while u_* is related to surface aerodynamic properties and atmospheric flow conditions (Shao, 2008). However, specific scenarios in the context of industrial open yards can

also influence these properties, as stockpiles geometries and structures in the stockpiles surroundings, as equipments, buildings and even other stockpiles. Turpin and Harion (2010), Ferreira and Fino (2012), Ferreira et al. (2013) and Furieri et al. (2012) have shown that the surroundings can influence the shear stress distribution patterns over the stockpile surface causing increase in the emitted mass depending on the distance and position of the object next to the pile in relation to the incident flow.

In the present work, wind tunnel experiments and numerical simulations were carried out to evaluate the physical behaviour of the fluid flow interacting with stockpiles and to quantify the emission of an stockpile in the presence of an isolated cubic building.

METHODS

The study was divided in two parts. In the first part, the experimental study was carried out in a wind tunnel with the following main dimensions: $H_s = 0.80$ m (height), $W_s = 1.50$ m (width) and $L_s = 8.12$ m (length). The dimensions of the sand stockpile model present a scale ratio of approximately 1:200 to a real one. The methodology of the experiments carried out is the same used in previous works. For more details, see the work of Furieri et al. (2013).

Sand with density equal to $\rho_p = 2,630 \text{ kg/m}^3$ was used to compose a bimodal granulometry mixture with 80% of white sand (56.0 to 194.2 μm) and 20% of black sand (700.0 to 1300.0 μm). Three parameters were varied during the experiments: (i) gap between the building and the pile equals 0.5 and 1.5 times the cubic model height H_b , (ii) orientation of the cube to the main flow, with angles equal 90° (face-on) and 45° (edge-on) relative to the pile, and (iii) free stream velocities, 7, 8 and 9 m/s.

In the second part, numerical simulations were performed to provide the wall shear stress distribution on the pile surface and the flow pathlines, which could be associated to the erosion patterns observed in the experiments and may be input data to mathematical emission models (de Moraes et al., 2018). Numerical simulations were carried out using the commercial software Ansys Fluent 15.0 to solve the three-dimensional equations of mass and momentum conservation. Turbulence effects were accounted using the κ - ω Shear Stress Transport (SST) model (Menter, 1994).

The inlet boundary conditions for velocity (u , v and w), turbulent kinetic energy (κ) and specific dissipation rate (ω) were obtained from previous numerical simulations (precursor empty domain) where a periodic streamwise flow was set to produce a fully developed channel flow. For the outlet boundary conditions, it was assumed that the flow is fully developed. For the upper boundary condition, symmetry was imposed. Smooth walls with no-slip conditions are set at lateral domain walls, as well, at stockpile, cubic building and ground walls.

FINDINGS AND ARGUMENT

Emitted mass measurements from the wind tunnel experiments with an isolated stockpile and a stockpile downstream a cubic building is showed in the Table 1. The results reveal that emissions considerably increase due to the presence of the building, that is, the isolated stockpile emits less than the pile downstream a cubic obstacle for all tested configurations. Furthermore, if the stockpile is downstream an edge-on cubic building, the impact is even stronger. However, as discussed above the isolated stockpile, that is, a stockpile far enough from any obstacle, emits less in all tested cases.

It is important to pointed out that there is an accumulation of sand on the ground between the cube and the pile for the tested cases. Therefore, the emitted mass can be higher than the estimated amount presented in Table 1 if the accumulated sand in the middle is considered.

Table 1. Emitted mass [g] measurements in wind tunnel

U_∞	Isolated pile	Gap	Face-on	Edge-on
7	140.3 ± 8.4	0.5 H_b	247.6 ± 14.9	282.7 ± 17.0
		1.5 H_b	209.3 ± 12.6	319.5 ± 19.2
8	247.8 ± 14.9	0.5 H_b	325.5 ± 19.5	413.0 ± 24.8
		1.5 H_b	336.2 ± 20.2	452.5 ± 27.2
9	387.4 ± 23.2	0.5 H_b	470.8 ± 28.2	518.5 ± 31.1
		1.5 H_b	455.4 ± 27.3	542.4 ± 32.5

Important analysis can be made we consider the angle (θ) at which the fluid flows over the stockpile surface to calculate the threshold friction velocity. Threshold friction velocity can be reasonably modified with the angle. For instance, dry sand on a flat surface presents $u_{*t} = 0.25 \text{ m/s}$. On the pile this value varies from 0.025 to 0.36 m/s. Numerical results in Figure 1(a) shows the distribution of the difference between the friction velocity and the modified threshold friction velocity over the stockpile surface for the case face-on and gap $0.5H_b$ at 7 m/s. The gray color indicate regions where $(u_* - u_{*t}(\theta)) < 0$, that is, the friction velocity did not reach the particle threshold friction velocity value leading the particles to not take-off.

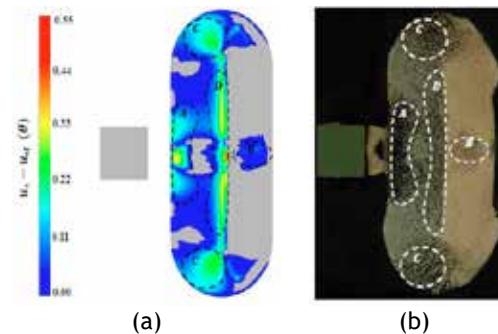


Figure 1. Face-on cubic building case for $0.5H_b$ and 7 m/s. (a) Distribution of $(u_* - u_{*t}(\theta))$ from numerical simulations and (b) photograph of the top view of the eroded sand stockpile after pavement.

The corresponding gray area of the Figure 1(a) in Figure 1(b) shows that, indeed, no erosion where experimentally observed. The highlighted areas A, B, C and D represent regions where $(u_* - u_{*t}(\theta)) > 0$, that is, the friction velocity reach the particle threshold friction velocity value leading the particle to take-off. The values of $(u_* - u_{*t}(\theta)) > 0$ varies from 0.055 to 0.55 m/s if we take a look on Figure 1(a).

Figure 2 shows the temporal evolution of wind erosion for face-on and edge-on cases. The photographs are compared for the same experimental time in order to be possible the assessment of erosion through a qualitative analysis of non-erodible particles behavior. The interaction between the pile and the cube also promotes an

accumulation of sand in the zone behind the building where shear stress is low. In addition, for the edge-on case, there is a more intense interaction between the vortices downstream the cube, leading the windward wall of the pile be even more impacted as can be noticed by the greater accumulation of black (non-erodible) particles. The leeward wall of the pile is more affected for an edge-on cubic building than the face-on case.

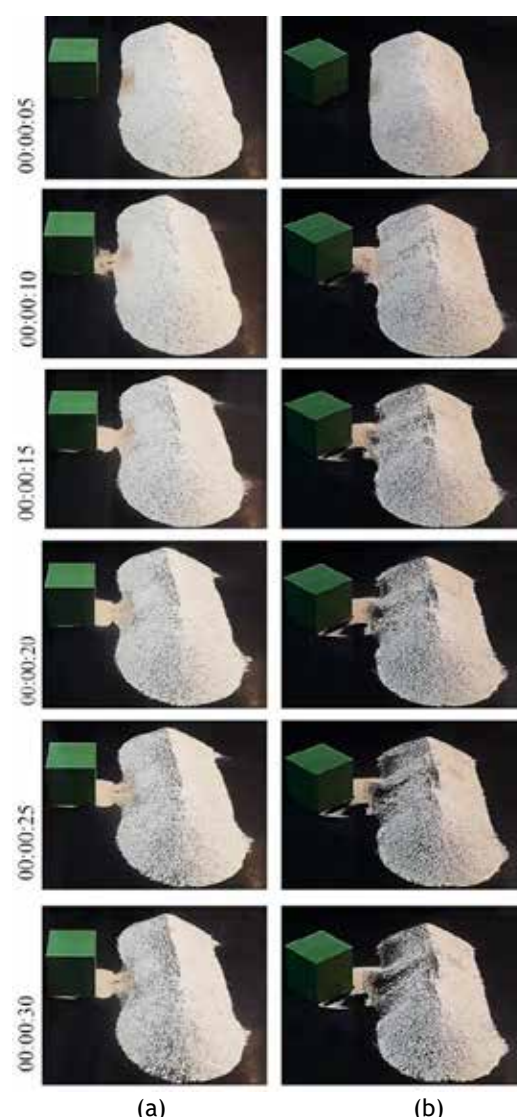


Figure 2. Temporal evolution of the erosion for a stockpile downstream a cubic building: (a) face-on and (b) edge-on, separated by gap of $0.5H_b$ for the upstream velocity of 8 m/s.

CONCLUSIONS

Comparing the obtained experimental results with those for the isolated stockpile configuration and observing the differences in the erosion patterns and emission estimates was possible to conclude that: (i) the emissions considerably increase due to

the presence of the building, mainly if stockpile is downstream an edge-on cubic building; (ii) the higher the free stream velocity, due to the presence of the obstacle, the more efficient the dynamics of the pavement process is and (iii) the increase of the gap between the building and the pile from $0.5H_b$ to $1.5H_b$ does not generate expressive changes in the emitted mass measurements. However, the analysis of the gaps reveals that smaller distances influence the particle distribution over the stockpile surface mainly downstream the cubic building showing areas where the erosion is more intense. These findings play an important role since it is possible to obtain an optimal industrial open yard configuration where fewer particles are emitted to the atmosphere. In open yards where reallocation of buildings or industrial structures and sources is not possible, to understand how the wind erodes the sources is very relevant leading the site management to constitute a method of particulate control.

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EFFECT OF ELECTROLYTES ON PARTICULATE SUPPRESSION

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Abstract: Increasing the humidity of the particulate material assists in the suppression of the dust emission, however, the addition of electrolytes increases the efficiency of this process, this is due to the electrolyte's ability to neutralize the electric charge of the dust, producing aggregates with the fine particulates. In this work the efficiency of the suppression of 5 types of electrolyte reagents in 2 different types of materials is analyzed, the pellet feed crushed with humidity of 6% and the iron ore's pellet, with and without the addition of 1% of fines , with different solution volume values, and with a cure time of 2 hours for both . In order to evaluate this suppression of the particulate emission, a bench and a methodology for the study of this emission during the handling in dynamic conditions were developed. The results are obtained with the aid of a particle counter for the range of the particle diameter of 5 μm and 10 μm , that are the respirable particulate diameters described by the regulation NR 15 , and are compared in order to verify which reagent has obtained the best performance for the suppression of dust emission for the two materials.

Keywords: Dust suppression, Dust tower, Particulate emission, electrolytes.

INTRODUCTION

Air pollution caused by dust generation during ore handling is a problem because of the risk associated with inhalation of dust and the nuisance it causes to the population. For this reason, in 1987 the EPA (Environmental Protection Agency) adopted standards to regulate the concentration of particles with 10 μm of diameter or smaller (PM10) and for particles with a diameter of 2,5 μm or less (PM2.5), since the greatest health risks come not only from particles that are easily inhaled, but from those that attach to the lung tissue, causing irritation or necrosis (EPA, 2006).

There are several solutions to control the emission of dust, such as surfactant solutions, sleeve filter, humidification with water, etc. The presence of water in the interstices of the particles can inhibit the generation of dust, since the weight of the particle and the capillary force are opposed to the shear force exerted by the air flow (Allen, 1970). Studies with iron ore showed that aqueous solutions of surfactants (glycols and esters) did not inhibit the generation of dust to a greater extent than the simple use of pure water (Copeland and Kawatra, 2005; Copeland, Eisele, Kawatra, 2009). On the other hand, these authors showed that the addition of solutions with electrolytes, such as CaCl_2 , were more effective in preventing dust generation than surfactants or even pure water (Copeland et al, 2009).

The dust suppression mechanism using these reagents may be associated with the neutralization of the electrical charge of the dust, causing its

aggregation. As the mass of the aggregate particles is greater than their individual mass, the aggregates settle, reducing the emission of dust.

In order to verify the efficiency of the electrolyte suppressors, a bench was used to study dust generation and control in dynamic conditions, based on the dust tower developed by Michigan Technological University - MTU (Copeland & Kawatra, 2011).

METHODS

The material used for the evaluation of the reagents was the pellet feed milled and pressed at a humidity of 6%, which was the material that presented a larger number of particles emitted in the tests with the dust tower. The electrolyte reagents were also evaluated for the suppression of iron ore pellets, without and with the addition of 1% fines, with a volume of solution of 10 ml and 16 ml, with a cure time of 2 hours.

For the tests with the pellet feed crushed. Humidification was done by adding material and the reagent solution in a mortar mixer, in order to guarantee a greater homogenization of the samples. With the pellet, the most spherical ones were selected, in order to keep the samples more homogeneous for the tests. Table 1 shows the reagents used with their molecular weight.

DUST TOWER TESTING

The methodology used to perform the tests as well as the bench for the experiments were developed by Copeland and Kawatra (2011), however, some modifications were made to meet some project

demands. This facility has a total of 5m, having a height falling of 2.4m, which is the height corresponding to the region where the sample traveled. To measure the PM10 and the finer particles, the particle counter of Particles plus 8306, connected to a suction duct, was used to obtain isokinetic sampling. Figure 1 illustrates the dust tower built at the Federal University of Pará.

Table 1. Reagents used as dust suppressors

Reagents	Chemical formula	Molecular weight
calcium hydroxide	Ca(OH)_2	74,09
ferric chloride	FeCl_3	162,2
Calcium chloride	CaCl_2	110,98
Aluminum sulfate	$\text{Al}_2(\text{SO}_4)_3$	342,15
Ferric sulphate	$\text{Fe}_2(\text{SO}_4)_3$	399,88

Reference: adapted from Santos Jr.(2018).

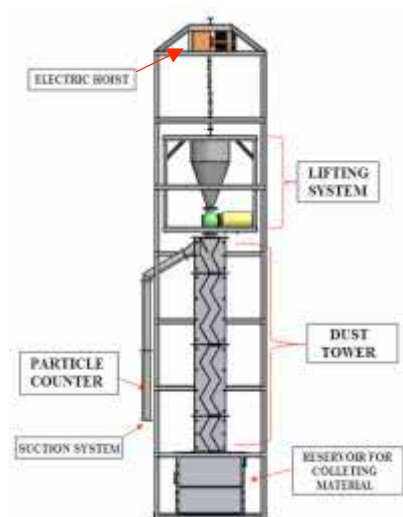


Figure 1. Dust tower facility.

The test consisted in releasing 1 kg of material in the tower, this material when passing by the tower, generates dust, which in turn is collected by a suction system that is next to the tower. An isokinetic sampling is done by a tube positioned in the central part of the suction duct, this tube is connected to the particulate collector, which returns us a result of the dust generated in the test in the bands of PM10 to PM0,3.

RESULTS

Figure 2 shows the variation of electric charge density, calculated for each reagent, in the two concentrations evaluated. It is observed that the increase in concentration significantly increases the values of electric charge density. In each series of experiments the volume and concentration of the electrolyte solution were constant, so the dosage was the same. However, since each reactant has a different molecular weight, and considering the valence of the cations composing them, the charge density (Coulombs / kg) assumes different values in each assay. It is also noted that ferric sulfate presents the lowest charge density for both concentrations, while calcium hydroxide presented the highest charge density.

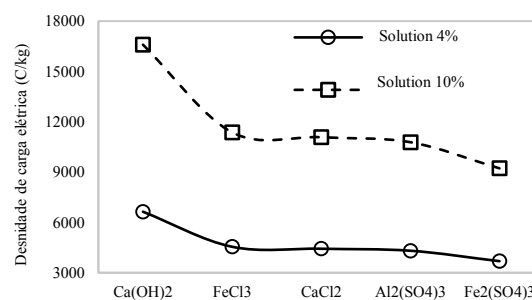


Figure 2: Electric charge density with solution concentration variation in pellet feed

The results of the assays with reagents for 5 µm pellet feed particles are shown in Figure 3.

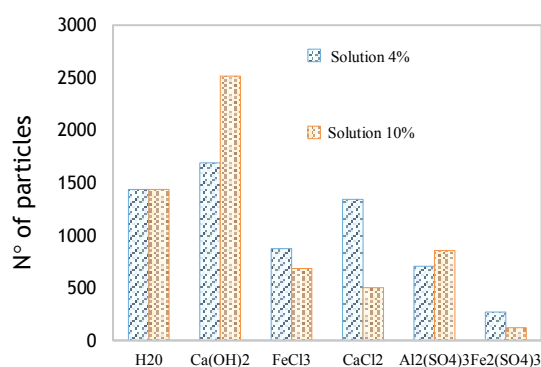


Figure 3: Influence of the use of reagents on the emission of Pellet Feed particles of 5 µm in diameter.

For the two concentrations, $\text{Fe}_2(\text{SO}_4)_3$ was the reagent that presented the best result, with a reduction of 81.3% at a concentration of 4% by mass and 91.6% at a concentration of 10% in relation to the number of particles emitted using only water. $\text{Al}_2(\text{SO}_4)_3$, CaCl_2 and FeCl_3 presented lower performance than $\text{Fe}_2(\text{SO}_4)_3$, although they reduced the number of particles when compared to water.

use performance. With increasing concentrations from 4% to 10%, CaCl_2 and FeCl_3 improved their performance. CaCl_2 decreased from 6.6% to 65%, and FeCl_3 decreased from 39.3% to 52.4% reduction, compared to the results obtained with water alone. However, $\text{Al}_2(\text{SO}_4)_3$, had its performance reduced with increasing concentration, going from 50.9% (the concentration of 4%) to 40.6%, the concentration of 10%. The reagent with the worst performance was $\text{Ca}(\text{OH})_2$, because the number of particles produced with the application of this reagent increased, in both concentrations, in relation to the values obtained with the use of water. At the 4% concentration, the increase was 17.6%, and at the 10% concentration, the increase was 74.9%.

The results of the assays with the reagents for particles of 10 μm of ground pellet feed are shown in Figure 4.

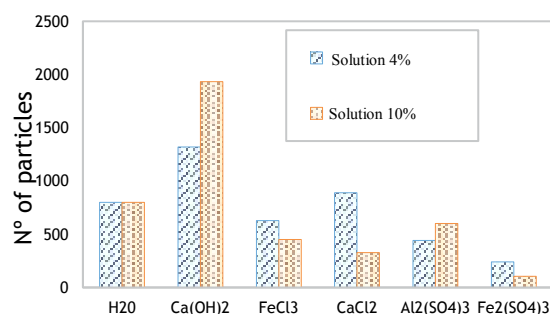


Figure 4: Influence of the use of reagents on the emission of Pellet Feed particles of 10 μm in diameter.

It was observed that the results had a similar behavior to those observed for the diameter of 5 μm , for all reagents, with $\text{Fe}_2(\text{SO}_4)_3$ having the best performance and $\text{Ca}(\text{OH})_2$ with the worst performance.

The figure 5 shows the variation of electric charge density, calculated for each reagent, for the two volumes of solution evaluated, 10 and 16 ml. The increase in solution volume (dosage) significantly increased the values of electric charge density. In all series of experiments the concentration of the electrolyte solution was constant (4% by mass), with only dose variation. However, since each reactant has a different molecular weight, and considering the valence of the cations composing them, the charge density (Coulombs / kg) assumes different values in each assay. It is also observed that ferric sulphate presents the lowest charge density for both concentrations, while calcium hydroxide presented the highest charge density, similar to the case with solution concentration variation (see figure 2).

The figure 6 shows the results obtained with the use of the reagents for PM10 pellet suppression. It is

observed that all the reagents were more efficient than the water in reducing the emission of particulates, in their respective dosages, except $\text{Al}_2(\text{SO}_4)_3$. The $\text{Ca}(\text{OH})_2$ was the reagent that presented the best result, in the two dosages of solution evaluated, although it was the reagent that presented the worst result for the pellet feed, fact that can be explained by the quantity of finer particles in the Pellet feed in relation to pellets.

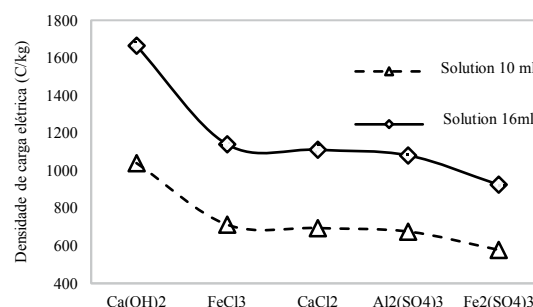


Figure 5: Density of electric charge with variation of solution volume for pellet testing.

The results also show that with higher volume of solution (16 ml), the concentration of particulates was reduced for all the reagents, and can be explained by the increased dosage and, consequently, increased humidity applied on the sample. Therefore, the solution dosage is an important factor to be investigated as it influences the charge density in the suppressor solution and in the suppression of particulates.

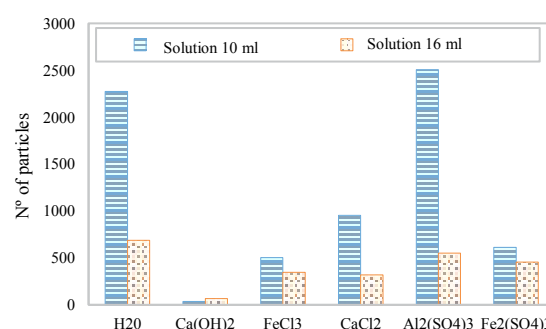


Figure 6: Influence of the use of reagents on the suppression of 10PM pellets.

The effect of the 2 hour curing time on the performance of the reactants in pellet suppression of pellets is shown in figure 7. The results reveal that curing time has been detrimental in suppressing particulate emission, with increasing concentration for most of the reactants. Those who did not increase in relation to the use of water alone had a similar behavior to water. The application of only water also passed the same curing time as the other reagents, ie, the natural drying effect is the

same for all reagents evaluated. The curing time also influenced the performance of the reagents in relation to the increase in the dosage of the solution. In this case, not all reagents improved their performance with increasing solution volume, behavior different from that found in the condition with no cure time.

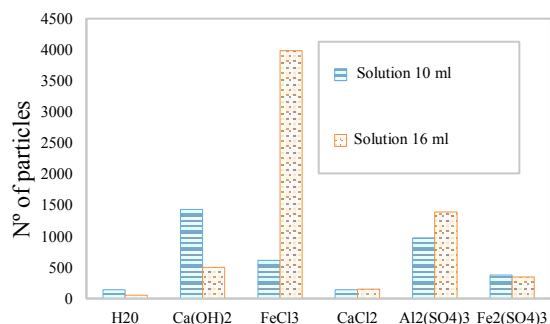


Figure 7: Influence of the curing time of the reactants on the suppression of 10PM pellets.

It was observed that some solutions during their preparation exhibited an exothermic behavior, which may influence the drying rate of the mixture, although a more detailed study of the characteristics of each reagent should be made. The figure 8 shows the effect of charge density on suppression of particulate emission by pellets.

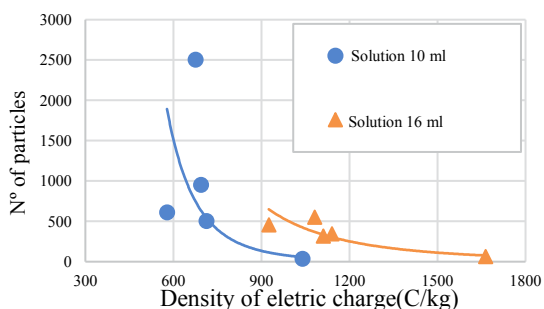


Figure 8: Influence of charge density on the suppression of pellets with diameters of 10 µm.

Each point in a series of experiments represents a reagent. For the 10 ml dosage the particulate emission is minimized by a charge density value between 750 and 1040 C / kg. For the dosage of 16 ml the minimum occurred between 1200 and 1700 C / kg. In the series of experiments with electrolytes, calcium hydroxide was the most approximating of the charge density associated with the lowest dust emission (1040 C / kg for the dosage of 10 ml and 1664 C / kg for the dosage of 16 ml). Ferric sulphate and aluminum sulphate were the most distant reactants of the optimum charge density, which explains the poor performance of these reagents. The worst result of aluminum sulphate may be

related to pH regulation, which was not measured in this experiment.

The results obtained from the dust tower tests with the addition of 1% pellet fines are shown in Figure 9, for the two dosages of solution evaluated, 10 and 16 ml. It is noted that the increase in the volume of the solution reduces the dust emission concentration for almost all the reactants, including water, except for Ca(OH)₂, which has an opposite behavior (increasing the number of particles with 16 ml solution), although this was the best performing reagent along with CaCl₂. Calcium chloride, however, had its performance improved by increasing the dosage of solution used, unlike the condition without the addition of pellet fines (Figure 6). Reagents Fe₂(SO₄)₃, FeCl₃ and Al₂(SO₄)₃, presented worse results than those obtained only with the use of water.

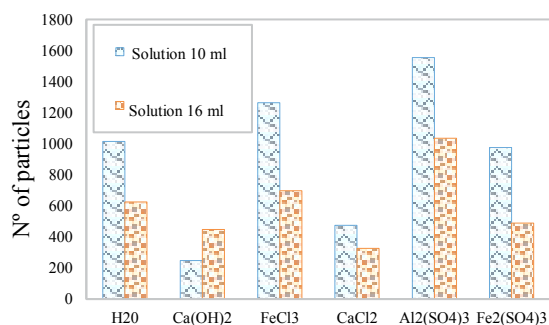


Figure 9: Influence of the use of reagents in the suppression of particles of 10PM pellets with addition of 1% fines.

The figure 10 shows the results obtained for pellets with 1% fine, with a cure time of 2 hours of the solution with reagents. These results are very important, since this is a situation similar to that used by Copeland and Kawatra (2011). The only reagent that presented better results than the water use in both volumes of solution was CaCl₂. The other reagents presented worse results than the use of water alone. No reduction in particulate emission was observed with increasing solution volume for aluminum sulfate and iron sulfate. For water, as expected, the increase in the volume of solution reduces the emission of particulates. For CaCl₂ the curing time had a great influence on the suppression of dust. The results show that the curing time favored the reduction of the particulate concentration, although it does not present the same behavior of reducing the emission near the reference line, where a concentration close to zero is observed, as found by Copeland and Kawatra (2011). Therefore, more experiments should be done to better evaluate the influence of the volume and cure time of the solution.

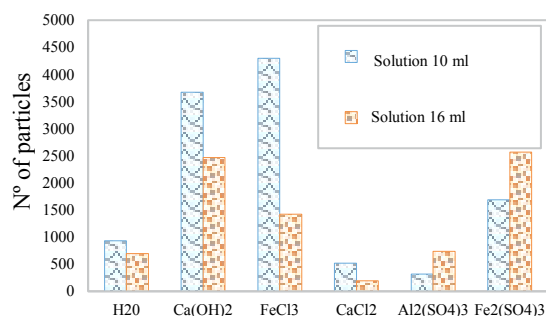


Figure 10: Influence of the curing time of the reactants on the suppression of particles of 10PM pellets with addition of 1% of fines.

CONCLUSIONS

For the pellet feed, it was observed that the reagent with the highest charge density at both concentrations Ca(OH)₂ emitted the largest number of particles, whereas the reagent with the lowest charge density (Fe₂(SO₄)₃) presented the best performance.

The results of all the series of experiments seem to indicate that there is a charge density that minimizes the emission of particulates, reiterating the necessity of new experiments exploring the dosage and density of charge for all the reagents.

For the pellet, the reagents closest to the charge density associated with the lowest dust emission were calcium hydroxide with 10 ml and calcium chloride with the dosage of 16 ml. Ferric chloride, ferric sulphate and aluminum sulphate were the most distant reactants of the optimum charge density associated with lower emission, presenting the worst performances among the reagents tested. The results with the addition of 1% of ball fines also indicate that there is a charge density that minimizes the emission of particulates, reiterating the need for new experiments to evaluate the optimum charge density for all reagents.

ACKNOWLEDGEMENT

The authors would like to thank Vale Institute of Technology - ITV for the financial support.

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INFLUENCE OF PARTICLE SIZE IN THE PERFORMANCE OF THE FILTER MEDIUM IN FILTERING BY BAG FILTER

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Abstract: Bag filters are widely used in the processes of many industries, mainly in the productive sector of steel industries to control air pollution. Most of the studies found in the literature are focused on the optimization of these equipments and there are only few studies on the effects of particle size of particulate matter on filter performance. Thus, this study aims to investigate the performance of a P84 filter medium by means of an equipment based on the VDI 3926 standard using two different particle sizes of powder. For this purpose, the maximum pressure drop was 100 mmH₂O and the operating conditions were those established in the standard mentioned above. The results of the filter medium characterization showed that the fibers had a mean diameter of 17.7 μm , with a very heterogeneous size distribution, air permeability equal to 12 m³/min/m² (under pressure drop of 196 Pa) and the porosity was 0.86. The collection efficiencies were calculated in cycles 1, 10, 20 and 30, in order to evaluate the performance of the filter media over the cycles and to compare the values for the finer and coarser particulate matter, and also we evaluate the residual pressure drop. According to the results, it was noticed that for the coarse particulate matter the collection efficiency was a little higher in the 1st and in the 30th cycles. In addition, the total filtration time for the coarser powder was higher than that finer and the residual pressure drop was higher for the finer powder.

Keywords: air pollution, bagfilter, particulate matter, particle size, collection efficiency.

INTRODUCTION

According to a study conducted in 2018 by the World Health Organization (WHO), air pollution causes the death of more than 7 million people worldwide each year. A specific survey showed people's exposure to particulate matter, which has caused great damage to health, such as lung cancer, cardiovascular ischemia and pneumonia (WORLDWIDE ORGANIZATION OF HEALTH, 2018). In this way, it is necessary to control the emission of particulate matter. This control can be made by many equipments, according to the process and based on the economic and environmental interests. Bag filters are widely applied to control air pollution because they present a high collection efficiency of particles to a huge granulometric range. The control of some filtering parameters in bag filter is of extreme importance for a good performance of the filter media, such as filtration velocity, pressure drop, temperature, humidity. Some characteristics of the filter media and of the particulate matter are also very important, such as permeability, porosity, particle size, shape and density, particulate matter loading, adhesion and cohesion forces. The particle size is a relevant characteristic because it influences the properties of the aerosol and the capture mechanisms of the particle. Larger particles form thicker filtration cakes, while smaller particles penetrate more into the filter medium and tend to form a cake with higher pressure drop (AL-OTOOM, 2005). Choi et al (2002), using fly ash with

particle size smaller than 10 μm , studied the effects of particle size on the pressure drop, concluding that the smaller particle size corresponded to a larger pressure drop. Li et al (2019) established a filtration and pulse-jet cleaning experimental system, with three kinds of particle sizes of particulate matters obtained by means of sieving. In this way, the effects of particle size and maximum pressure drop on the performance of pleated cartridge filter were studied. These authors found that under the same maximum pressure drop, for the larger particle size, the average pressure drop, the number of pulse-jet cleaning and the average dust emission concentration all decreased. Based in the literature, this present study aims to analyze the influence of particle size in the performance of the filter medium P84 in filtering by bag filter. This investigation is relevant because the particle size can help reduce the emissions in the stacks of industries.

METHODS

Powder characterization

The fine particulate matter was the powder from the real sinterplant. The coarser particulate matter was obtained by mixing the fine powder with hydrated lime. These materials were characterized in the Malvern Mastersizer equipment, that provided the volumetric diameter. The granulometric distribution of powders showed a

polydisperse material, with median volumetric diameters equal to 6,52 μm and 15,62 μm .

Filter medium characterization

The filter medium (aromatic polyimide - P84) was characterized in terms of mean diameter of fibers, air permeability, porosity, and collection efficiency of particles. The experimental air permeability was calculated using Darcy's equation, considering measurements of pressure drop as a function of the gas velocity, without particles, Equation 1:

$$\frac{\Delta P}{L} = \frac{\mu v_s}{K_1} \quad (1)$$

where L is the filter medium thickness, μ is the fluid viscosity, and K_1 is the constant of permeability of the porous medium. The mean fiber diameter of the filter medium were determined by scanning electron microscopy (SEM) images with manual analysis using the software Image-Pro Plus 7.0. Further information can be found in Barros et al (2015) and Bortolassi et al (2017). The porosity of the filter medium was obtained using Equation 3.

$$\varepsilon_{\text{superficial}} = \frac{A_{\text{total}} - A_f}{A_{\text{total}}} \quad (3)$$

where $\varepsilon_{\text{superficial}}$ is the porosity considering only the filter medium surface, A_{total} is the total area of the SEM images and A_f is the area occupied by fibers in the images. The collection efficiency of the filter medium was calculated by gravimetry according to Equation 4 (SÁNCHEZ et al, 1997).

$$E = \frac{\Delta M_{FT}}{\Delta M_{FT} + \Delta M_{FA}} \times 100\% \quad (4)$$

where ΔM_{FT} and ΔM_{FA} are respectively the mass retained in the test filter medium and the mass retained in the absolute filter, both weighted before and after the filtration cycles.

Experimental system

The filtration cycles and cleaning pulses were performed in the equipment based on the VDI 3926 standard, that simulates in laboratorial scale the industrial filtration. The filter medium (P84) was tested using powders with different granulometries. The experimental conditions were based in the same standard mentioned above. The filtration tests were carried out keeping the operational parameters constant: filtration velocity equal to 2 m/min, maximum pressure drop of 100 mmH₂O, cleaning pulse time of 60 ms and cleaning pulse pressure of 5 bar. The number of cycles was 30 for each powder.

FINDINGS AND ARGUMENT

Figure 1 shows the SEM image of the filter medium P84.

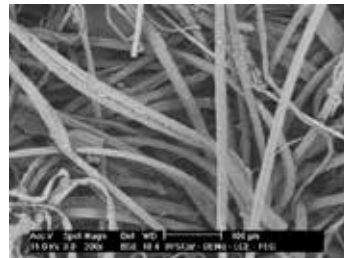


Figure 1. 200x SEM image of the filter medium.

As can be seen in Figure 1, the fibers are very heterogeneous in shape and diameter. It means that there are some regions with more opened porous and others with more closed porous, so that these more opened porous can be possible areas where the powder passes through. The mean fiber diameter was calculated following the steps presented in the study of Bortolassi et al (2017) and the obtained value was 17.7 μm . The air permeability for the virgin filter medium was 12 m³/min/m² (under the pressure drop of 196 Pa and the filtration area of 40 cm²); the calculated porosity of the filter medium was 0.86. Figure 2 shows the evolution of pressure drop within the time to complete 30 cycles for two kinds of particle sizes under the maximum pressure drop of 100 mmH₂O.

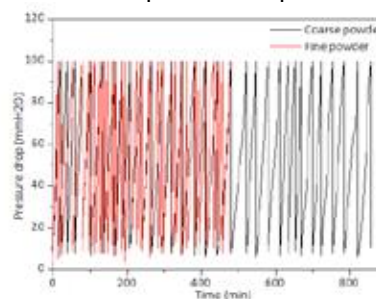


Figure 2. Pressure drop as a function of filtration time for two different particle size (fine and coarse powder).

Figure 2 exhibits the filter medium starting the filtration under a clean condition. The electromagnetic pulse valves were turned on for pulse-jet cleaning when the pressure drop of the filter medium reached the maximum pressure drop. The pressure drop decreased instantly after pulse-jet cleaning, and the minimum value was called the residual pressure drop, showed in Figure 3.

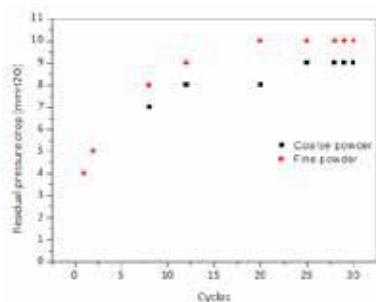


Figure 3. Residual pressure drop as a function of the number of pulse-jet cleaning under two different particle sizes.

Analyzing Figures 2 and 3, it can be observed that as filtration and pulse-jet cleaning goes on, the filtration cycle decreased while the residual pressure drop increased. The larger the residual pressure drop is, the worse the effect of pulse-jet cleaning gets, and the shorter the next filtration cycle will be. These results are consistent with data obtained by Li et al (2015, 2017). Under the same maximum pressure drop, the residual pressure drop of fine particulate matter was greater than that of coarse ones. This is probably because it is easier for fine particulate matter to enter the filter medium. This fact also explains the lower total time of 30 cycles for the fine powder in Figure 2. The collection efficiencies were calculated in cycles 1, 10, 20 and 30, in order to evaluate the performance of the filter medium over the cycles and to compare the values for the finer and coarser particulate matter.

Table 1. Collection efficiency of P84 for fine and coarse particles

Collection efficiency (%)		
Cycle	Coarse powder	Fine powder
1	99,79	99,67
10	99,47	99,84
20	99,82	99,81
30	99,96	99,95

As can be seen from the Table 1, there are no huge differences in the collection efficiencies over the cycles for both powder. However, the great difference between the two powders lies in the lifespan of the fabric, since the coarse powder provides longer cycles which reduces the number of cleaning pulses under the same maximum pressure drop and considering an specific total time. In addition, according to Li et al (2019) the coarse powder provides a lower emission, which is very important for the industries.

CONCLUSIONS

Our findings highlight the importance of the particle size in the performance of bag filters, since a larger

particulate matter can provide better lifespan of the filter medium and also it reduces the emissions. In terms of collection efficiency the difference in particle size is not so great but the main result found is related to the lifespan of the fabric and emission, that are very relevant factors for the industries to reach the established emission limits in the stacks and also the industries can save money with the change of the bags.

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CFD SIMULATION OF THE FLUID FLOW INSIDE AN INDUSTRIAL CYCLO FILTER

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Abstract: In addition to the most common air pollution control equipments in industry, the cyclo filter is an another important technology to capture particulate matter. It associates the advantages of a cyclone separator with the efficiency of a bag filter, in order to increase the filtration efficiency. This equipment has a great application in systems of pneumatic transport, mainly as a relief filter for storage silos. However, there are not many available studies in the literature about this equipment and, in an industrial case, this one has been presenting several failures, such as low service life of the bags. In this context, this work presents a CFD analysis to evaluate the behavior of the gas flow inside an industrial cyclo filter, according to its design parameters. The simulations were performed using the ANSYS Fluent v18.0, which applies the Finite Volume Method. In the computational modeling, the mesh was predominantly polyhedral and an URANS approach was used to model the turbulence, with the appliance of the Reynolds Stress Model (RSM). The simulations revealed that, because of this cyclo filter geometry, the flow dynamics inside the equipment were a little different when compared to a conventional cyclone separator flow pattern. As a result, the distribution of the flow in the bags is non-homogeneous and presents high filtration velocities in some regions, indicating one of the main causes for premature wear observed in the bags.

Keywords: Computational Fluid Dynamics, Cyclone separator, Bag filter, Reynolds Stress Model, Polyhedral mesh.

INTRODUCTION

With the increasing urban growth and industrial activity, air pollution has become a global concern. Pollution from particulate matter represents the 6th leading cause of premature deaths, according to studies conducted in 2015 (FOROUZANFAR *et al.*, 2016). Its negative effects leads to restrictions imposed by environmental agencies, making the industries look for robust and efficient technologies in order to respect the maximum tolerable levels of pollutant emissions. In this context, the cyclo filter, also called just as bag filter, is a technology that associates the advantages of a cyclone separator with the efficiency of a bag filter, which can reduce the upward velocity of the flow in the interior and the load of particulate matter on the bags. With great applications in systems of pneumatic transport, this equipment works also as a relief filter for storage silos. However, in an industrial case, this equipment has been presenting several failures, such as low service life of the bags, which raises their operating and maintenance costs.

The study of cyclo filters using numerical simulations is very recent in the literature. Solari *et al.* (2017) studied the application of a bag filter in-

stalled inside a cyclone with the perform of CFD simulations. The turbulence model used was the *Realizable k-ε*, which includes two extra transport equations to represent the turbulent properties of the flow, and the results were compared with experimental measurements. The flow was modeled as steady-state and some different inlet velocities were tested. The Porous Jump conditions were used to model the fabric filter. For the purpose of studying the behavior of the flow inside this cyclone with a bag filter, the comparison was satisfying. However, for the cyclone separator, many numerical and experimental studies have been conducted in the literature to investigate its flow pattern. Initial researches of cyclone separators using numerical simulations made by Boysan *et al.* (1982) and Hoekstra (2000) have shown the 3D dimension nature of the flow inside a cyclone. The high anisotropy and the strong swirling flow demands an adoption of turbulence models more expensive in computational resources, such as the Reynolds Stress Model (RSM) (CORTÉS, GIL, 2006; SHUKLA, SHUKLA, GHOSH, 2011). This model is capable to produce reasonable and qualitative agreement with the experimental data, because it can calculate the effects of stream curvature, rotation, swirl and rapid changes in strain rate

(GUINBUM, 2008). In the other hand, the numerical simulations of the flow in bag filters are well predicted using two equations turbulence models, as seen in recent works of Damian (2004), Rocha *et al.* (2014) and Pereira *et al.* (2016).

In this context, the objective of this work was to investigate the behavior of a single-phase flow inside an industrial cyclo filter using the Computational Fluid Dynamics (CFD) techniques.

METHODS

In this work, an analysis was made in a cyclo filter existing in an industrial plant. This equipment, working as a relief filter for a storage silo, is located in a primary dedusting system plant which is responsible for the capturing of particulate matter generated in a blast furnace cast house. The simulations were performed using the software ANSYS Fluent v18.0. Information about this cyclo filter design parameters are presented in Table 1.

Table 1. Cyclo filter design parameters

Flow rate (Am^3/h)	2484
Inlet velocity (m/s)	39,05
Height (mm)	4245
Larger cone diameter (mm)	1740
Tube sheet diameter (mm)	1500
Number of bags	39
Bags inner diameter (mm)	152
Bag's height (mm)	2500
Air-to-Cloth ratio (m/min)	0,89
Bag thickness (mm)	1,9

Computational domain and Mesh

The computational domain was defined as a 3D geometry designed using the software ANSYS SpaceClaim. In this case, a prolongation of both inlet and outlet ducts was considered in order to avoid recirculation at the domain outlet and to ensure the fully developed flow. For this case, the computational domain, presented in Figure 1, was divided in fluid and porous. The porous domain was used to model the fabric of the bags, which introduces a pressure drop to the flow. After the definition of the computational domain, a mesh independence test was performed. Because of the complexity of the flow, smaller meshes did not obtain a result due to a characteristic error in "Multigrid" solvers caused by insufficient elements in places with high gradients. Increasing the refinement in these regions, it was possible to obtain a result with a mesh containing 18.2 million elements. Larger meshes were not possible to compute because of the computational cost limitation also occasioned by the RSM turbulence model. The

chosen mesh consists mostly of polyhedral elements. This type of mesh combines the advantages of the hexahedral element and the tetrahedral mesh. In other words, the polyhedral element allows the exchange of mass over a larger number of faces, reducing numerical diffusion and resulting in accurate solution with rapid mesh generation (SOSNOWSKI, KRZYWANSKI, GNATOWSKA, 2017). In the near wall regions, the mesh has triangular elements inflated in the normal direction, with bigger refinement, where it is necessary to calculate the boundary layer. In the porous domain, the mesh consists only of hexahedral elements, making possible the optimization of the mesh number of elements, once the gradients founded in this region are less critical. The meshes were generated in the software ANSYS Meshing and the conversion to the polyhedral mesh was performed in ANSYS Fluent. A mesh detail is presented in Figure 2.

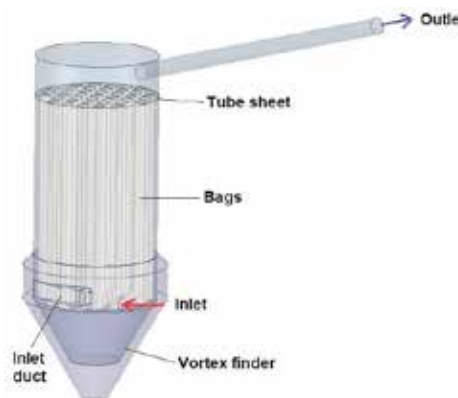


Figure 1. Computational domain

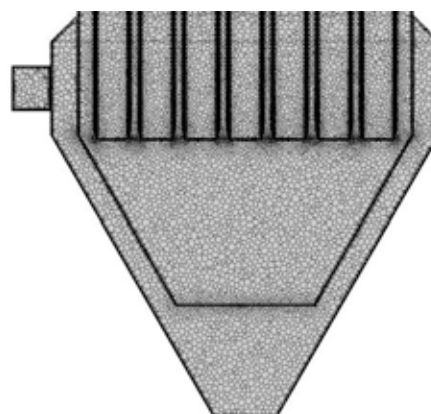


Figure 2. Mesh detail in the cyclone region

Turbulence Modeling

Since the cyclo filter works as a cyclone separator, the turbulence model used in this simulation was the Reynolds Stress Model (RSM). This model is the most complex between the RANS models and its use is essential when the flow characteristics of

interest are the result of the anisotropy of the Reynolds stresses (FLUENT, 2013). The governing equations for mass and momentum conservation were solved. Since the flow is evaluated as three-dimensional, where $u_i = (u_x, u_y, u_z)$ and $x_i = (x, y, z)$, transient, isothermal, incompressible and without body forces, the continuity and Navier-Stokes equations for turbulent flows can be expressed as (FERZIGER, PERIC, 2012):

$$\frac{\partial(\rho \bar{u}_i)}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial(\rho \bar{u}_i)}{\partial t} + \frac{\partial(\rho \bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right] + \frac{\partial(-\rho \bar{u}_i' \bar{u}_j')}{\partial x_j} \quad (2)$$

where $u_i(t) = \bar{u}_i + u_i'$ is the instantaneous velocity, $\bar{u}_i$ is the time-averaged velocity, u_i' is the fluctuating velocity, x_i is the position, $\bar{p}$ is the time-averaged pressure, ρ is the constant gas density and μ is the dynamic viscosity. This additional term, $\tau_{ij} = -\rho \bar{u}_i' \bar{u}_j'$, is called Reynolds Stress tensor and it appears in the Reynolds-Averaged equations due to interactions between turbulent fluctuations. In the RSM model, instead of the Boussinesq assumption of isotropic eddy-viscosity, the transport equations of a dissipation rate and individual Reynolds stresses are solved. The generalized transport equations for Reynolds stresses can be expressed as (SHUKLA, SHUKLA, GHOSH, 2011; FERZIGER, PERIC, 2012):

$$\begin{aligned} & \underbrace{\frac{\partial \tau_{ij}}{\partial t}}_{\text{Local time derivative}} + \underbrace{\frac{\partial(\bar{u}_k \tau_{ij})}{\partial x_k}}_{\text{Convection}} \\ &= - \underbrace{\left(\tau_{ik} \frac{\partial \bar{u}_j}{\partial x_k} + \tau_{jk} \frac{\partial \bar{u}_i}{\partial x_k} \right)}_{\text{Stress production}} + \underbrace{2\mu \left(\frac{\partial \bar{u}_i'}{\partial x_k} \frac{\partial \bar{u}_j'}{\partial x_k} \right)}_{\text{Dissipation}} \\ & - \underbrace{p' \left(\frac{\partial \bar{u}_i'}{\partial x_j} + \frac{\partial \bar{u}_j'}{\partial x_i} \right)}_{\text{Pressure strain}} + \underbrace{\frac{\partial}{\partial x_k} \left(\nu \frac{\partial \tau_{ij}}{\partial x_k} \right)}_{\text{Molecular diffusion}} \\ & + \underbrace{\frac{\partial}{\partial x_k} (\rho \bar{u}_i' \bar{u}_j' \bar{u}_k + p' \bar{u}_i' \delta_{jk} + p' \bar{u}_j' \delta_{ik})}_{\text{Turbulent diffusion}} \quad (3) \end{aligned}$$

where p' is the fluctuating pressure and δ is Kronecker delta. The terms before equality are the terms of production and do not require approximation or modeling. The terms of dissipation, pressure strain and turbulent diffusion need to be modeled. The most common and simplest model for modeling the dissipation tensor (ε_{ij}) is to treat this term as isotropic, i.e.:

$$\varepsilon_{ij} = \frac{2}{3} \varepsilon \delta_{ij} \quad (4)$$

Thus, a dissipation equation is solved together with the equations of the Reynolds stresses. In this case, the dissipation equations of the $k - \varepsilon$ model were used. Terms of turbulent diffusivity are generally modeled using a diffusion gradient approximation type. For the Pressure strain modeling, in this work the Linear Pressure-Strain model was used. The deductions can be seen in Fluent (2013).

Boundary conditions and convergence criteria

To perform this simulation, some hypotheses were adopted. The fluid was considered as a single-phase, incompressible (air at 25°C) with isothermal conditions. In the region of the bags, the porous media was modeled according to the generalized Darcy's law, which generates a pressure loss linearly proportional to the flow velocity in the region (DAMIAN, 2004). The flow was modeled as transient, because it was not possible to achieve the convergence with the adopted turbulence model in steady state. A time step of 0.0002 seconds was used to achieve the convergence with a minimum residual of 1×10^{-4} for all the variables, calculating 14 iterations per time step. The total flow time calculated was 4.0 seconds, in order to consider the flow fully developed. Boundary conditions are presented in Table 2.

Table 2. Boundary conditions

Inlet condition	Inlet velocity=39,05 m/s
Outlet condition	Zero pressure gradient
Walls	No slip condition
Porosity	81%
Permeability (m ²)	$4,211 \times 10^{-11}$

The simulations were performed in a 128Gb RAM cluster with 36 processing cores, located in the Computational Transport Phenomena Laboratory at Federal University of Espírito Santo.

FINDINGS AND ARGUMENT

The evaluation of the results is based primarily in an analysis of the streamlines and the velocities in the cyclone region. Then, an additional analysis of the flow behavior in the bags is made, evaluating the filtration velocity and the mass flow distribution. A final analysis of the equipment is made by evaluating the total pressure loss generated in the system by the cyclo filter.

Streamlines

It is possible to observe, in Figure 3, the flow pattern inside this cyclo filter. It is noted that, at the entrance, when the section of the duct changes,

there is a small expansion of the flow, reducing its velocity from 39 m/s to 30 m/s approximately. Posteriorly, the flow enters tangentially in the cyclone region and begins a rotational motion. There is a gradual velocity reduction, but, due to the conic geometry, the flow accelerates near the entrance of the vortex finder tube, with velocities around 40 m/s. It happens because the flow is concentrated in a region with a smaller section and, therefore, it suffers acceleration. It is also observed that, when the flow leaves the cyclone region, it presents a velocity around 10 m/s, showing that the ascending velocity is very high.

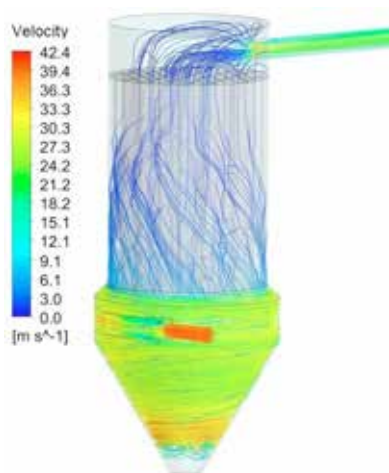


Figure 3. Streamlines from inlet

In Figure 4, streamlines from the vortex finder entrance are presented. According to a source of engineers, it was understood that the inner vortex was smaller and directed to the central bags. But, as can be observed, the flow suffers an expansion when entering the inner vortex region, favored by the vortex finder conical geometry, ascending by the sides with a considerable velocity. Therefore, the air flow reaches the lower region of the bags located closer to the cyclo filter walls with a very high velocity, around 12 m/s, showing that, possibly, these ones are more affected by this characteristic of the flow.

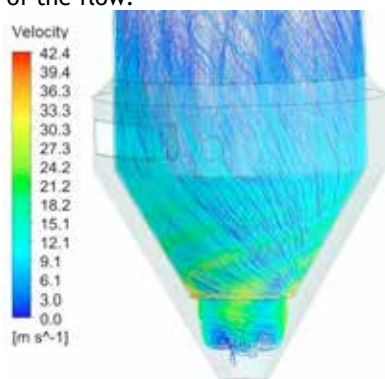


Figure 4. Streamlines from the vortex finder entrance

Velocities in the cyclone region

In the Figure 5 are presented the normalized velocity vectors of the flow in a reduced scale, located in a longitudinal plane in the cyclo filter center. It is possible to verify that, in the lower regions of the bags, there is a downward flow. In other words, a part of the flow follows in the opposite direction of the expected, returning and recirculating in the central region of the vortex finder. When the flow ascends on the sides, most part of the gas flow enters the bags in half of its length (Figure 5-a). Thus, a part of the flow continues in direction to the tube sheet, while another portion follows in descending direction. This downward flux, when it encounters the flow in the other direction, creates several small recirculation zones in the cyclone region, especially near the bottom of the bags and the vortex finder (Figure 5-b).

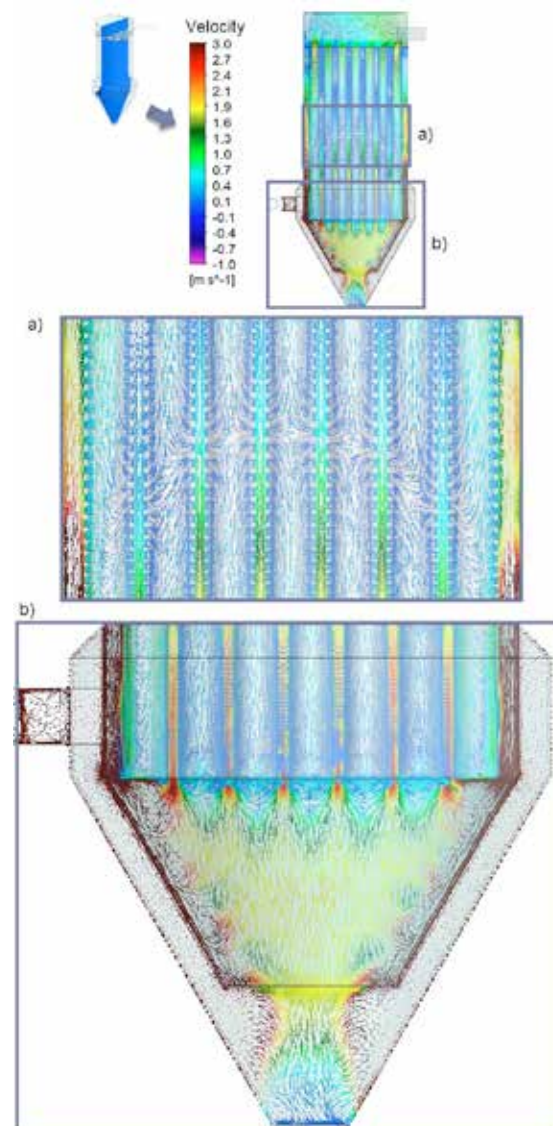


Figure 5. Velocity vectors from a longitudinal plane (reduced scale)

Filtration velocity

The filtration velocity, or Air-to-Cloth ratio, is one of the most important project parameters of a bag filter. In this case, the project value of filtration velocity is 0.89 m/min (0.0148 m/s). In Figure 6-a are presented the filtration velocity contours on the bags of the cyclo filter with a scale variation of $\pm 20\%$ of the design value. It is observed that the Air-to-Cloth ratio is lower than the project value mainly in the lower region of the bags. In general, the regions with filtration velocity higher than the project value represent 64,87% of the total filtration area, which the highest value reached was 1.5 m/s in the upper part of the bags. In Figure 6-b it is possible to verify, with a scale adjustment, the distribution of the Air-to-Cloth ratio values that are at least 20% higher than the project value. The higher values (above 0.1 m/s) are concentrated in the region where the bags are fixed in the tube sheet and in the proximity of the bottom of the bags, however, along its length, it is possible to observe that, especially in the bags located closer to the cyclo filter walls, the filtration velocity achieves values around 0.04 m/s, i.e., almost 3 times higher than the project value. The probable cause of these high values of filtration velocity in a great part of the filtration area is due to the upward velocity of the flow, which is still high. High filtration velocities lead to a small filtration time, but it increases the penetration of the particles in the fabric, which makes it difficult to remove the filter cake and increase the pressure drop during filtration and after removal of the cake (due to the residual pressure). Consequently, there is a reduction of the fabric service life (DONOVAN, 1985). It is also important to highlight that, in some regions, negatives values of filtration velocity were observed, i.e., the flow is passing through the bags in the opposite direction of filtration. It is possible to verify, in Figure 7, the filtration velocity contours with an emphasis to the negative values. It is observed that these ones are concentrated in the lower region of the bags not located close to the cyclo filter wall, representing 13.1% of the total filtering area. In this case, it is necessary to point out that, in the real dynamic of the flow with particles, this behavior is quite dependent on the particle relaxation time and the formation of the filter cake, since it causes an additional pressure loss in the filter (PEREIRA et al., 2016). In the simulated case, the analysis is based on a cleaned fabric, i.e., without the agglomeration and impregnation of particles, which makes possible this negative flux. Therefore, a study using particles in addition to experimental data would be necessary to improve this result.

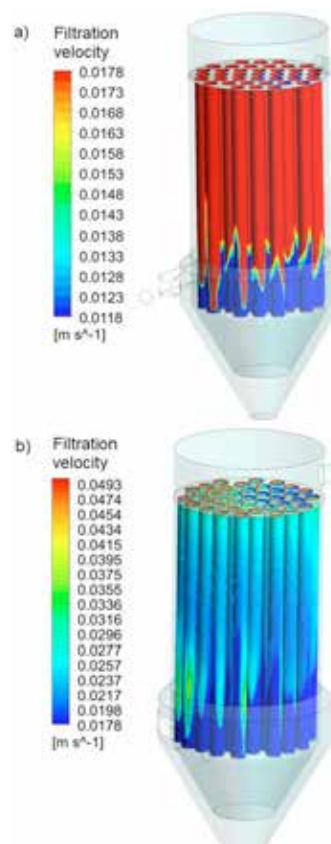


Figure 6. Filtration velocity contours

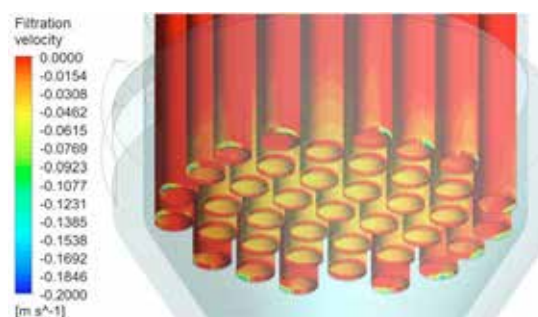


Figure 7. Negative values of filtration velocity

Mass flow distribution

Another way of evaluating the filtration velocity is the analysis of the flow distribution in the bags. As discussed before, the bags located near to the cyclo filter walls present higher values of Air-to-Cloth ratio. The Figure 8 presents the maximum values of mass flow calculated in each bag of the cyclo filter. Similarly, it is verified that the bags located in the central region of the equipment have received a maximum value of 0.017 kg/s of mass flow, approximately, and values around 0.026 kg/s were observed in the more external bags. In these last ones, a maximum value of 0.031 kg/s was reached.

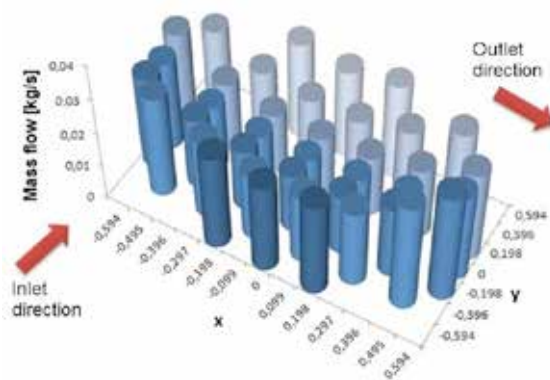


Figure 8. Mass flow distribution

Pressure drop

As a way to analyze the influence of each component of the cyclone filter, in the Figure 9-a are presented the pressure contours analyzed from a longitudinal plane in the center of the equipment. The total pressure drop in the cyclone filter was calculated in 1805.29 Pa, equivalent to 184.08 mmH₂O, which varies from a positive value in the entrance to 23.6 Pa in the outlet of the cyclone filter, according to the outlet conditions. When changing the section in the inlet duct, the flow suffers a small expansion and, therefore, gains static pressure, thus the pressure passed from 1828.89 Pa to 2071 Pa. Following the movement of the outer vortex, it is observed that the pressure drops from 2071 Pa to 450 Pa, approximately, when entering the inner vortex. In the Figure 9-b are presented the pressure contours with a scale adjustment for the same longitudinal plane of reference. In the inner vortex region, it can be observed regions of lower pressures, confirming the existence of a downward flow in the central region of the cyclone filter.

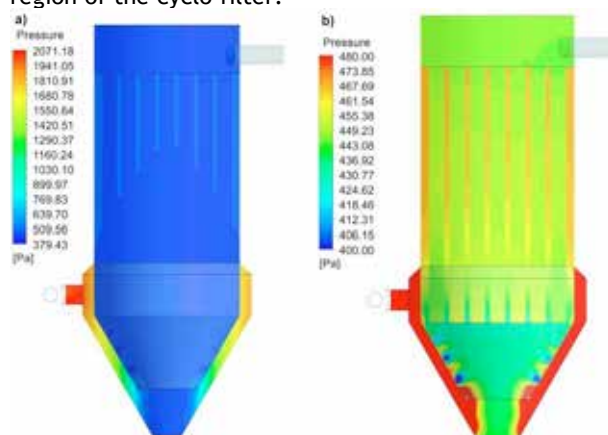


Figure 9. Pressure contours on a longitudinal plane: a) Full scale; b) Modified scale

In a general analysis, it is verified that this geometry of the cyclone region provides a pressure drop around 1355.30 Pa (138.1 mmH₂O), representing

75% of the pressure drop generated in the system by the cyclone filter. However, it is important to note that this analysis does not take into account the formation of the filter cake, since the fluid was modeled as a single-phase. This is responsible for a considerable pressure drop in a bag filter, so a further particle addition analysis is needed to improve this result.

CONCLUSIONS

According to the results obtained in the simulation of the cyclone filter, the accentuated conic geometry of the cyclone region is the parameter of greatest influence on the flow behavior. In a general way, the geometry of the vortex finder provides an expansion in the flow, causing it to travel at high speeds on the sides of the cyclone filter, initially reaching the bags located near the edges. Due to the high upward velocities of the flow, it is concluded that the mass flow distribution and, similarly, the filtration velocity, are not homogeneous along the bags. Some regions in the bags present Air-to-Cloth ratio values higher than the design value and these are concentrated in the bags located near the cyclone filter walls. It is suggested that this non-homogeneous distribution of the filtration velocity is one of the main causes of the low service life of the bags observed in this equipment. It is also concluded that the greatest pressure gradients inside the cyclone filter are located in the cyclone region, which is responsible for a great part of the pressure drop generated by the equipment. In general, the Computational Fluid Dynamics is very important in the study of complex flows, as in the case of this cyclone filter. In this way, the great potential of its applicability is reiterated, which makes it possible to obtain improvements of processes and new or existing equipments.

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ELECTROSTATIC PRECIPITATION OF NICKEL OXIDE NANOPARTICLES DISPERSED BY NEBULIZATION

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Abstract: In studies on the electrostatic precipitation of metal oxide nanoparticles (especially NiO, a commercially interesting material in this particle size range), the dispersion of metal oxide nanoparticles by pneumatic atomization is not commonly used due to the insolubility issues, besides the agglomeration and sedimentation of the particles. Therefore, the aim of this work was to evaluate the performance of a wire-plate electrostatic precipitator in the collection of NiO nanoparticles produced by nebulization of aqueous suspensions pre-treated with ultrasound bath. Electro-fluid dynamic phenomena were analyzed and discussed. Increase of voltage enhanced the efficiency in the particle size range observed.

Keywords: Electrostatic Precipitator, Environmental Control, Metal Oxide Nano-aerosols, Nanoparticulate Matter, Metal Oxide Nebulization.

INTRODUCTION

Researches on the performance of electrostatic precipitators (ESPs) collecting metal oxide nanoparticles have used different techniques to disperse nano-aerosols. Kulkarni *et al.* (2002) used a combustion furnace to obtain particles of Fe₂O₃, TiO₂, and SiO₂ of diameters from 20 to 600 nm. Domat *et al.* (2014) obtained SnO aerosols with electrical mobility equivalent diameters less than 60 nm from the vaporization of the solid material with subsequent carrying of a gas stream and condensation.

Although being a simpler and cheaper technique to disperse nano-aerosols than the abovementioned methods, the atomization of aqueous suspensions of metal oxides is barely used due to the insolubility of these particles and their agglomeration and sedimentation in the liquid mixture. However, these agglomerates can be fragmented due to the ultrasonic acoustic forces (Ivanov, 2012).

Studies on the electrostatic precipitation of NiO were not found, despising its high applicability. In nanometric scale, this material has been used in the development of hybrid films with graphene for supercapacitors (Xia *et al.*, 2011) and in nanowires of high specific surface area to collect ions of heavy metals and organic dyes from liquid effluents (Zhao *et al.*, 2015), for example. Therefore, this work aimed to study the performance of an ESP collecting nickel oxide nanoparticles, which were produced by atomization of aqueous suspensions by a commercial atomizer (TSI, 3076) after pre-treatment with ultrasound bath.

METHODS

Figure 1 shows a flow sheet of the experimental setup used.

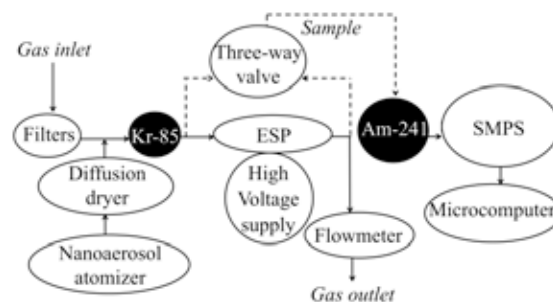


Figure 1. Experimental Setup

In the tests, air (25°C, 92 kPa) was fed by the compressor and passed through the filters in order to retain impurities. An internal compressor of the air atomizer also injected air into a vessel containing the metal oxide suspension. The nanoparticles produced passed through the diffusion dryer to remove humidity. The dried aerosol was mixed to the main air stream before passing through the Kr-85 source, which neutralized the aerosol charge in order to not interfere with the measurement of the particle concentration by the SMPS. Then, the aerosol passed through the electrostatic precipitator (Figure 2), which was made of acrylic and contained two copper plates and eight stainless steel wires with 0.3 mm of diameter. The ESP was connected to the high voltage source in order to generate the negative corona current. Particle samples in the inlet and outlet of the ESP were continuously withdrawn by controlling a three-way valve, thus the sample passed through the Am-241 source in order to neutralize its charge before entering the SMPS (Scanning Mobility Particle Sizer Spectrometer), which classified particles by size and counted the particles concentration by their electrical mobility.

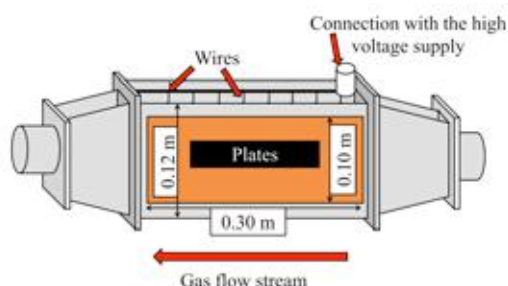


Figure 2: Sketch of the electrostatic precipitator

The suspensions were prepared by mixing the NiO powder (Aldrich, 99.8% of purity) in deionized water. The dielectric constant of NiO was equal to 11.9 (Young and Frederikse, 1973 apud Lide, 2015). An ultrasound bath was used in order to break the agglomerates in the suspension, as reported by Ivanov (2012). Previous experiments of nanoaerosol dispersion were performed in order to evaluate the homogeneity of the suspension and the reproducibility of the dispersion. Times of ultrasound bath of 30 and 60 min were evaluated and it was observed that 60 min was sufficient to break the aggregates and mitigate sedimentation of the NiO suspensions, providing higher aerosol concentrations and homogeneous dispersion.

In order to evaluate the effect of the applied voltage, a 0.01% wt NiO suspension was prepared and voltages of -8.0 (1.1 μ A), -8.5 (30.6 μ A), and -9.0 kV (76.0 μ A) at 23.5 L/min of air (residence time of 3.1 s) were evaluated.

The grade collection efficiency (η) was calculated from the inlet (ce) and outlet (cs) concentrations of the ESP for each diameter measured by the SMPS:

$$\eta (\%) = 100 \times (ce - cs) / ce \quad (1)$$

The N_{EHD}/Re^2 ratio was also calculated in order to evaluate the influence of the ion flux on the gas flow pattern into the ESP. The electrohydrodynamic number (N_{EHD}) and the Reynolds number (Re) are expressed according to IEEE (2003). The time $t_{90\%}$ for the particle to achieve 90% of its saturation charge was calculated by the definition presented by Riehle (1997). Since the dynamic charging is independent of the particle size when a homogeneous electric field is considered (Riehle, 1997), the same value of $t_{90\%}$ was considered for all the particle size range evaluated.

FINDINGS AND ARGUMENT

Figure 3 presents the particle size distribution of the ESP inlet (a) and the grade efficiency of the tests for different voltages at 23.5 L/min. It is possible to see that the increase of voltage enhanced the efficiency under the experimental conditions used. The particle charging inside the ESP occurs from two main mechanisms that prevail in different size ranges: field and diffusion charging. In the field

charging, ions generated by the corona discharge follow the electric field lines. When the particle of dielectric material passes through the electric field, it causes the distortion of these lines, promoting the collision of the ions with itself and the subsequent charge transfer (Hinds, 1998). Therefore, the high value of dielectric constant of the NiO possibly promoted high concentration of the field lines around the particles, enhancing the charge transfer and subsequently the collection by the ESP. However, the particle size range used here was below 200 nm. According to Riehle (1997), the diffusion charging prevails for particle sizes less than 200 nm and, at first analysis, this mechanism does not depend on the particle material. In the diffusion charging, particles acquire electrical charge from the ions by the random collisions due to the Brownian motion when the particle is extremely small (Hinds, 1998).

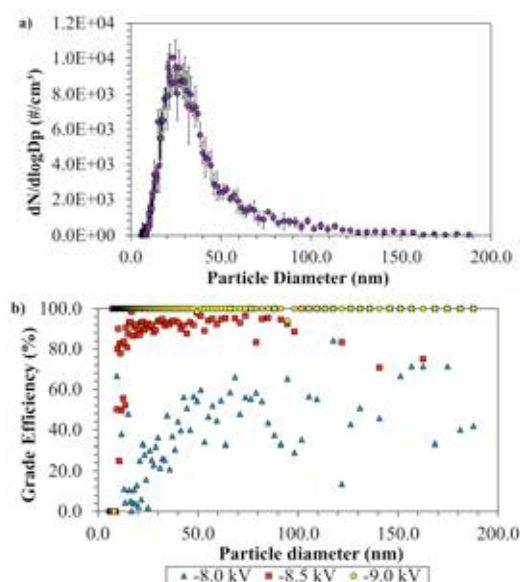


Figure 3: Particle size distribution in the ESP inlet (a) and grade efficiency (b) of tests at -8.0, -8.5, and -9.0 kV

In order to elucidate the prominence of both mechanisms, Figure 4 exhibits the particle electrical mobility for diameters up to 1000 nm at 23.5 L/min and -8.0 kV, calculated from the equations presented by Hinds (1998, p. 325) from the number of electrical charges a particle could acquire for each mechanism individually. The total number of charges acquired by both mechanisms simultaneously was obtained by the correlation of Lawless (1996). The same calculations were performed for NaCl and KCl, which dielectric constants are respectively equal to 5.9 and 4.86 (Young and Frederikse, 1973 apud Lide, 2015), thus the mobilities provided by field mechanism and by both mechanisms for these materials were also plotted (since diffusion charging does not depend on the dielectric constant, it was plotted once).

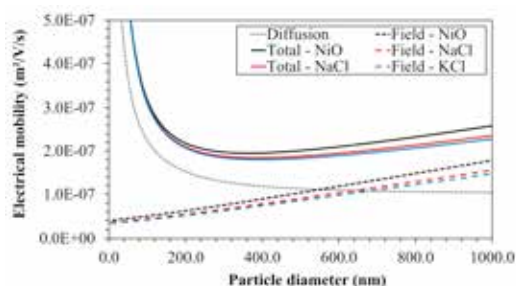


Figure 4: Electrical mobility by diffusion, field and both mechanisms for NiO and by field and both mechanisms for NaCl and KCl

From Figure 4, it is possible to observe that the material with higher dielectric constant (NiO) provided major influence of the field mechanism on the electrical mobility of the particle, even in the range of prominence of the diffusion mechanism. It is also verified that the field mechanism acts prominently over diameters greater than 480 nm for NiO, while this occurs for diameters between 630 to 640 nm for the other materials, with smaller dielectric constants. Although not being prominent for particle size range less than 200 nm, this mechanism also acts on the particle charging, as exhibited in Figure 4, justifying the importance to study the nanoparticle collection efficiency of ESPs for different materials, as metal oxides.

The time $t_{90\%}$ required to the particles to achieve 90% of their saturation charge was equal to 6.9, 0.26, and 0.11 s respectively for the tests at -8.0, -8.5, and -9.0 kV. This parameter indicates that the increase of voltage provides the increase of the electric field inside the device and the increase of the ions generated, which enhances the charge transfer and decreases the time needed to completely charge the particles (Riehle, 1997). By comparing with the residence time at the experimental conditions used here (3.1 s), it is verified that the voltages of -8.5 and -9.0 kV were sufficiently high to charge the particles before they pass through the ESP, at a first analysis.

The N_{EDH}/Re^2 values for tests at -8.0, -8.5, and -9.0 kV were respectively equal to 0.30, 8.53, and 21.2. According to Podliński *et al.* (2006), values of N_{EDH}/Re^2 higher than 1 mean high influence of the ion flux (from wires to plates) on the gas flow pattern, promoting the appearance of local turbulences in wire-plate ESPs. This phenomenon needs to be considered, since the increase of the voltage strongly enhanced this parameter, meaning a strong increase of the gas turbulence and possibly a enhanced mixture between ions and particles inside the ESP, which could have contributed to increase the charge transfer by diffusion and subsequently increasing the particle collection.

CONCLUSIONS

It was possible to perform a study of electrostatic precipitation of metal oxide nanoparticles by using

the method of atomization to disperse the nanoaerosols, since it provided reproducible data. The increase of voltage decreased the time required to totally charge the particulate and increased the influence of the ion flux on the gas flow pattern, which enhanced the process.

ACKNOWLEDGEMENT

The authors are grateful for the financial support provided by CNPq (131744/2017-8) and CAPES (001).

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THE IMPORTANCE OF STATE INSPECTION AND VEHICLE MAINTENANCE PROGRAMS IN AIR POLLUTION CONTROL

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Abstract: Air pollution in urban areas is associated with acute and chronic human health problems. Automotive vehicles are among the most significant sources of atmospheric pollutants, contributing to air quality degradation in many Brazilian cities. There are several substances harmful to man and the environment that are emitted into the atmosphere by motor vehicles. Individually, the emission of a vehicle may be small. However, the concentration of millions of vehicles generates tons of pollutants everyday. According to RMRJ Road Vehicle Emissions Inventory, published in 2016, it is estimated that 15 thousand tons/year of non-methane hydrocarbons, 42 thousand tons/year of nitrogen oxides and 888 tons/year of particulate material. In the 1980s, the Air Pollution Control Program for Automotive Vehicles (PROCONVE) was implemented in Brazil, which aims to reduce and control the pollution caused by vehicular sources. In addition, to establishing technological requirements for domestic manufacturers and imported vehicles and improving fuel quality, it has made it mandatory to implement Inspection and Maintenance Programs for Vehicles in Use (I/M Program) to states whose objective is to identify vehicles in use, having as reference the original specifications of the vehicle manufacturers that cause increased emission of pollutants, therefore, encourages corrective and preventive maintenance of the vehicles and discourages the adulteration of emission control devices. The fleet of the state of Rio de Janeiro is estimated to be almost 7 million vehicles, with about 70% of these registered in the RMRJ. The average age of the state fleet is approximately 9 years of use. This paper will show some results obtained in the scope of I/M Program of Rio de Janeiro state, analyzing the results of approximately 3 million surveys conducted in the period from 2014 to 2017 of Otto cycle vehicles. Of this total of inspections, about 24% were of disapproval. In addition, it can be observed that the variation between the corrected hydrocarbon (HCC) and corrected carbon monoxide (COC) emission averages of vehicles failing when compared to the HCC and COC averages of vehicles of approved vehicles was 6 times more (COC) and 10 times more (HCC). Therefore, it can be concluded that due to the lack of preventive and corrective vehicles maintenance, the emission levels are quite high, which makes it difficult to reduce the pollutants required for each new phase of PROCONVE, making it less efficient.

Keywords: I/M Program, vehicle inspection, pollution, emission, air quality

INTRODUCTION

There are several substances harmful to man and the environment that are released into the atmosphere by motor vehicles, mainly due to the process of burning fossil fuels, causing air pollution (LI et al., 2011; WANG et al., 2010; GUO et al., 2013).

According to Kampa and Castanhas (2008), air pollution in urban areas is associated with acute and chronic human health problems, depending on the time of exposure, ranging from small irritations in pathways superior to chronic heart diseases, lung cancer, and of problems associated with premature mortality and reduction of life expectancy.

In view of the adverse health effects of the population, it is becoming increasingly important to have Vehicle Inspection and Maintenance Programs in use (I / M Program), which verify if the emissions of the vehicles that circulate in the cities, especially in the are within the emission limits set forth in environmental resolutions, such as those issued by the National Environmental Council (CONAMA), in

order to control the release of pollutants into the atmosphere.

An I/M Program aims to identify nonconformities of the vehicles in use, having as reference the original specifications of the vehicle manufacturers (CONAMA, 2009). In addition, it has as main purposes to encourage the corrective and preventive maintenance of the vehicles and to discourage the adulteration of the emission control devices (VENTURA et al., 2016). The lack of maintenance and incorrect maintenance of vehicles can be responsible for the increase of pollutant emissions and the consumption of fuels, which cause health problems in the population (CONAMA, 2009).

Vehicle environmental inspections are regularly conducted by 51 countries worldwide, including the United States, Japan and the European Union. In Latin America they already carry out this type of inspection in Uruguay, Argentina, Chile, Peru, Costa Rica and Peru (MMA, 2018).

In Brazil, CONAMA Resolution No. 418/09 establishes the guidelines for I/M Program, bringing in its scope the pollutants that must be measured during the

annual vehicular inspection, as well as specifying the emission limits to be met, as a function of its manufacture years, motorization and fuel.

For vehicles with Otto cycle engines, ie gasoline, ethanol or flex-fuel vehicles, as well as those equipped with the natural gas vehicle (NGV) kit, HC, CO and dilution factor of exhaust gas (FD) must be measured.

However, CONAMA (2009) establishes emission measurement standards for FD, and CO and HC corrected, the latter two being products by the FD with CO and HC measured, respectively.

Thus, the objective of this work is to present results of the I/M Program implemented in Rio de Janeiro state, in order to demonstrate the importance of this type of Program for air pollution control and the maintenance of public health, as well as (PROCONVE) since the first edition (CONANA Resolution No. 18/1986).

METHODS

For the analysis of the characteristics of vehicles fleet registered and circulating in Rio de Janeiro state, DETRAN-RJ (2018) data were adopted. In addition, the maintenance status of the light vehicles evaluated in the inspections of the I/M program in Rio de Janeiro state was analyzed using the corrected HC and CO data measured during supervision conducted between 2014 and 2017 at DETRAN-RJ stations and compared to limits established by CONAMA Resolution N.418/09.

FINDINGS AND ARGUMENT

The results obtained through an exploratory analysis of Otto cycle survey data between the years 2014 and 2017 will be presented under the Inspection and Maintenance Program (I/M) of Rio de Janeiro state.

Table 1 shows the fleet average age of Rio de Janeiro State by vehicle type. It can be observed that most of the fleet, about 70%, is composed of automobiles that have a relatively high average age. Then, it must be considered that the consolidation of the PROCONVE phases take place more slowly, which evidences the constant need for vehicles maintenance.

Also noteworthy is the average age of approximately 14 years for trucks that, despite representing only 3% of the fleet, is the main responsible for particulate material emissions among all vehicular emissions.

Table 1. Fleet average age of Rio de Janeiro State licensed in 2015

Vehicle type	fleet	Average age

Heavy vehicles	93,622	14
Bus	397,983	6
Utility	50,826	7
Light vehicles	2,306,543	8
Motocycles	466,749	5

Font: DETRAN-RJ (2015)

Figure 1 represents the percentage of vehicles disapproved in the inspections conducted at DETRAN/RJ stations during 2014 to 2017. It is noted that approximately 1.1% of the vehicles are disapproved in the visual inspection, most of these failures being caused by leakage of fluids in the engine block, smoke emission and deterioration in the catalytic converter or in the exhaust system.

The highest vehicle failure rate is observed in the gas inspection, approximately 22.5%. In this inspection, the emissions of CO, HC and FD are evaluated according to CONAMA (2009) limits.

Therefore, from Figure 1, it can be verified that about 24% of the vehicles fail at any of the environmental criteria, evidencing the need to maintain them for the emissions control of polluting gases.

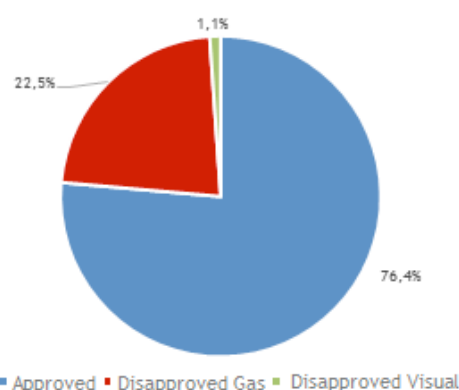
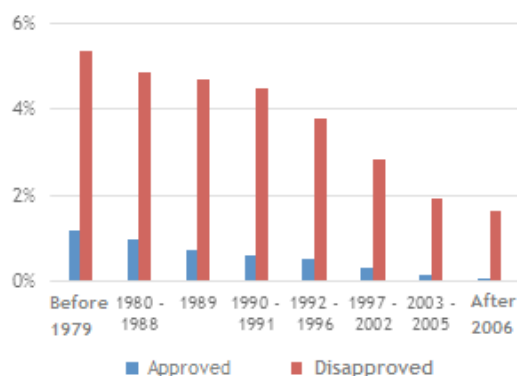
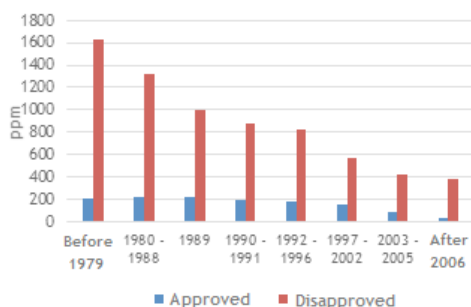


Figure 1. Failure indexes in the inspections carried out in Rio de Janeiro vehicle fleet from 2014 to 2017.

Figure 2 presents the results by manufacture years of the average emissions of COc (a) and HCc (b) in the inspections from 2014 to 2017. It is necessary to show that the ranges proposed in Figure 3 are based on the same phases of CONAMA (2019).



(a)



(b)

Figure 2. Average Emissions of COc (a) and HCc (b) for the vehicles approved and disapproved by groups of manufacture years in the inspections carried out between 2014 and 2017.

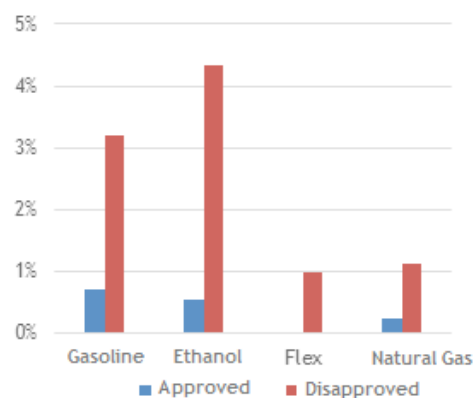
It is noted that for both average COc and HCc emissions there are quite significant differences between approved and failed vehicles. It is revealed that in the range of vehicles whose manufacture year is 2006 onwards, the average COc emission is about 20 times higher in the reprovved vehicles while the average emission of HCc is about 10 times higher for this same group of vehicles.

It is known that newer vehicles are designed to emit less pollutants. However, what Figure 2 shows is that the lack of preventive and/or corrective maintenance on the vehicles, raises emission levels greatly, which makes it difficult to reduce the pollutants that these vehicles were projected, thus making PROCONVE less efficient.

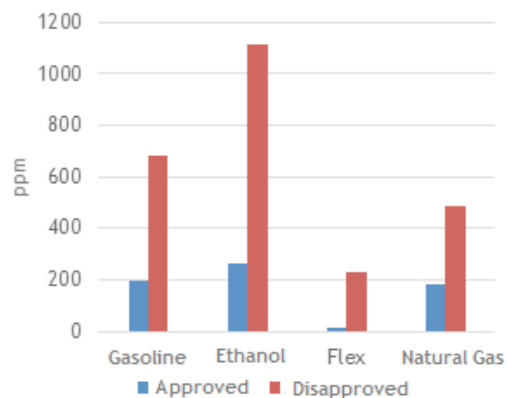
Figure 3 also shows a high difference in the average emissions of COc (a) and HCc (b) between approved vehicles and failed vehicles, being the first one with the lowest indexes. In this figure, there is a greater difference between vehicles approved x disapproved in ethanol fuel in both pollutants (COc

and HCc). This fact can be explained due to ethanol vehicles being older. Therefore, they have less advanced technology.

It is also shown in Fig. 3 that NGV vehicles which have been approved in inspection centers have also been disapproved, and the average COc and HCc emissions from these vehicles are approximately 3 times higher than those of approved vehicles.



(a)



(b)

Figure 3. Average Emissions of COc (a) and HCc (b) for the vehicles approved and disapproved by fuel type in the inspections carried out between 2014 and 2017.

CONCLUSIONS

PROCONVE aims in the first phase to improve the quality of commercial fuels and the technology of engines and atmospheric emissions control systems of vehicles during the manufacture. In addition, it counts that the states implant I/M programs for the control of the pollution of the vehicles in use in the second phase, with the objective of maintaining the

technological gains already achieved, once the owners carry out preventive and/or corrective maintenance of their vehicles for licensing purposes. These sets of federal and state actions aim at improving air quality indices, especially in urban areas with air pollution problems.

The results of I/M Program implemented in Rio de Janeiro state showed that 24% of the fleet inspected from 2014 to 2017 were disapproved. This shows the lack of maintenance of the circulating vehicles in the state, which greatly increases (3 to 20 times) CO and/or HC levels emitted by light vehicles in relation to the environmental limits recommended by CONAMA, which makes PROCONVE less efficient in its strategy to reduce vehicular pollution, and consequent improvement of air quality and public health.

Finally, an I/M Program, if properly implemented, can be an effective instrument for the reduction of emissions of gaseous and particulate pollutants by the circulating fleet of motor vehicles, according to the National Air Quality Control Program - PRONAR, as well as and of the PROCONVE.

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FILTRATION PERFORMANCE OF A SINGLE NANOFIBER LAYER ADDED TO A FILTER MEDIA BY CENTRIFUGAL SPINNING

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Abstract: The inhalation of nanoparticle is relate to heart and respiratory diseases and premature death. The aim of this work was to investigate the filtration performance of a single nanofiber layer added to a filter media by centrifugal spinning. 12 wt.% polyacrylonitrile was dissolved in dimetilformamide. The solution was spun on filter media by Forcespinning (FS) equipment using vacuum collection system as collector. The nanofiber layer were analyzed through scanning electron microscopy images using ImageJ software to obtain fiber diameter, pore size, superficial porosity and density of fiber intersections. The filtration performance was measured experimentally in filtration apparatus. The pressure drop was measured by digital manometer and permeability was calculated by the Darcy equation. The collection efficiency was calculated from particles that ranged from 5 to 100 nm, with face velocity 4.8 cm/s, and filtration area 5.2 cm². The nanofiber layer presented a fiber diameter 1.04 µm, pore size 9.20 µm, superficial porosity 86% and density of interaction 0.01 int/ µm². The fiber diameter ranged from 0.11 to 3.68 µm. The covered filter media resulted in 36% of collection efficiency, pressure drop of 2.6 Pa and permeability of 1.48 10⁻⁷ cm². As expected the collection efficiency and pressure drop increased and the permeability of the filter media decreased. However, the addition of a single nanofiber layer in the filter media promoted increase the collection efficiency 19% with the small increase pressure drop, 2.0 Pa, compared with only the filter media.

Keywords: centrifugal spinning, nanofiber, nanoparticle, pollution, collection efficiency.

INTRODUCTION

Particle with diameter smaller than 100 nm contribute around 90% of particle concentration in urban areas. The nanoparticles, when inhaled, can reach the deeper respiratory tract, and the whole body, through the lymphatic and blood circulation, causing serious health problems (Choi and Kim 2018). Particles with this size were related to health problems, lung cancer, stroke, heart diseases, and premature death (World Health Organization 2006).

Spun nanofiber had been researched for filtration application with good performance (Zhu et al. 2016; Leung, Hau, and Choy 2018). Nanofiber was high surface-to-volume ratios, small pore sizes, and small fiber diameters (Ahn et al. 2006; Gibson, Schreuder-Gibson, and Rivin 2001). These characteristics promoted an increasing on collection efficiency of micro and nanoparticles. Centrifugal spinning has been a promising method of produce polymeric nanofibers. This method increase the materials choice, high productive and reduce production costs (Padron et al. 2013; Sarkar et al. 2010). Thus, the aim of this work was to analyse filtration performance of nanoparticle promoted for the addition of a single nanofibers

layer by centrifugal spinning in low performance filter media.

METHODS

The nanofibers were spun by Forcespinning (FS) equipment using vacuum collection system (VCS) as collector. 12% wt polyacrylonitrile was dissolved in dimetilformamide on stirring and heating. The solution were spun over the filter media with follow operational conditions: 26 gauge half-inch needle, 10 cm needle-collector distance, rotational speed 4000 rpm, 60 s collection time, VCS on 100% power.

The characteristics of nanofiber layer were measured by image analysis performed on scanning electron microscope (SEM) - Inspect S50, FEI Company - to determine the fiber diameter, the fiber diameter distribution, the superficial porosity, the density of intersections and the pore size performed on ImageJ software.

The filtration apparatus were used to perform collection efficiency of nanoparticles, permeability and pressure drop of filter media. The nanoparticles were generated from a solution of 0.1 g/l NaCl. The concentration of the particles before and after the filter media was determined

by the scanning mobility particle size spectrometer, one hour after the start of the test. The face velocity was maintained at 4.8 cm/s and the filtration area was 5.2 cm². The collection efficiency was calculated by the equation 1.

$$E = \frac{C_0 - C_1}{C_0} \quad (1)$$

where, E is collection efficiency, C_0 is the particle concentration before filter media and C_1 is the particle concentration after filter media. The permeability was calculated by the Darcy equation used in the case of purely viscous flows, as can be seen on equation 2.

$$\frac{P}{L} = \frac{\mu v_L}{k} \quad (2)$$

where, ΔP is the pressure drop, L is the filter media thickness, μ is the fluid viscosity, v_L is the face velocity and k is the permeability constant of the filter media.

The pressure drop was measured by the digital manometer (TSI 9555 P). The thickness of the filter media was measured by optical microscope - BX60, Olympus.

FINDINGS AND ARGUMENT

The filter media was composed of polyester. The filter media was 17% collection efficiency, 0.6 Pa pressured drop and $3.34 \cdot 10^{-7}$ cm² permeability (Table 1). Figure 1 shows the image of filter media and covered filter media with 200x of magnification.

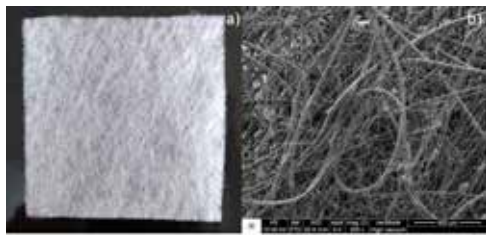


Figure 1. a) Filter media and b) SEM image of covered filter media with 200 x of magnification.

The nanofiber layer was fiber diameter 1.04 μ m, the superficial porosity 86%, the density of intersections 0.01 int/ μ m² and the pore size 9.2 μ m, Table 1.

Fibers on nanometric dimension promotes greater interaction with particles and the fiber, because the mean free path of gas molecules is comparable with the fiber diameter, the gas fluid will slip over the fiber surface, which increases the collection efficiency (Grafe and Graham 2002; Graham et al. 2002).

(Payen et al. 2012; Zhang, Shim, and Kim 2009) reported that fiber diameter distribution influence on collection efficiency. A better analysis of fiber diameter was done in Figure 2 a). The fiber diameter of nanofiber layer ranged from 0.11 to 3.68 μ m. The diameters most frequently were between 0.7 and 1 μ m.

Figure 2 b) present collection efficiency of particle that ranged from 5 to 100 nm performed on filter media and covered filter media. The shape of the curves can be explained for the change of the collection mechanisms. The inertial impaction and interception mechanisms decrease for particle size from 1 to 0.1 μ m, while diffusion mechanism became dominant for small particles smaller than 0.1 μ m (Yang 2012). This causes decay in the curve during the change of mechanisms. The addition of nanofiber layer promotes increase on collection efficiency over the whole range of evaluated particles. Covered filter media was 36% of collection efficiency, 2.6 Pa of pressured drop and $1.48 \cdot 10^{-7}$ cm² of permeability (Table 1).

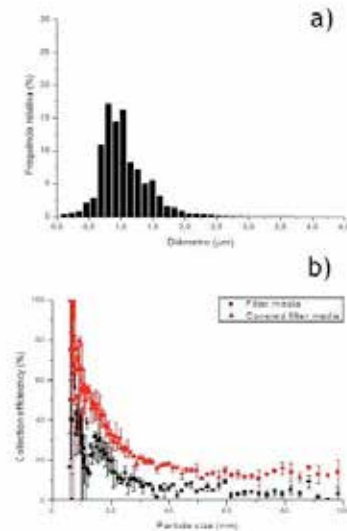


Figure 2. a) Fiber diameter of nanofiber layer distribution and b) collection efficiency of filter media and covered filter media.

Table 1. Filtration performance employed on filter media and covered filter media and characteristics of fiber layer.

	Filter media	Covered filter media
Fiber diameter (μ m)	-	1.04
Superficial porosity (%)	-	86
Density of intersection (int/ μ m ²)	-	0.01
Pore size (μ m)	-	9.2
Collection efficiency (%)	17	36
Pressured drop (Pa)	0.6	2.6
Permeability (cm ²)	$3.34 \cdot 10^{-7}$	$1.48 \cdot 10^{-7}$

CONCLUSIONS

Nanofibers promote good interaction between particles and fiber. The addition of a single nanofiber layer to a filter media increasing efficiency 19% with the small increasing pressure drop, 2.0 Pa, compared with only the filter media. Thus, the addition of the nanofiber layer can be an alternative to increasing filtration performance. Centrifugal spinning can be a good alternative of nanofiber production for filtration application.

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EVALUATION OF AIR FLOW AND DISTRIBUTION IN THE INLET DUCT OF A BAG FILTER THROUGH COMPUTATIONAL FLUID DYNAMICS (CFD)

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Abstract: To minimize the impact on the environment, air pollution control systems such as local exhaust ventilation systems are used. In these systems, the use of equipment as bag filters stands out. In order for these equipments to function satisfactorily and to meet the purpose for which they were designed, it is fundamental that the air inlet conditions in the filter are the closest to the idealized design. With the technological advances in computation, associated to the popularization and greater access to hardware and software, Computational Fluid Dynamics (CFD) has become an important tool for the design and verification of the operation of processes, equipment and products that involve the flow of fluids. In view of this scenario, the present work intends to contribute to the study of the flow in bag filters inlet ducts, using CFD techniques, from the case study of a duct used in a local exhaust ventilation system in a industry. The real case studied consists of a local exhaust ventilation system section composed of a duct that forks giving rise to an outlet and to a section with a derivation, giving rise to two other outlets. Each outlet has an expansion section and is located in the lower section of the bag filter. For the modeling, it was necessary to create a domain in 3 dimensions. Thus, in this present work, the duct geometry was constructed using Autodesk Inventor Professional 2016 3D CAD software. The mesh was created using the ANSYS Meshing module, and tetrahedral cells were chosen for a better description of the flow, considering the large velocity gradients in this duct section. The mesh used has about 12 million nodes. The boundary conditions for the flow solution in the studied duct are essentially the inlet mass flow rate (Q_m), the non-slip condition on the duct walls and the pressure at the duct exits. The simulation was performed in two computers due to the reduced computational resources available, being a Notebook with 2 cores of processing of 2.0GHz and 4 GB of RAM and a desktop with 2 cores of processing of 3.4 GHz and 8GB of RAM belonging to the Department of Sanitary and Environmental Engineering of UFMG (DESA - UFMG). Through the results obtained with the simulation of the flow in the inlet duct was observed the non-uniformity in the air flow distribution along the duct and its outlets. It is also possible to observe the presence of large recirculation vortices near the bifurcation of the duct and in the 3 outlets, being able to cause the deposition of materials and increase of the loss of load in these sections. The concentration of the flow in specific regions of the outlets collaborates for high speeds in these regions, causing the air to enter in the filtration chamber with a velocity capable of offering risks of rupture to the sleeves and wear of components. These results confirm the reports obtained by industry employers about the problems with this bag filter.

Keywords: CFD, air pollution control, bag filters ducts, case study.

INTRODUCTION

Nowadays, industrial processes are one of the major causes of deterioration of air quality through the emission of pollutants into the atmosphere (MMA, 2018). These substances are often toxic or harmful to the environment and/or human health. To minimize the impact on the environment, air pollution control systems such as local exhaust ventilation systems are used. In these systems, the use of equipment as bag filters stands out. In order for these equipments to function satisfactorily and to meet the purpose for which they were designed, it is fundamental that the air inlet conditions in the filter are the closest to the design idealized. With the technological advances in computation, associated to the popularization and greater access to hardware and software, Computational Fluid Dynamics (CFD) has become an important tool for the design and verification of the operation of processes, equipment and products that involve the flow of fluids. (VERSTEEG & MALALASEKERA, 2007). In view of this scenario, the present work intends to

contribute to the study of the flow in bag filters inlet ducts, using CFD techniques, from the case study of a duct used in a local exhaust ventilation system with this type of air pollution equipment control.

METHODS

The real case studied consists of a local exhaust ventilation system section composed of a duct that forks giving rise to an outlet and to a section with a derivation, giving rise to two other outlets, as can be seen in Figure 1.

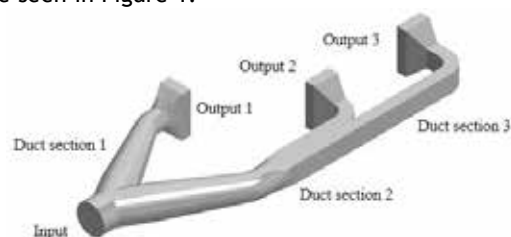


Figure 1 - Studied inlet duct 3D model.

Each outlet has an expansion section and is located in the lower section of the bag filter. The construction and design details of the duct section are shown in Table 1.

Table 1 - Duct section technical features.

Parameter	Unit
Flow	31.000 m ³ /h
Inlet diameter	780 mm
Outlets dimension	600 x 1100 mm
Duct section 1 diameter	490 mm
Duct section 2 dimension	600 x 470 mm
Duct section 3 dimension	300 x 470 mm

The computational modeling follows the governing differential equations of mass and momentum conservation, discretized for each control volume of the domain in the three dimensions (x, y and z). For the numerical solution of the differential equations is used the Element based Finite Volume Method (EbFVM). In order to contemplate the effects of the turbulence in the flow, it is necessary to use specific methods, in this work the RANS model.

For the modeling, it was necessary to create a domain in 3 dimensions. Thus, in this present work, the duct geometry was constructed using Autodesk Inventor Professional 2016 3D CAD software. The mesh was created using the ANSYS Meshing module, and tetrahedral cells were chosen for a better description of the flow, considering the large velocity gradients in this duct section. The mesh used has about 12 million nodes.

The boundary conditions for the flow solution in the studied duct are essentially the inlet mass flow rate (Q_m), the non-slip condition on the duct walls and the pressure at the duct exits. In this way we have:

- $Q_m = 10,21 \text{ kg/s}$
- Pressure condition at the outlets:
 $P_1 = P_2 = P_3 = 1 \text{ atm}$
- Non-slip condition: $u_1 = u_2 = u_3 = 0$

The simulation was performed in two computers due to the reduced computational resources available, being a Notebook with 2 cores of processing of 2.0GHz and 4 GB of RAM and a desktop with 2 cores of processing of 3.4 GHz and 8GB of RAM belonging to the Department of Sanitary and Environmental Engineering of UFMG (DESA - UFMG).

FINDINGS AND ARGUMENT

Through the analysis of the current lines, it is possible to verify the existence of recirculation zones and low velocity and pressure, propitious to the detachment of the boundary layer of flow along the duct, as shown in Figure 2.

The existence of these zones may lead to the appearance of recirculation phenomena, as shown

in Figure 3, causing an increase in energy dissipation through the shear stresses created in the vortices. In addition, the presence of zones with low velocities can propitiate the deposition of the particulates present in the airflow, creating pockets of waste inside the pipe. In the long run, these materials can interfere with the flow dynamics, encrusting in the duct and progressively strangling the section.

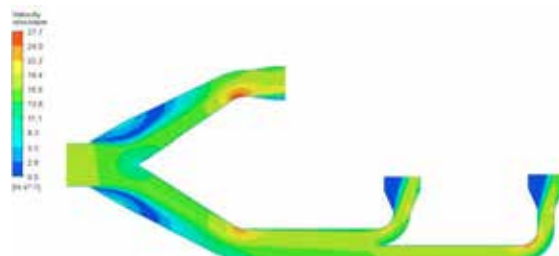


Figure 2 - Speed distribution in the horizontal plane to the average height of the duct.

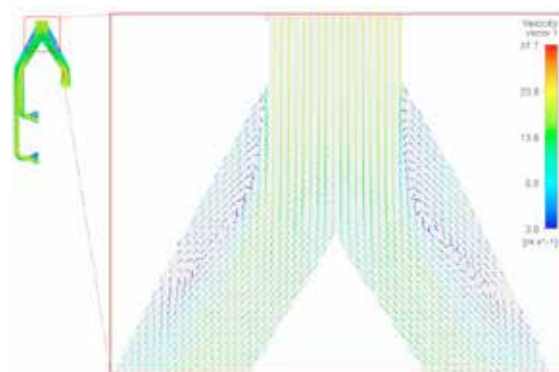


Figure 3 - Airflow vectors in the recirculation zone near the bifurcation.

The duct outlets have specific characteristics regarding the velocity and flow distribution, as shown in Table 2. Observing the distribution of the mass flow in the exits, we noticed that although the Outlet 1 area is smaller than the Outlet 2 and 3 areas, it has a mass flow rate of about 60% greater. These data show the imbalance in the distribution of airflow at the outlets.

Table 2 - Flow and velocity distribution at the duct outlets.

Localization	Area (m ²)	Mass Flow (kg/s)	Volume Flow (m ³ /h)	Average Velocity (m/s)
Inlet	0,48	10,20	31000	18,02
Outlet 1	0,66	4,46	13553,3	5,70
Outlet 2	0,72	2,83	8612,4	3,35
Outlet 3	0,72	2,91	8834,3	3,43

The flow lines, shown in Figure 4a, point to a concentration of the flow in the central portion of Outlet 1. This centralization of the flow demonstrates that the expansion at the end of the duct does not effectively fulfill the flow expansion

function due to the high velocity with which the flow gets at the outlets, the stretch being more elongated or having a smaller opening angle in the expansion. Moreover, this centralization at the inlet of the bag filter causes the air to enter at a high velocity, of the order of 20 m/s, according to the velocity distribution shown in Figure 4b, overloading the sleeves located in that region and increasing the probability of his breakup.

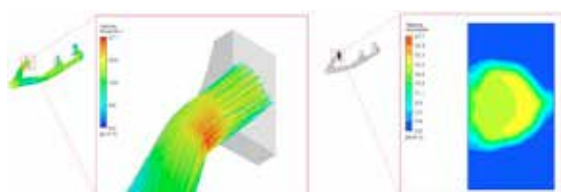


Figure 4: a) Flow lines distribution at Outlet 1. b) Velocity perfil at Outlet 1.

The distribution of velocities, shown in Figures 5a and 5b, indicate a flow distribution only on the sides of Outlets 2 and 3. This distribution can be associated with an abrupt derivation angle, which forces the flow layer to detach and concentrate it on the opposite side of the outlet duct. From this, the average velocity values presented in Table 2 doesn't correspond to a homogeneous distribution, as expected in design, but rather an irregular distribution that reaches velocities close to that of the duct inlet.

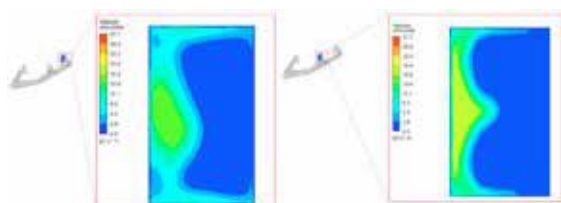


Figure 5 - a) Velocity perfil at Outlet 2. b) Velocity perfil at Outlet 3.

The concentration of the airflow at the side of the duct and the existence of low velocities throughout the surroundings of Outlets 2 and 3 contribute to the formation of large recirculation zones, as observed in Figures 9 and 10. The presence of recirculation zones can to provide not only the deposition of particulates from the outlet duct, but also the return of these materials from the inside of the filtration chamber.

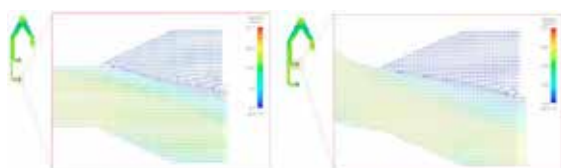


Figure 6 - a) Plan view of the recirculation vortex zone at Outlet 2. b) Plan view of the recirculation vortex zone at Outlet 3.

CONCLUSIONS

Through the results obtained with the simulation of the flow in the inlet duct was observed the non-uniformity in the air flow distribution along the pipe and its outlets. It is noticed that the air distribution in the 3 outlets is not balanced, with Outlet 1 receiving a flow surplus of approximately 60% in relation to Outlets 2 and 3. It is also possible to observe the presence of large recirculation vortices near the bifurcation of the duct and in the 3 outlets, being able to cause the deposition of materials and increase of the loss of load in these sections. The concentration of the flow in specific regions of the outlets collaborates for high speeds in these regions, causing the air to enter in the filtration chamber with a velocity capable of offering risks of rupture to the sleeves and wear of components. These results confirm the reports obtained by industry officials about the problems with this bag filter.

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DEVELOPMENT OF CONTROLL POLICIES ON ATMOSPHERIC EMISSIONS FROM STATIONARY SOURCES AT RIO DE JANEIRO STATE

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Abstract: In the last few decades pollutants emissions gradually increased, due to the urban and industrial quick growth, specially at metropolitan areas, causing side effects over society, economy and environment. Some brazilian states developed numerous regulatory steps as a initiative to future federal laws, following international tendency, to implement air pollution control acts and air quality degradation preventive efforts. Subsequently, the state of Rio de Janeiro has implemented, to industrial sources by an institution named State Foundation for Environment Engineering (FEEMA), in 1986 a regulation named DZ-545 - Atmospheric Emissions Self-monitoring Program (PROCON-AR) composing Pollutant Activity Permits System (SLAP), in order to monitor effective or potential pollutant activities emissions that alter air quality. This program (PROCON-AR) main purposes are, among others: improve air pollution control actions of Rio de Janeiro's environmental agency, named Environment Institute of Rio de Janeiro State (INEA), verify compliance with the applicable local and national emissions standards and support the development of appropriate atmosphere emission control strategies. The referred Guidance Document content was improved in 2010, already among the responsibilities of the Institute, and from there on the PROCON-AR was replaced by Atmosphere emissions of Stationary Sources Monitoring Program (PROMON AR), established by an Operational Standard, called NOP-INEA-01, approved by CONEMA n° 26 at 22/11/2010 Regulation, standardizing the analysis procedures and sample handling, as well as giving information feedback directly to the environmental agency. In 2018, CONEMA n° 26/2010 Regulation was revoked and replaced in 17/10/18, by CONEMA n° 84/2018 Regulation. This new Regulation simplified Sample Reports analysis and sign up procedure bringing automation, also updating methodological references, improving Sampling Schedule, and so forth. Accordingly, in this research it is introduced a review of pollution prevention policies in stationary sources at Rio de Janeiro state, as well as the benefits accomplished with the progress and its trends.

Keywords: Atmospheric emissions, emissions monitoring, stationary sources, PROMON AR.

INTRODUCTION

Human activity was always connected to environment transformation. Environment, according to Environmental National Policy, Law n° 6.938, august 31 of 1981, is defined as the circumstances, laws, influences and physical, chemical and biological interactions, that shelters and guides life in all of its forms. This widespread word, encompasses concepts about the reality of the world.

According to MMA (2018), atmospheric pollution can be defined as any matter or energy form with intensity, concentration, time or any other characteristics that the presence in the air causes nuisance or harm to human life, animal life or vegetation, inconveniences public welfare, damages materials or is harmful to safety, the use and enjoyment of property and communities' life quality. Air pollution emphasized at this paper, is

generated by burning fossil fuels, resulting in pollutants that for their chemical and physical characteristics and under meteorological parameters influences, can reach different locations, harming public health and the environment. Those conditions amplify the impact range, that goes beyond local, reaching regional and global.

The concept includes human activities and/or natural activities that causes deterioration of the atmosphere's original condition. There are many air pollutants, that can be defined by BRETSCHEIDER and KURFÜRST (1987) by: (1) a place where pollutants substances escape from (chimneys, ducts, air discharge, etc.); (2) Production processes and/or equipments (boiler, oven, production line, combustion chamber, etc.); (3) an area as a set of points and/or processes and equipments in a specific region, capable of releasing matter or energy to the atmosphere, polluting it.

Developed countries, driven by the constant incidents of air pollution, structured systems of environmental policies by adopting standards of environmental quality - air quality and emission standards - that combined with the development of more efficient control systems were able to bring benefits to the quality of life of the urban population. It is noticeable a tendency to modernize industrial installations as a result of environmental permits, aiming to reduce atmospheric emissions.

Rio de Janeiro's metropolitan region, with 22 cities, has the second highest industry and vehicles (mobile sources) concentration of the country, and also presents the worst air quality of the state. (INEA, 2013) According to FEEMA's second inventory in 2004, 23% of atmospheric emissions are derived from stationary sources, while petrochemical, marine, chemical, food and beverage and energy transformation are the predominant sectors.

Accordingly, stationary sources pollution control perform an important role in air quality management. Two fundamental approaches are able to accomplish it: control through emissions dilution in the atmosphere due to dispersion effects, and control in the source with the control equipment implementation and/or actions able to decrease emissions (PAINTER, 1974).

Hence, this paper presents a review of prevention policies for stationary sources pollution at Rio de Janeiro state, as well as benefits obtained with progress and its tendencies.

METHODS

This paper is the outcome of research, mostly from environmental regulations and policies from Rio de Janeiro's state and the country, about the thematic of stationary sources atmospheric emissions, aiming to obtain historical data about the main public policies, which presents an analysis since the first version of the ongoing legislation, in 1981. Also, highlights the achieved benefits with public policies progress and its tendencies.

FINDINGS AND ARGUMENT

The federal constitution of 1988 - set of laws of higher hierarchical level in the country - acknowledges the environment as a indispensable character at the development of economical activities, deepening this relation, recognizes that the environment protection is essential to assure a proper use of resources and a higher quality of life to the population. According to the constitution, it's the Union's responsibility to establish general rules and the states' to only specify them.

Aiming to establish control, prevention and recovery of air quality strategies on national territory, respecting Law n° 6.938 of 31/08/81 which instituted the National Environmental Policy, was declared in July 15, 1989 the Air Quality Control National Program - PRONAR.

The PRONAR was defined as one of the fundamental instruments to environmental management of populations health, protection of well being and improvement of quality of life, aiming to economically and socially develop the country in an environmentally safe manner, by the limitation of pollutants emissions through atmospheric pollution sources, therefore improving air quality, the established procedures attendance and non commitment to air quality in non degraded areas.

According to Federal Law 6938/81, article 10, construction, installation, ampliation and functioning of institutes and activities that uses environmental resources considered effective or potentially polluting, as well as capable of environmental degradation in any way, will require previous licensing by the qualified State Agency, member of Environment National System (SISNAMA) and Brazilian Institute of the Environment and Renewable Natural Resources (IBAMA), on supplementary basis, without injury of any other licenses/permits.

Considering National approach, the applicable emissions limitations were predicted by CONAMA n° 05/89 for definition and use purposes. The same regulation establishes emissions limits as guidance and service of control actions defined by PRONAR. The text also mentions that "highest emission limits will be distinguished by means of classification by intended use to varied areas and also more severe to new pollution sources" (CONAMA, 1989).

In the following year, the CONAMA n° 03/90 Resolution determined, in Brazil, air quality standard, based on scientific studies of criteria pollutants effects in the atmosphere. Some compounds are internationally known as indicators of air quality such as are sulfur dioxide (SO₂), particulate matter in suspension (PM), carbon monoxide (CO) and photochemical oxidants such as ozone (O₃), total hydrocarbons and nitrogen oxides (NO_x).

Furthermore, CONAMA's resolution n° 08/90 established emissions limits to air pollutants (emission standards) to new stationary sources registered of external combustion processes with total nominal load of 70 MW or higher. The resolution established values only to combustion processes assuming that this type of source was predominant, and also established only sulfur

dioxide, total particulates and colorimetric density analysis (smoke).

The 7^o article of this referred resolution, mentions that the inspection of national emissions limits attendance, when provided the Operating Permit (LO), can be realized by environmental agency licensed or, by the licensing company, since the referred agency conduct the supervision (CONAMA, 1990b).

The analysis procedures of environmental licensing evaluates atmospheric emissions for criteria pollutants and its corresponding air quality impacts at the companies' surroundings (CAVALCANTI, 2003). The evaluations are accomplished using as foundation one of the CONAMA's resolution, the n^o 08/90 with the emission limits, and the n^o 03/90 that establishes air quality standards.

CONAMA's Resolution n^o 05 of june 15, 1989, recommended the establishment of Emission Limit arranged by source typology and majority pollutants, at january 02, 2007, published at DOU n^o 1 the Resolution CONAMA n^o 382 of december 26, 2006, establishing atmospheric pollutants Emissions Limits to all stationary sources arranged by its installation date.

In order to fulfill this regulation, published on december 26, 2011 at the DOU N^o 247 the Resolution CONAMA n^o 436 of december 22, 2011, which establishes the atmospheric pollutants Emission Limits to stationary sources already installed or with permit order of installation before january 02 of 2007.

Currently, air quality standards are established by CONAMA Resolution n^o 491/2018, that dismissed and replaced CONAMA n^o 3/1990.

National public policies establishes how the state will develop its activity, specifying public agencies' fundamental actions concerning environmental protection, improvement of goals, principles and mechanisms of environmental control.

The State Foundation of Environmental Engineering (FEEMA) was established at Rio de Janeiro's state though Decree-Law n^o 39 of march 24, 1975, to implement control actions and environmental management.

In 1977, FEEMA instituted the Pollution Activities Licensing System - SLAP, through Decree No. 1633, which served as support for the registration of the main sources of air pollution in the State (Pires, 2005).

In 1985, the DZ-525-R1 was approved, which establishes criteria for formulation of control

requirements and establishes emission standards for industrial activities that pollute the air. This guideline considers that although SLAP was established on 12/21/77, there were still no limits on the amount of pollutants to be released into the atmosphere by different types of sources, which makes it vital for that system to issue. Thus, Technical Standards (TS) were published establishing emission standards for groups of industrial activities installed on Rio de Janeiro. Table 1 presents these groups and the corresponding TNs.

Table 1 - Industrial Activities and Technical Standards

	Industrial Activities	Technical Standards (TS)
1	Production of hot-rolled asphalt concrete	NT-506.R-6
2	Production of primary aluminum by electrolytic process	NT-521.R-3
3	Manufacture of cement	NT-508.R-3
4	Extraction of blocks and Production of gravel	NT-526.R-2
5	Manufacture of glass	NT-530.R-1
6	Steel mills	NT-536.R-2/533.R-1/539.R-2/524.R-2/546.R-1/
7	Calcium carbide fabrication	NT-550.R-1
8	Sulfuric acid production	NT.554.R-1
9	Catalytic cracking at petroleum refineries	NT.557.R-1
10	Secondary foundries of metals and alloys	NT.563.R-3
11	Sugarcane bagasse boiler	NT. 570.R-3

Furthermore, in 1986 the FEEMA implemented the guideline DZ-545 - Atmosphere Emissions Self-Control Program Implementation Guideline - PROCON-AR, contained at the Pollutant Activities Licensing System - SLAP, to monitor the facilities emissions, among other goals: amplify INEA's control inspection at air pollution facilities, verify attendance to pollutants Emissions Limits (LME) and support emissions control strategies.

The FEEMA was officially combined to State Superintendent of Rivers and Lakes (SERLA) and to State Forestry Institute (IEF) at january 12, 2009, originating The State Environmental Institute (INEA), by means of the State Law N^o 5.101/07.

Under the responsibility of INEA, the content of the DZ-545 - PROCON AR - was improved in order to include new procedures, updating the program and bringing more reliability to the presented results, being then replaced by the Emissions Monitoring Program Fixed Sources for Atmosphere - PROMON AR.

Thereby, it was published the Resolution CONEMA nº 026/2010 at official journal in december 7, 2010 that approves the rule NOP-INEA-01 - Atmosphere Emissions of Stationary Sources Monitoring Program (PROMON-AR). NOP-INEA-01's main purpose is to establish general procedures to associate pollutant companies to the referred program. The stationary sources that comprehend specific emission to atmosphere, included at the Resolution CONEMA nº 26/2010, must have their sources sampled regularly, at least twice per year.

The PROMON AR is one of the support documents and direction/guidance to PRONAR, and it is an Air Pollution Control State Program aiming to: (1) Amplify INEA's supervision at air pollution control; (2) Verify attendance to air pollutants Emissions Limits (LME); (3) Create control requirements; (4) Assist the establishment of proper Emission Limits at Rio de Janeiro state; (5) Subsidy atmosphere emissions control strategies elaboration, through most significant sources identification and the amount of pollutants emitted; (6) Subsidy environmental licensing and INEA's inspection control through technical report quantitatively consolidated and (7) Subsidy national database elaboration of atmospheric emissions.

CONAMA Resolution nº 26/2010 was revoked and replaced, through official journal at october 17, 2018, by the Resolution CONEMA nº 84/2018. The aforementioned resolution, provided automation of sending procedures and sampling report analysis, brought more efficient schedule samplings, among others.

CONCLUSIONS

Since the late 80's, stationary sources atmospheric emissions regulamentation has been the target of heated arguments between governments, industry agents and civil society peaking at the development of policies aligned to the country's reality.

The arguments that culminated to the Resolutions editions, that corroborated with air quality and environmental preservation, pointed out what's ahead considering emissions and control limits, and monitoring pollutants.

The application of air pollution management can be through enhancing the regulamentation by implementing methods such as environmental quality standards, continuous development of technical controlling systems, and also, measures of inquiry according to standards defined through monitoring programs. Furthermore, the mentioned implementation is absolutely important in the matter of emissions escape to atmosphere, to achieve a level of effectiveness capable of providing

real benefits, as consequence of atmospheric pollution.

The establishment of environmental legislations that control stationary sources pollution gradually advances, in national scope, through National Environment Council (CONAMA), such as in Rio de Janeiro's state, through State Environment Council (CONEMA), performing especially over the monitoring procedures and standard attendance improvement.

With CONEMA nº 84/2018 as current resolution, PROMON AR is improving, which had close to 110 companies associated in 2018, referred to large and small-sized companies. The benefits achieved were: more simplified and fluid association and monitoring procedure of stationary sources; higher reliability of the results presented; increased transparency and efficiency in meeting the deadlines established on the rule.

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NUMERICAL STUDY OF WIND-FENCE EFFICIENCY IN CONTROLLING PARTICULATE MATTER EMISSIONS FROM COAL STOCKPILES IN A INDUSTRIAL SITE

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Abstract: Particulate matter as an atmospheric pollutant has been studied because it can cause adverse effects to human health (CHAN et al., 2008; CHAMBLISS et al., 2014) and environment, such as: visibility reduction (HYSLOP, 2009), climate change (LIOU, 2002; KONDRATYEV et al., 2006), vegetation injuries (RAHUL AND JAIN, 2014), wear of buildings, works of art and monuments (HU et al., 2006), besides the nuisance caused by dust fall particles (SANTOS E REIS, 2011; CONTI, 2013; MELO, 2015).

Fugitive emissions of particulate matter (PM) in stockpiles occur due to aeolian erosion, potentially carrying the material to far distances, depending on the physical characteristics of the particle (size and density) and meteorological conditions (wind speed and turbulence). This phenomenon represents a large part of the emissions of an industrial complex stockpile yard (coal) and to comply with legislation the industry uses methods designed to control air pollution. One of the most up to date methods is wind fences, which aim to reduce the magnitude of the wind velocity incident on stockpiles, thus minimizing the emission of the material into the atmosphere.

The present study aims to evaluate the PM control efficiency from a wind-fence with 47% porosity, located in an industrial park in the coastal region of the city of Vitória, Espírito Santo, Brazil. The AIM software developed by Ansys was applied and the simulation was performed by solving the transport and turbulence equations using the standard k-ε model (finite volume method). The turbulence model and the computational mesh were validated by comparing the velocity magnitude profiles obtained by the numerical simulations and the wind tunnel experiments that were developed by Chen et al. (2010).

Simulations were performed for five wind directions (East, Southeast, South, Southwest and West) considering the wind gust speeds (acquired from the years 2015, 2016 and 2017 meteorological data provided by Aeroporto (SBVT) station, located in Vitória/Espírito Santo) for each of these directions, since they are the directions intercepted by wind fence. Two different scenarios were studied: i) the coal stockpile yard without the porous barrier and ii) the coal stockpile yard with the porous barrier. The objective of the scenarios analysis was to analyze the behavior of the runoff in an industrial stockpile yard and to determine the efficiency of wind fence in reducing the magnitude of the wind velocity incident on the storage cells and, consequently, the emission of particulate matter into the atmosphere. The wind fences efficiencies were calculated by comparing the two scenarios analyzed using the methodology proposed by the United States Environmental Protection Agency (USEPA, 2006), section 13.2.5.

The simulations shows that the principal factors exercising influence in air flow around the coal yard were i) the geometry and position of physical barriers, such as stacks, buildings and vegetation around the yard, in the formation of low pressure zones and interceptions; ii) the position and geometry of the wind fence in relation to the direction of flow in order to cause greater or lesser effect in decreasing the magnitude of the flow velocity; and iii) the magnitude of the incoming wind velocity, since higher velocities tend to generate greater erosivity potential on the piles surface.

It was concluded that porous barriers are a good method of controlling emissions of particulate matter, although its efficiency varies considering different wind directions and velocities. The efficiencies obtained in the simulated wind directions were equal to 13% for the East, 39% for the Southeast, 33% for the South, 59% to the Southwest and 50% to the West, finally achieving an average efficiency of 42%.

Keywords: Air pollution control, Computational fluid dynamics, Wind erosion, Wind-fence, Stockpile.

INTRODUCTION

The increase in the global population has caused a rise in the exploration of natural resources and in the global pollution levels. This fact called the attention of environmentalists, government policy makers and academic institutions that, with the pollution emission standards creation, have pressured industries to invest in better pollution control equipment.

Open-air industrial yard, which contains storage of large loads of materials, emit particulate matter (PM) from granulated material storage piles. These fugitive emissions caused by wind erosion in addition of the social-environmental impacts, can also generate economic impacts, such as the substantial loss of stored material (CONG *et al.*, 2012).

Porous barrier, also known as wind fences, are also widely used in this context because they have a similar purpose as the green belt, with the advantage of demanding less area and costs in the installation phase.

As the study object of the current project is an industrial unit, the fluid dynamics approach is promising, since it promotes versatility and efficiency to analyze the proposed situations.

The present work proposes to study numerically the behavior of the runoff in an industrial plant of iron and steel that contains 6 stockpiles of coal storage, a greenbelt around the yard and its located in the coastal region of the city of Vitória, Espírito Santo, Brasil. Simulations were done in two different scenarios: i) without the presence of the wind fence and ii) with the presence of the wind fence. The simulations on these two scenarios provided discussions on the influence of obstacles on the air flow around the stockpiles and, by comparing them, to calculate the efficiency of the porous barrier using the emission factor proposed by the US Environmental Protection Agency (USEPA, 2006).

METHODS

The numerical simulation used in this study is based on three main steps: the geometry and mesh creation, the numerical procedure to solve the governing equations starting from the prescribed boundary conditions through a meteorological study, and finally the post processing the results.

The finite volume method was used and the simulation performed from the solution of the transport and turbulence equations using the standard $k-\epsilon$ model developed by Launder-Sharma (1974).

The turbulence model and the computational mesh were validated by comparing the velocity magnitude profiles obtained by the numerical simulations and the wind tunnel experiments by Chen *et al.* (2010).

The simulations were performed for five wind directions (East, Southeast, South, Southwest and

West), since they are the directions intercepted by wind fence, using two scenarios (without and with the presence of the porous barrier). The maximum wind velocity magnitude (wind gust) for each of the simulated directions obtained in the three-year sampling period (2013, 2014 and 2015) was used in order to predict the most critical scenarios possible for each direction studied.

To calculate the emission from the stockpiles using the model proposed by USEPA (2006), it is necessary to use the Equation (1).

$$E = k \sum_{i=1}^N P_i S_i \quad (1)$$

Where k is the multiplier relative to particle size, N is the number of disturbances suffered by the surface of the pile during a time interval (the study considered 24 monthly disturbances), P_i is the erosion potential corresponding to the highest wind speed between the disturbances (gm^{-2}) and S_i is the area of the exposed surface (m^2). And the erosion potential of the exposed area can be obtained by Equation (2).

$$P = 58(u^* - u_t^*)^2 + 25(u^* - u_t^*) \quad (2)$$

Where u_t^* is the limiting friction velocity of the material stored in the cells (m s^{-1}), u^* is the friction velocity at the cell surface (m s^{-1}) and the values 58 and 25 are empirical constants of the model.

The established value of the particle size multiplier was $k = 1,0$ (USEPA, 1995) and the number of disturbances was deployed by the industry equal to 24 per month. The threshold friction velocity value (u_t^*) is given in function of various physical characteristics of the material of the coal stockpile. Topic and Zitnik (2010) experimentally studied threshold friction velocity values for various coal granulometries and, therefore, the value adopted was $u_t^* = 0,18 \text{ m s}^{-1}$. As certain areas of the stockpiles are more susceptible to wind erosion due to exposure to different rates of friction (USEPA, 2006), a weighting was performed for each area of the stack (exposed to a given friction velocity range).

As the objective of the study is to determine the efficiency of wind fence in reducing the erosive potential in the stockpiles of coal, the numerical simulations and the emission calculation was carried out for the two proposed scenarios (with and without the presence of wind fence). Thus the efficiency of the porous barrier (with 47% porosity) is given by the comparison between the emissions without the control method and with the control method.

FINDINGS AND ARGUMENT

The results were obtained by applying equation (2) to calculate the erosion potential and equation (1) to calculate the emissions of the patio of coal. The

analysis of the friction velocity in the stockpile yard showed that physical obstacles drastically change the flow behavior. The presence of the green belt caused a remarkable reduction in the magnitude of the friction velocities for all the simulated directions. The **Figure 1** shows the decrease of the friction velocity in the southwest direction due to the presence of wind-fence.

The efficiency of the wind-fence was calculated by the comparison between the scenarios with the presence of the wind-fence and without wind-fence. The highest average efficiency was observed for the Southwest wind (59%). The average between all the simulations corresponds to a 42% reduction in the total emissions from the site.

Mechanisms such as recirculation zones, wake turbulence and interferences of the vegetation barrier and some factors such as the geometry of the stacks and the position of the buildings were responsible for the reduction of efficiency in the other directions analyzed. The **Figure 2** shows the interference of the buildings located southwest of Stack 1 in the distribution of the friction

velocity. The results of the calculated efficiencies are shown in **Figure 3** below.



Figure 1: Normalized friction velocity contour for simulation a) Without Wind-fence b) with Wind-fence in the southwest wind.

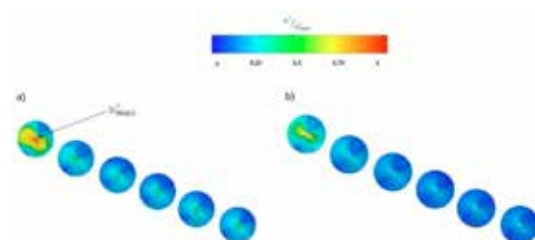


Figure 2: Normalized friction velocity distribution for simulation a) Without Wind-fence b) with Wind-fence in the southwest wind.

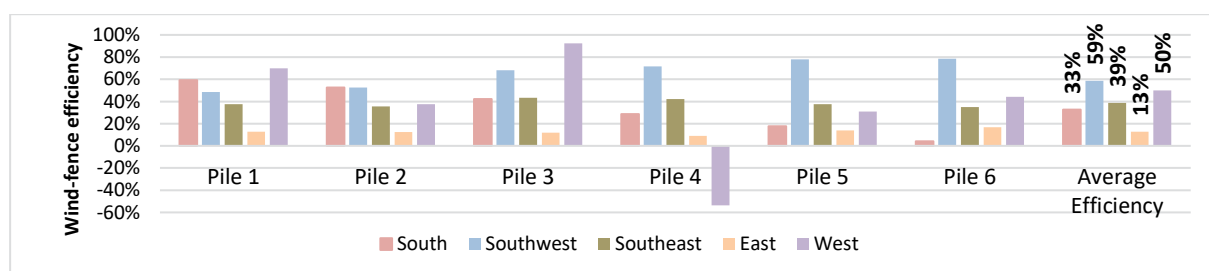


Figure 3: Efficiency of the porous barrier in each storage pile (1 to 6) for the South, Southwest, Southeast, East and West winds and the average efficiency.

CONCLUSIONS

The study demonstrated that porous barriers presents itself as a good method of controlling the emission of particulate material, presenting an average efficiency of 42% in the reduction of the emissions of the batteries of the patio of coal. This result justifies the implementation of the porous barrier as a method of controlling the emission of particulate matter, mainly in patios where the representativeness of the emissions of the stockpiles are significantly high compared to the other emitting sources.

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EVALUATION OF PARTICULATE MATTER EMISSIONS IN RAILROADS EQUIPED WITH A SPRINKLING SYSTEM FOR THE ASPERSION OF POLYMERS DURING TRANSPORTAION

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Abstract: The railway transportation is an important tool of the Brazilian national industry, principally for the transportation of commodities like grain, iron ore and coal. Particularly, the mining sector contributes significantly to the economy, which makes it a centerpiece of the national policy. Nevertheless, the environmental impacts generated may cause severe damage to human health and environment. The emission of particulate matter during railway transportation occurs due to factors like wind erosion and spilled ore on the railway tracks. In order to mitigate particulate matter emissions during the transportation of iron ore between the federal states of Minas Gerais, Rio de Janeiro and São Paulo by an important railway logistics-operator, a sprinkling system for the aspersión of polymers on train wagons was constructed and is in full operation to prevent the material from being carried or dropped away. This study aimed to evaluate the occurrence of particulate matter emissions in railway wagons and the efficiency of the sprinkling system for the aspersión of polymers, located in the city of Barra Mansa - RJ, for particulate matter control.

The monitoring of particulate matter emissions was performed continuously with an air quality monitor (GM 5000 developed by Thermo Fisher Scientific) with an optical particle counter which is able to detect and quantify total particulate matter (TPM), particulate matter smaller than 10 µm (PM₁₀) and smaller than 2,5 µm (PM_{2.5}). The equipment was installed in the back parts of three lined-up train wagons. In addition to the GM 5000 equipment, there was also a video monitoring of the wagons with a camera installed on the locomotive.

The temporal evolution of the particulate matter emission was registered every minute and synchronized simultaneously with the geographic position (GPS), allowing the assessment of the mean spatial concentration per minute of emission. Regarding the polymer application efficiency, the average concentrations measured in the wagons analyzed before and after the application point were: 7672,03 µg/m³, 829,98 µg/m³ and 85,22 µg/m³ before and 1051,70 µg/m³, 263,79 µg/m³ and 38,64 µg/m³ after the application, respectively for TPM, PM₁₀ and PM_{2.5}. The Pearson correlation coefficient was used to check the affinity between the monitoring wagons. Besides the monitoring considerations, the acquisition of meteorological data was performed in order to achieve more reliable results by identifying the possible interferences of the climate.

The monitoring of PM emissions was performed on the 5th of April, 2018, between the counties of Bom Jardim de Minas - MG and Mangaratiba - RJ, starting at 10:51 o'clock until 21:59 o'clock of the same day. The obtained results indicate more emission of particulate matter during an increasing speed of the wagons, whereas all three parameters analyzed in this study were significantly reduced after the application of polymers. Considering the average values of the results before and after the application of polymers, the concentrations of emissions were reduced by 86,30% for TPM, by 68,00% for PM₁₀ and by 54,66% for PM_{2.5}. The monitoring of the air quality in cities next to the railway showed satisfying values referring to the law, whereas the highest values were found at the railway station of Bom Jardim de Minas due to more train traffic.

It was concluded that the sprinkling system for the aspersión of polymers managed to reduce substantially the emissions of particulate matter coming from sinter feed transportation. Regarding the granulometry of the particulate matter, the efficiency of the system was better for particles with bigger diameter. Such results prove the efficiency of the sprinkling system for aspersión of polymers, which enables the system's extension to other points before the city of Barra Mansa - RJ.

Keywords: Pollution control, railway transportation, particulate matter, emission of pollutants, aspersión system.

INTRODUCTION

The discharge of iron ore through rail transport generates significant contributions in emissions of atmospheric pollutants. Concentrations of particulate matter can generate impacts on human health, especially in regions surrounding the railway, in addition to the disturbances caused by the emission of particulate matter. In view of the above considerations control and air quality standards have become increasingly demanding.

From the perspective of emission control, the present study sought to investigate the dispersion of pollutants in ore transportation, of the sinter feed type in a railroad linking the states of Minas Gerais and Rio de Janeiro, located in the southeastern region of Brazil. In addition to the characterization of fugitive emissions, the study sought to evaluate the efficiency of the spray of polymers to control the emission of particulate matter.

METHODS

AQMesh continuous measurement equipment was used for the monitoring of particulate matter. The monitor is capable of measuring total particulate matter (TPS), particulate matter less than 10 μm (PM_{10}), particulate matter less than 2.5 μm ($\text{PM}_{2.5}$), and other atmospheric pollutants. Particle detection is by the incidence of a laser beam in a sample. The signal generated by the light detector is sent to a microprocessor which interprets and calculates the amount of particles contained in the air sample.

Three equipments were installed along the iron composition. The definition of the positioning of the equipment during the installation was based on studies by Conell Hatch (2008) and Ferreira et al. (2003), considering the effects of downwash in the first wagons, the emissions due to the fuel consumption in the locomotives, the fugitive emissions due to the longitudinal drag and the distribution of the flow velocity throughout the composition.

In addition to monitoring through the AQMesh, video-monitoring was carried out through a camera coupled to the auxiliary locomotive in order to identify the sections with visible emissions.

The results were compiled in the form of graphical maps of temporal and spatial evolution of the concentration parameters. The maximum, minimum, standard deviation before and after the

application of the polymer was also raised, as well as the percentage reduction in emissions after spraying.

FINDINGS AND ARGUMENT

Figure 1 presents the means of the time evolution of the monitored parameters PTS, PM_{10} and $\text{PM}_{2.5}$ throughout the monitoring.

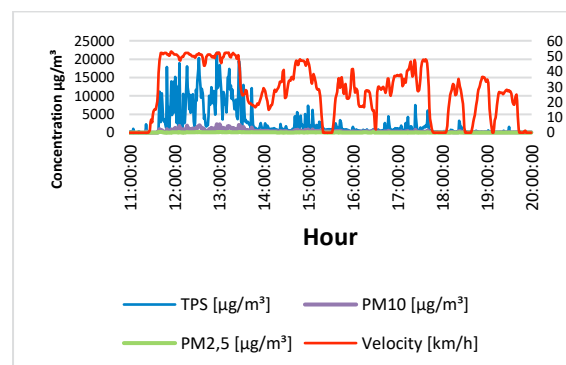


Figure 1: Concentration of TPS, PM_{10} and $\text{PM}_{2.5}$ along the railroad in relation to the velocity of the composition.

The analyzed parameters, TPS, PM_{10} and $\text{PM}_{2.5}$, obtained similar behavior along the displacement of the train. The monitoring showed higher emissions of particulate matter from the increased speed of the wagons (speeds above 45 km/h), which is due to the increase of the drag speed caused by the movement of the train. The temporal evolution of the graph demonstrates the reduction of emissions of particulate matter from the point of application of the polymer, located in the municipality of Barra Mansa - Rio de Janeiro, demonstrating its immediate effect as a measure of pollution control.

Data analysis showed that after polymer application the reductions reached mean percentage values of 79.46% for TPS, 30.09% for PM_{10} , and 6.31% for $\text{PM}_{2.5}$. It should be noted that rainfall occurred, which contributed to a greater reduction of the average calculated after the application of the polymer, but this fact did not disqualify the reduction of emissions of particulate matter.

With the concentrations and the real time localization of the composition it was possible to generate maps of temporal evolution along the monitored path. Figures (2), (3) and (4) represent the means in minutes and in hours of concentration during the course of the train.

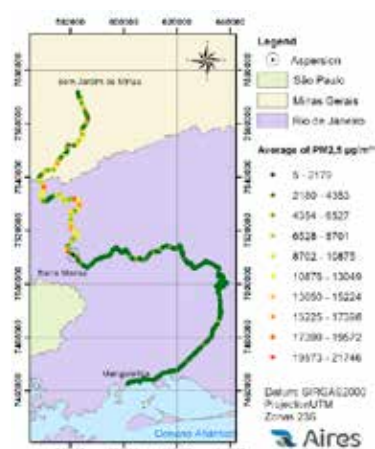


Figure 2: Spatial evolution of TPS concentration.

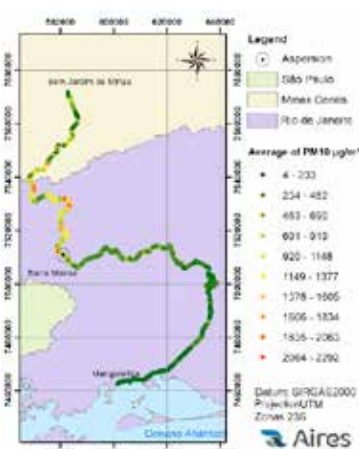


Figure 2: Spatial evolution of PM₁₀ concentration.

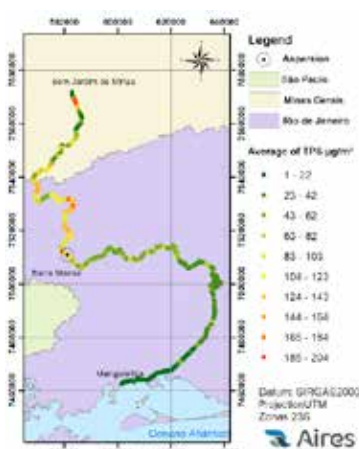


Figure 3: Spatial evolution of PM_{2.5} concentration.

From the above figures it is possible to see that concentrations tend to increase in places where there is a greater sinuosity of the route, especially sharp curves. In addition, after the polymer application point, the concentration reductions were observed, a fact clearly observed in the maps representing the spatial evolution of the hourly mean of the concentrations.

In line with the monitoring carried out by AQMesh, it was possible to detect, from the filming, the visible emissions during the railway transport of sinter feed. Table 1 shows the concentration values and the points at which particulate matter emissions were observed to the naked eye.

Table 1: Mean concentration of visual emissions.

Event	Duration [s]	Speed [km/h]	Mean concentration [µg/m ³]		
			TPS	PM ₁₀	PM _{2.5}
1	38	51	10731,9	1180,5	117,5
2	47	50	9922,8	1086,0	108,8
3	11	48	7161,4	956,4	104,9
4	12	51	6609,6	827,2	90,61
5	12	52	15434,4	1649,7	152,2
6	28	50	11288,6	1230,1	123,0
7	21	33	7481,8	811,6	84,55

The points cited in Table 1 are located upstream of the point of application of the polymer, located in Barra Mansa. After spraying the polymer there was no visual emission record for the remainder of the course.

CONCLUSIONS

The behavior of the emissions during the transport of iron ore elucidates the increase of the concentrations from the gain of speed of the composition, factor explained due to the elevation

of the drag speed. In addition to the high velocities, changes of direction also led to the increase of emissions of particulate matter due to the action of centrifugal and inertial forces.

Based on the analysis of the results and the maps generated, the significant reduction in pollutant emissions after the pollinating of the polymers in the municipality of Barra Mansa / RJ was observed, reducing the emissions from sinter feed transport in gondola type wagons in 79 , 46% for TPS, 30.09% for PM₁₀, and 6.31% for PM_{2.5}. This result suggests the increase of more points of spray of polymers, mainly in points upstream of the municipality of Barra Mansa where still high emission rates of particulate matter occur.

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BIOFILTRATION SYSTEM FOR THE REMOVAL OF H₂S AND NH₃ USING ORGANIC PACKING MATERIAL

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Abstract: There are several industrial/treatment activities which produce offensive odours involving negative effects over life quality of the surrounding population. In wastewater treatment plants (WWTP), these odours are caused mainly by the emission of hydrogen sulfide, ammonia and volatile organic compounds. To treat these contaminants, biofiltration offers an economic alternative of high efficiency and low generation of additional waste. In this project, the removal efficiency of H₂S and NH₃ was evaluated using several compost mixtures as packing material in a laboratory biofiltration system. Chicken manure, as main compost component, was mixed with three types of lignocellulosic materials (rice husk, waste from pruning and sugarcane bagasse) at a weight ratio of 1:1. The gas concentration levels were fixed according to the ones found in the emissions of a WWTP sited in Bogotá, Colombia. After one week of acclimation at low concentrations of H₂S and NH₃, the removal efficiency of H₂S was 100% in all biofilters. An increase of the gas concentration up to the maximum level found in the WWTP (20 ppm of NH₃ and 250 ppm of H₂S) did not affect the removal efficiency for the three organic beds. However, the performance of the compost from manure with pruning bed along the biofilter showed that it has less elimination capacity than other beds. Thus, compost from manure with rice husk or sugarcane bagasse are highly recommended as packing materials for biofilters due to their high removal efficiency for H₂S and NH₃. These materials represent a reduction in system costs due to their low cost and availability as commercial by-products.

Keywords: Biofilter, compost, hydrogen sulfide, ammonia

INTRODUCTION

Wastewater Treatment Plants (WWTPs) are considered important sources of gaseous emissions, including offensive odours and greenhouse gases. The main compounds that generate odour in the WWTP are volatile compounds of sulphur such as H₂S, nitrogen compounds such as NH₃ and volatile organic compounds (VOCs) (Easter *et al* 2005, Alfonsin *et al* 2015). To reduce these emissions and to accomplish with air quality regulations, there are a variety of technologies, including biotechnology alternatives, that require low capital and operating costs and are environmental-friendly compared to physicochemical technologies. Among the available biotechnologies, biofiltration is the most commonly used in industries due to its ease of implementation, low cost and diversity of designs and studies (Lebrero *et al* 2014). In this type of bioreactor, the gases pass through a wet porous bed and are diffused into the aqueous phase of a biofilm containing microorganisms for contaminants degradation, as well as nutrients and oxygen, in aerobic systems. The packing material is one of the factors that affect the biofilter performance, so several desirable characteristics have been established in them to be used in the biofiltration process: 1) high specific surface area (300-1000 m²/m³); 2) high porosity (0.4-0.9); 3) good water retention capacity to maintain the humidity of the biofilter between 40-70%; 4) presence and intrinsic

availability of nutrients; and 5) presence of a large and diverse microbial community. Materials such as compost, peat and wood chips are the most used as beds because they meet most of the criteria (Muñoz *et al* 2015). In addition, since they are natural materials, the bed is usually less expensive and available (Delhoménie and Heitz 2005). However, these materials may lose its water retention structure and capacity due to gradual deterioration and the consumption of nutrients, in such a way that it can decrease the efficiency and lifespan of the supports (Muñoz *et al* 2015). For this reason, materials like straw, wood chips (Hou *et al* 2016), pruning waste (Cabeza *et al* 2015) and rice husk (Forero *et al* 2018) have been used in mixtures with compost as bulking agent. The objective of this work was to evaluate different mixture of compost with lignocellulosic materials (rice husk, waste from pruning and sugarcane bagasse) as packing material for the biofiltration of a stream with hydrogen sulphide and ammonia.

METHODS

1. Materials

The mixtures of compost with lignocellulosic materials was obtain from the composting of poultry manure with rice husk (CA), waste from pruning (CP) or sugarcane bagasse (CB) in a 1:1 volume ratio. The final composted mixture went

through a screening step to select particles with more than 2 mm before their use as biofilter beds.

2. Biofiltration system

The pilot system phase consisted in six biofilters (two biofilters per bed) constructed in PVC pipes with a diameter of 10.16 cm. The biofilters were divided into 3 sections, each of 27 cm height and a volume of 0.002 m³; between each section there was a sampling port. An inlet flow rate of 6.5 L/min was fixed to each biofilter to obtain a retention time of 60 s. The flow was verified with flowmeters (Flowtron), and it was adjusted through valves installed in the biofiltration system. The bed moisture was established in each material and adjusted to 40% adding water in each section. The evaluation of the beds was carried out by exposure to different concentrations of the contaminants: 7, 32, 75, 120 and 250 ppm for H₂S and 0, 2, 8, 15 and 20 ppm for NH₃. These concentrations were established as a result of a previous monitoring in the pre-treatment zone of the WWTP - El Salitre, Bogotá, Colombia.

3. Gas sampling

A portable multi-gas monitor (MultiRAE- PGM-6228 RAE Systems) was used for H₂S and NH₃ measurements, which were made at the inlet, outlet and sampling ports along the biofilter. These were taken until stabilization of the gas concentration. The gas sampling was performed for a 2-month period, and three measurements were made throughout the day, obtaining the data of gas removal, with a daily average. The removal efficiency percentage (%RE) was calculated for each gas using Equation 1:

$$\%RE = \frac{(C_i - C_o) \times 100}{C_i} \quad (\text{Eq. 1})$$

where, C_i: gas input concentration (ppm), and C_o: gas output concentration (ppm).

4. Chemical analysis

The composted material was characterized by the evaluation of pH, bulk density, particle size distribution by sieving, water holding capacity (Chen *et al* 2012), buffer capacity (Costello and Sullivan 2014), organic matter content by combustion, and nitrogen content by Kjeldhal. Moisture in biofilters was determined daily using established procedures CEN-EN 13040 (CEN-EN 2007).

RESULTS AND DISCUSSION

1. Mixture compost properties

According to Table 1, compost CA showed the highest buffer capacity which indicates that it can better avoid the bed acidification produced by the biological oxidation of H₂S, making it promising for this gas biofiltration.

The results obtained for water retention capacity, show that these composts could help to maintain the moisture content of the biofilter system without

continuous water addition, avoiding the formation of dry areas in the bed that could lead to poor microbial growth and thus reduced removal efficiencies (Dorado *et al* 2010).

Table 1. Characteristics of the different mixtures of compost material evaluated.

Characteristics	CA	CP	CB
Density, g/L	796.66 ± 0.58	850.45 ± 2.66	753.30 ± 1.53
pH (1:25)	9.45 ± 0.18	9.57 ± 0.11	10.03 ± 0.08
% Size particle distribution, > 4.75 mm 4.75 - 2.36 mm 2.36 - 1 mm 1 - 0.6 mm 0.65 - 0.25 mm < 0.25 mm	24.40 19.02 21.64 11.51 9.15 8.20	77.32 2.08 10.30 0.78 0.73 0.81	46.60 16.56 9.74 8.15 6.83 3.51
Water retention capacity (WHC), gH ₂ O/g material	1.68	1.02	1.20
Buffer capacity, mol H ⁺ /kg material	2.80	0.24	0.37
% Total Nitrogen	3.3 ± 0.3	3.6 ± 0.6	3.2 ± 0.2
% Organic matter	44.77 ± 0.63	52.75 ± 0.49	38.17 ± 1.03
C/N	16.67	13.15	19.62

The particle size is important for the selection of a biofiltration bed since it must have enough area for an efficient mass transfer, but it must not be too small that it can generate problems of compaction or high resistance to the gas flow (Dorado *et al* 2010). As the size particle distribution was greater than 50% for size higher than 2 mm in all materials, it can be concluded that these are suitable for use in biofiltration and could avoid compaction problems. In addition, in a study carried out with similar compost, there were no compaction problems (Forero *et al* 2018).

The organic matter and nitrogen in the compost would allow, inside the biofilters, for microorganisms to survive periods of pollutants low emissions (Dorado *et al* 2010), a common situation in industrial emissions.

2. Biofiltration

In the first week, when the H₂S concentration was low, the removal efficiency for H₂S and NH₃ in all biofilters was 100% (Figures 1 & 2). Initially, this is due to physicochemical processes of the gases on the bed, since their hydrophilic nature allows them to be easily adsorbed, but once saturated, the

removal process is biological. In this period, called acclimatization, occurs the growth of specialized microorganisms that adapt to biofilter conditions such as pH, temperature, nutrients and pollutants, (Muñoz *et al* 2015).

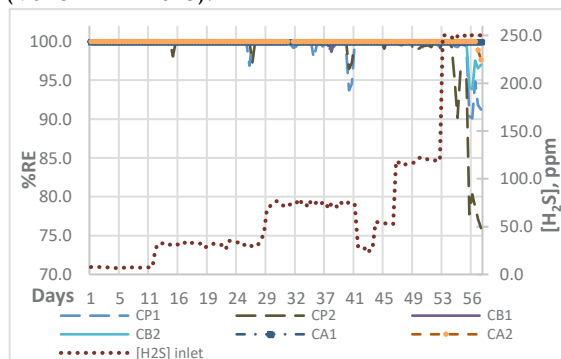


Figure 1. H₂S inlet concentration and removal efficiency in biofilter systems. CA, manure + rice husk; CP, manure + pruning waste; and CB, manure + sugarcane bagasse (numbers 1 or 2 indicate replicate biofilter system).

Even when the concentration of H₂S was increased to 120 ppm, all biofilters, except for CP2, maintained the removal efficiency by 100%. Increasing the concentration to 250 ppm, decreased the removal efficiency in all beds, although it remained above 90%, except for the CP bed, which showed the lowest efficiency.

The observed positive performance can be attributed to the high mass transfer of the gas phase mixture to the biofilm, where the pollutants are consumed by the microorganisms.

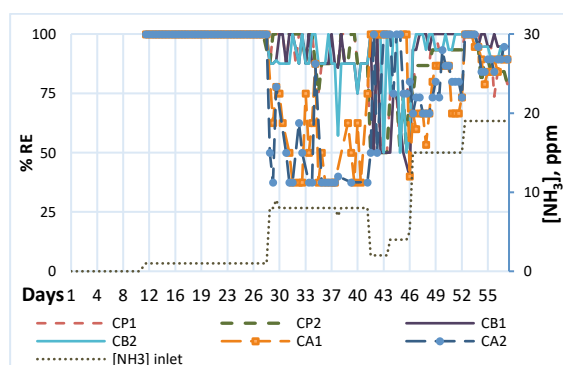


Figure 2. NH₃ inlet concentration and removal efficiency in biofilter systems. CA, manure + rice husk; CP, manure + pruning waste; and CB, manure + sugarcane bagasse (numbers 1 or 2 indicate replicate biofilter system).

According to the results found in the physicochemical properties and biofiltration performance, compost CA and CB are suitable for use in a WWTP, since they showed high H₂S and NH₃ removal efficiency at the evaluated WWTP emission concentrations. Further, these materials are economical and do not require constant addition of water and nutrients. An *in-situ* study will allow to determine if the biofilters maintain a high removal efficiency under transient emission conditions, as

well as the presence in the air stream of other pollutants such as hydrocarbons and organic acids.

CONCLUSIONS

The materials used as biofiltration beds achieved H₂S and NH₃ eliminations above 90%, which is adequate to continue the studies with the addition to the mixture of more pollutants known to be produced in the water treatment plant.

The CB filter bed showed the best performance at different concentrations of H₂S and NH₃, with 100% and 93% efficiency removals, respectively. This indicates that it is possible to continue the studies with this compost using a higher pollutants concentration or flow rate.

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**PROCEEDINGS OF THE
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Session 12
**Air Pollution at Critical
Infrastructure Sites and
Its Influence for the Society**

AIR QUALITY STUDIES AT THE ALCANTARA LAUNCH CENTER

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Abstract: The Alcantara Launch Center (ALC) is the Brazil's gate to access the space. From this range, the Brazilian rockets (and may be others foreign rockets in the near future) are launched to the atmosphere. During its propulsive stage near the ground (or in the case of an explosion), some material (toxic gases for instance) can be released to the atmosphere and its dispersion requires investigation, as there are staff working for the launching as well as small villages and inhabitants around. The air quality issue at ALC is being a topic of investigation about 10 years by a group of Brazilian organizations. The topics explored by this group is to understand better the couple of the atmospheric flow (including the atmospheric turbulence) on the dispersion and the air quality of the region. The strategy adopted was to conduct field measurements (for data validation), wind tunnel essays and numerical modelling using an atmospheric meteorological models and computation fluid dynamics (CFD) techniques. For the field measurements, there were 2 field campaigns held at ALC in order to collect data that describes the spatial and temporal evolution of the flow. From this data-set, some parameters of the turbulence were derived and used at the model simulations as input and boundary conditions. For the wind tunnel essays, a mock-up of the topography (including the assembly building - Torre Móvel de Integração) was constructed and the flow and turbulence were studied using hot wire anemometer and particle image velocimetry sensors. Some preliminary studies using a mesoscale meteorological model (WRF-CHEM) were already done about the dispersion of toxic gases - like HCl released by the Brazilian's rocket for different scenarios (daytime/nighttime) and wet/dry conditions. Some of their findings are that the personnel involved with the launching should wait 15 min after the launching to leave the blockhouse for other activities. Currently, a CFD is being under development and the results are being compared with observations, wind tunnel essays and meteorological forecast using WRF-CHEM. The final objective of this project is to have an operational software that can be run at ALC to help decision makers about the best meteorological conditions to launch a rocket, which will have the lower impact to the surrounding society.

Keywords: Fluid rocket launching, infrastructure critical, modelling studies, wind tunnel essays.

INTRODUCTION

The Alcântara Launch Center (in Portuguese Centro de Lançamento de Alcântara -CLA) is the Brazilian main space center, located in the north part of

northeast Brazil. The Launch Pad Area (in Portuguese Setor de Preparação e Lançamento -SPL), where all activities associated with the rockets are conducted, is located close to the coastline (around 150 m far), on an irregular cliff.

Therefore, some important characteristics for the atmospheric flow acting on this place can be observed: an internal boundary layer (IBL) created by the abrupt change of roughness (from a smooth surface of the ocean to a rough surface of the continent) and topographic variation caused by the irregular cliff. Furthermore, the launching platform (Figure 1) has some obstacles nearby necessary for rocket integration as the Mobile Integration Tower (TMI), where the space vehicle is prepared and assembled. Once the rocket is at the launching pad, it is subject to the wind and atmospheric turbulence coming from the ocean (upwind).

It is well known that the flow around obstacles is dominated by shear-generated mechanical turbulence. In this way, the presence of buildings modifies the flow pattern, causing the formation of characteristic regions as the separation and recirculation areas and the turbulence wake behind the obstacle (ARYA, 1999). Thus, the understanding of the flow pattern around the launch pad buildings and how the flow changes due to the geography of the region are important to establishing the conditions in which the CLA is exposed and providing the necessary basis for the development of rockets as well as the procedures during the launches.



Figure 1. Launch Pad Area (SPL) and its location at coastline.

During the launching operations of orbital vehicles, large plumes of exhaust products are released on the surface of the launch pad. These hot gases rise, mix with the atmosphere and then cool until they reach an approximate thermal equilibrium with the ambient temperature, and simultaneously are transported and dispersed by the wind in the lower atmosphere. These emissions occur only during a few seconds after the ignition of the rocket engines, but a large amount of pollutants (on the order of 10^5 kg of material) is liberated during this process to generate the necessary thrust for the vehicle to take off from the surface and achieve the required orbital speed to escape the Earth's gravitational field.

The spacecraft VLS (in portuguese Veículo Lançador de Satélites) is the largest Brazilian rocket engine vehicle driven by solid propellant that was designed to release small satellites (up to 380 kg). The exhaust gas is composed of the products of the combustion of a hydroxylated polybutadiene resin (HTPB) and aluminium (Al), which reacts in the atmosphere and can impact not only the launch pad area but also its vicinity, including nearby villages and cities.

In this context, field measurements, experimental essays in wind tunnel (WT) and numerical simulations using high resolution atmospheric models and Computation Fluid Dynamics (CFD) codes are important tools and they have been used in order to understand better the coupling between the atmospheric flow and the air quality in the CLA region.

METHODS, FINDINGS AND ARGUMENT

This section will be splitted in a) field data observations, b) wind tunnel essays and c) numerical models.

a) Field observations

Since de mid of 90s, many field work has been conducted at CLA, in order to describe the atmospheric flow, including its turbulence. For instance, Marciotto et al. (2012) has analyzed the wind data from a tower (70m) and some special observations made during field campaign. At Figure 2, there is a picture about the cliff as well as the representation of the *in situ* measurements.

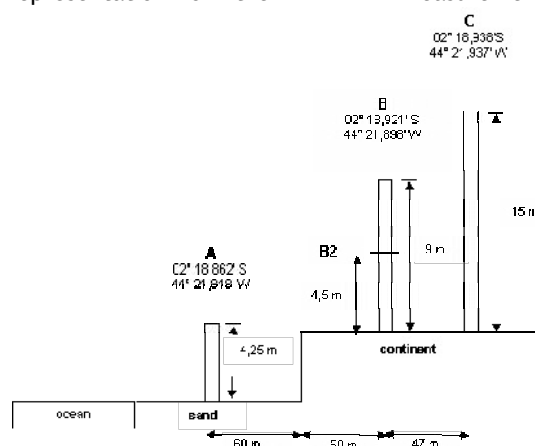




Figure 2. Conceptual scheme of the observations (a) made during ECLICLA 2 and the wind mast erect at the observations point (b).

From the analysis, an conceptual model for the Internal Boundary Layer developed was proposed where the upper layer is usually characterized with the oceanic upwind (Figure 3). Moreover, recently, Ramos et al. (2018) has concluded that the thermal stability is at neutral conditions, most of the time (more than 95% of the time), with no influence of the daily cycle (daytime or nighttime) or seasonal cycle (during dry and wet seasons).

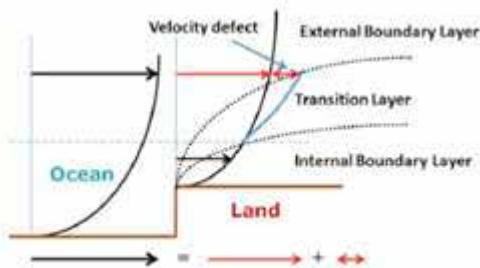


Figure 3. The conceptual model of the development of the IBL.

b) Wind tunnel Essays

As a complementary approach to study the atmospheric flow at SPL, some wind tunnel (WT) essays have been made and detailed described by Robalo et al. (2009), Pires et al. (2010) and recently by Faria et al. (2019). The WT The test cases are based on an experiment recently conducted by Faria, Avelar and Fisch (2019) in a boundary-layer wind tunnel, with a free-stream flow with velocity of $U_\infty = 20\text{m/s}$, Reynolds number of 4.3×10^5 and 0.05 to 0.10 turbulence intensity. The windprofile was created using a combination of spires and roughness and its obey a neutral atmosphere (or logarithmic profile). Figure 4 presents the frontal and superior view of the apparatus used for the WT essays.

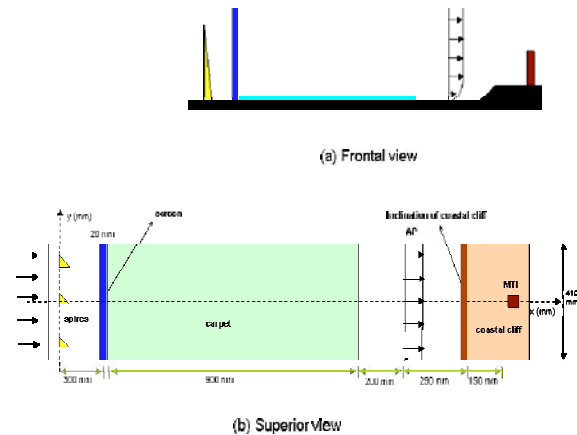


Figure 4. XZ (Frontal) and XY plane (Superior view) of the WT essays for inclination cliff of 75° and wind direction of 90° .

The Figure 5 presents the wind flow and the turbulence (described by its vorticity) for a case study (inclination cliff of 90°). A recirculation zone can be observed at the edge point and behind the TMI, producing strong turbulence (around 1500 s^{-1}).

a) Numerical Models

For the numerical model analysis, 2 different approaches have been chosen: use of a high resolution atmospheric model (The Weather Research and Forecasting (WRF) model and a Computational Fluid Dynamic CFD code.

The WRF model is considered the state of the art for limited-area weather-prediction systems. It is designed for atmospheric research and operational forecasting that can be applied to a wide range of meteorological problems with scales from tens of metres to thousands of kilometres. The meteorological and chemistry calculations in the WRF are made online (without loss of information due to asynchronous time integration), and with a proper methodology they can be used to calculate the transport and chemical reaction of the rocket launch's effluents into the atmosphere. Another advantage is that the process of transport, radiation and reactions is fully coupled (interacting with each other) and solved simultaneously without any type of interpolation.

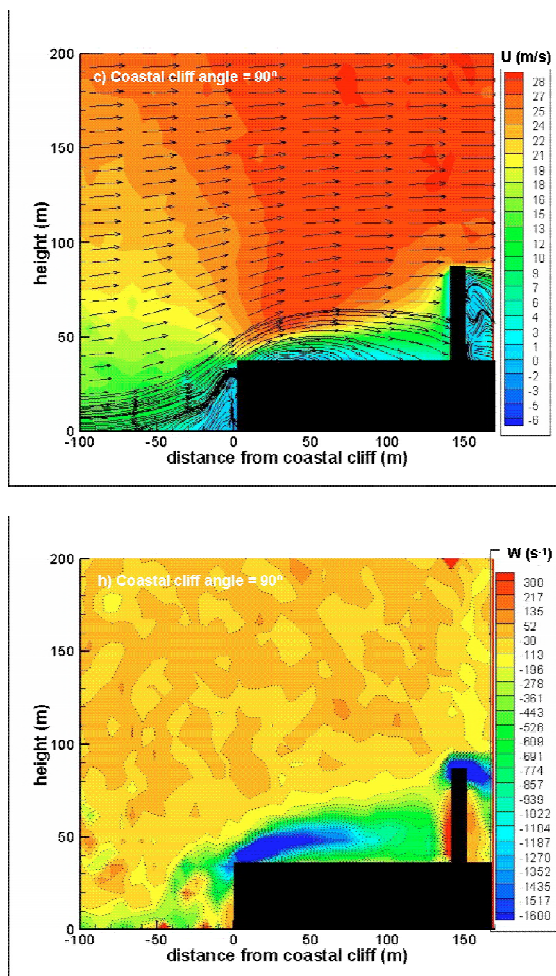


Figure 5. The wind flow (a) and vorticity field (b) for inclination cliff of 90° and wind direction of 90° . The arrow indicates the wind direction.

In order to conduct the numerical simulations, three nested domains (Figure 6) centred on the CLA. The outer domain (d1) was a 100×100 grid point with 9 km of horizontal spacing; the middle domain (d2) was a 70×70 grid point with 3 km of spacing; and the inner domain (d3) was a 40×40 grid point with 1 km of horizontal spacing. All domains had 43 vertical levels, from the surface up to 30 km, distributed mainly close to the surface (19 levels up to 3000 m). The static data (e.g. topography, land mask, vegetation) used was provided by the United States Geological Survey (USGS) at http://www.mmm.ucar.edu/wrf/src/WPS_files/geog.tar.gz with a spatial resolution of $30''$.

The simulated concentrations of hydrogen chloride (HCl) at the surface level: (a) 1 min, (b) 10 min, (c) 20 min and (d) 30 min after the launch at different positions at and around CLA are shown at Figure 7a. The time series of those results are also shown at Figure 7b. This simulation was characterized by a nighttime (at 00 UTC) launching during the wet season, with typical values of windspeed between 5.1 and 8.5 m/s. Considering the exposure concentration of 5 ppmv for a minimal effect on human health, Figure 7b shows a plot of HCl as a function of time for the different points inside and outside CLA. e arrows show the wind direction, which does not vary significantly in this time period, and the mean wind speed is 6.1 m/s on the launch pad, varying by < 0.5 m/s along the plume's path. The higher levels are 3768 ppmv at the SPL and 120 ppmv at the SMT, the nearest locations to the launch pad. The inhalation of these levels, even for a short time period (≤ 1 hr), can be dangerous (especially in the SPL). The maximum concentration at the ALC was 30 ppmv, which is a concentration close to strong throat irritation. The concentrations were safe at the VTA (with values < 2 ppmv).



Figure 6. Computational domain of WRF simulations.

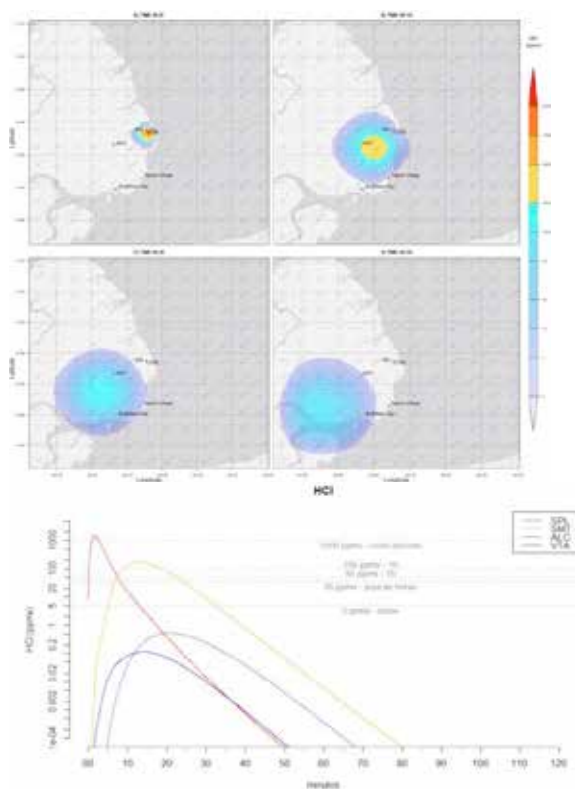


Figure 7. Some results from a simulation of gas HCl released at CLA: spatial dispersion (a) and time series (b). The contour areas are HCl concentrations.

For the CFD simulations, they were performed using the commercial software Fluent Ansys, which employs the finite volume method to discretize the conservation equations. A second order scheme was chosen to spacial discretization of momentum, specific dissipation energy rate and Reynolds stresses variables. The Figure 8 presents the computational domain.

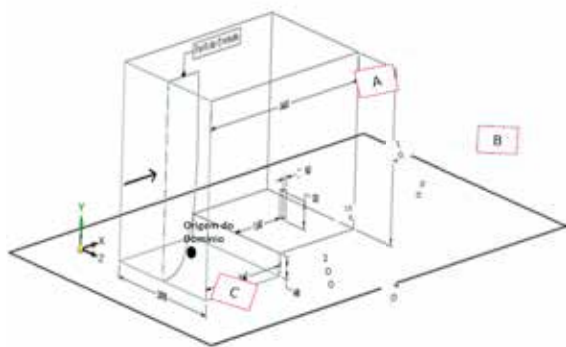


Figure 8. The CFD computational domain.

Although cliff inclinations β (45° , 70° and 90°) and two incident wind directions α (90° and 135°) were

considered, only one simulation will be presented (More details at Souza et al., 2015 and Klippel et al., 2019). At the outlet boundary, a zero pressure derivative boundary condition is adopted. Symmetry boundary conditions are applied to the lateral boundaries. At the top a free slip condition is applied. No-slip boundary condition is applied to all solid surfaces.

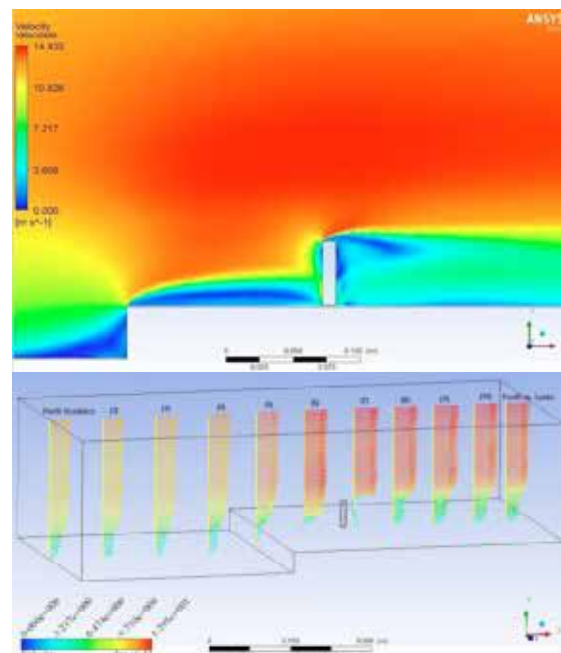


Figure 9. An aerial view of the SPL and the CFD computational.

The outputs obtained (presented at Figure 9) are very similar of the results done at WT by Faria et al. (2019). As expected, the higher vorticities (close to 1500 s^{-1}) were found at flow separation points in the cliff and behind the TMI. The wind profile (Figure 10) also shown good match between the CFD simulations and WT, especially at mid of test section.

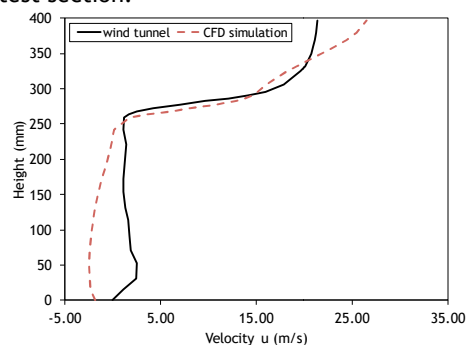


Figure 10. Comparison between the wind tunnel results and the numerical simulation in the TMI wake and for 90° wind direction and cliff inclination. Extracted from Klippel et al. (2019).

CONCLUSIONS

The final objective of this project is to have an operational software that can be run at CLA to help decision makers about the best meteorological conditions to launch a rocket, which will have the lower impact to the surrounding society, especially associated with air quality procedures (like the HCl released by the combustion of the solid propellents).

ACKNOWLEDGMENTS

This work is financially supported by CAPES (Pró-Estratégia n. 2240/2012) and CNPq (Edital Universal 2016 n. 403899/2016-8) projects coordinated by the first author (GF)

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Air pollution emission effects of changes in transport supply. The case of Bogotá, Colombia

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Abstract: Transportation policy and planning decisions, including decisions on new infrastructure and public transport improvements, will significantly impact urban socio-economic development, but will also affect local and global environmental conditions. New highway investments aim to upgrade connectivity between Bogotá and the surrounding regions, reducing congestion, associated fuel consumption, and air pollution emissions. Previous studies concerning air pollution in Bogotá have focused on evaluating different command-and-control strategies to reduce traffic-related air pollution levels, but implications of other transportation policies, such as changes in road infrastructure, need to be assessed. The literature shows that the potential air pollution benefits of capacity enhancement depend on the impacts of vehicle travel and changes in speed. If highway investments lead to an increase in vehicle trips, there would be little improvement in traffic flow and increases in total Vehicle-Kilometers-Traveled (VKT) would offset reductions in emissions per vehicle kilometer. However, if vehicle trips remain constant at pre investment levels, highway investments could reduce congestion and thus improve mobility and reduce air pollution. This work studies the effect of increased road capacity on traffic-related emissions in Bogotá using a tool that couples a transportation model with emission factors from COPERT IV. We followed a parametric approach varying transport supply and demand, comparing two supply and demand scenarios: Scenario-1 incorporates five highway capacity-enhancement projects in Bogotá and assumes insensitive travel demand; Scenario-2 incorporates the same highway projects, but assumes a demand increase of 13% in vehicle trips with private cars. This increased demand represents the amount of new traffic that would offset the travel time savings from road-capacity enhancement (e.g., average travel time of private vehicle in Scenario-2 is equal to baseline of year 2015). Results include daily and annual values of traffic-related emissions of five criteria air pollutants, CO, NO_x, PM₁₀, SO₂, VOC for the Baseline, Scenario-1, and Scenario-2. We report a reduction on emissions after adding capacity on highways and assuming inelastic demand (Scenario-1). Scenario-1 results in a 15% reduction in PM₁₀ emissions and a 10% reduction in NO_x emissions. Such emissions reductions are a result of reductions in VKT in Scenario-1. In contrast, the Scenario-2 results in increased emissions for all criteria air pollutants. For example, VOC and CO emissions increase by 21% and 22% compared to the Baseline scenario, respectively. Increased emissions are a result on increased VKT and lower speeds than the Baseline in the network. Therefore, the new traffic demand would eliminate the emissions savings observed in Scenario-1, and could potentially further degrade air quality in Bogotá. While an exact estimate of induced demand that may result from highway expansion in Bogotá is not available, this analysis highlights that such projects could lead to an increase in emissions unless there is a combined effort to limit growth in vehicle demand.

Keywords: Transport supply and air pollution, traffic-related emissions, Bogotá.

INTRODUCTION

Transportation policy and planning decisions affect many aspects of a city's environment. Planning decisions often involve trade-offs between conflicting objectives. For example, strategies to increase travel speed often increase crash risk, or a decision to expand on-road parking supply can degrade walking and biking conditions, later increasing congestion and pollution emissions. As a result, while aiming to promote solutions for urban transportation, planners often implement a mix of policies that can have conflicting results. Some of the benefits and costs, of transportation policies, like travel time and operation costs, are widely studied and their estimates are often accessible [1]. Other impacts (e.g., changes in walking conditions, crashes, and air pollution) are more difficult to quantify and are often dismissed by policy-makers as intangible [2]. This research

intends to contribute to a more comprehensive discussion of transportation policy by assessing the impact on air pollution from changes in transport infrastructure.

Over the last decade, Bogotá has implemented different strategies to achieve a sustainable, equitable, environmentally and financially sustainable transportation system. Interventions such as reductions of the oversized bus transit fleet, implementation of a high-capacity bus-rapid system (Transmilenio), provision for an extensive bike-lane network, and improvement of diesel quality, have had positive impacts on the air quality of city, by reducing traffic-related pollution [3]-[5]. However, air pollution remains an important public health issue for Bogotá. Activities that are contributing to pollutant emissions include poorly managed land-use and transportation planning in the northern and eastern suburban areas; fast growing motorcycle and light-duty vehicle fleets predominantly powered by diesel and gasoline; low penetration of

clean vehicle technologies; and limited air quality management capacity [6].

Previous studies have focused on evaluating different strategies to reduce air pollution. In 2005, Zarate (2007) [7] used an air quality model to evaluate repercussions of three abatement strategies targeting heavy-duty vehicles: i) restriction of trucks during morning rush hours, ii) reduction of bus fleet by 20%, and iii) improvement in diesel's quality. Zarate reports changes over the mixing ratios of CO, NO_x, VOC, and O₃ concluding that primary pollutants decrease proportionally with the decrease of emission in all three strategies, whereas a combined strategy to reduce VOC emissions and NO_x emission from light-duty vehicles are necessary to reduce high levels of O₃. In 2009, Rodriguez and Behrentz, measured real-world emissions factors for converted natural gas vehicles and found no reduction on emissions factors when compared to gasoline-powered vehicles [8]. In addition, in 2009 the Environmental Authority of Bogotá, designed the Clean Air Plan for Bogotá, which contains strategies to decrease air pollution between 2010 - 2020 [3]. Some of these strategies are: requiring exhaust emission control systems for trucks and motorcycles, voluntary inspection and maintenance programs for transit buses, educational programs for drivers, restricted use of old buses without catalytic converters, among others. Our work expands on previous research by evaluating the effect on emissions from interventions that directly affect the city's transportation system. We used a bottom-up model that couples detailed activity data from a travel-demand model and traffic-assignment model (typically used by transportation planning agencies) with COPERT IV emissions factors to develop a high-resolution road traffic emissions inventory for Bogotá. We then investigate the effect on emissions from a highway-capacity enhancement program. To the best of our knowledge, none of the prior work to evaluate the impact of expanded infrastructure capacity for Bogotá has accounted for the impacts on air emissions.

METHODS

Our analysis aims to assess the effect of increased road capacity on traffic-related emissions in Bogotá. We followed a parametric approach varying transport supply and demand. Specifically, we compared two supply and demand scenarios: Scenario-1 incorporates five highway-capacity enhancement projects in Bogotá and assumes insensitive travel demand; Scenario-2 incorporates the same highway projects, but assumes a demand increase of 13% in vehicle trips with private cars. This increased demand represents the amount of new traffic that would offset the travel time savings from road-capacity enhancement. (e.g., average travel time of private vehicle in Scenario-2 is equal to baseline of year 2015). It is worth noting that

private vehicle trips increased an average of 3% per year between 2010 and 2015 according to the household travel survey [9]. To get a 13% increase would take between 4 and 5 years.

We included five major highway which are shown in Figure 1: Viaducto Autopista Sur (Elevated South Expresway - Hwy-1); Autopista Longitudinal de Occidente ALO Tramo Sur (Longitudinal West Highway, South segment, Hwy-2); Autopista Regional de Occidente Jose Celestino Mutis (Jose Celestino Mutis Regional West Highway, Hwy-3); Avenida Centenario (Centerario Avenue, Hwy-4); and Avenida Boyaca (Prolongation of Boyaca Avenue, Hwy-5). We modeled traffic behavior under these infrastructure scenarios using EMME 4.0, a transportation planning software, and estimated air emissions using the COPERT IV emission factors.



Figure 1. Geographic localization of five highway infrastructure projects with access point.

Table 1. Relevant specification of highway infrastructure projects

ID	Name	Total length [km]	Number of lanes by direction	Capacity [Veh/h per direction]	Number of access
Hwy-1	Elevated South Expresway	9	2	3,000	4
Hwy-2	Longitudinal West Highway - South segment	21	2	3,000	4
Hwy-3	Jose Celestino Mutis Regional West Highway	23	2	3,000	11
Hwy-4	Avenida Centenario	14	2	3,000	6
Hwy-5	Prolongation of Avenida Boyaca	8	2	3,000	6

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Table 2 shows travel time and vehicle-kilometer traveled in the baseline scenario, the Scenario-1 (highway capacity plan with no change in demand), and Scenario-2 (capacity plan with 13% increase in private vehicle trips). As expected, adding highway capacity to the network decreases the daily distance traveled, because travel routes are optimized using new highways. For the Scenario-1, VKT reductions occur for taxis (21%) and private vehicles (7%). VKT for fixed-route modes like buses and trucks do not change significantly because their route choices are highly inflexible (i.e., defined by operational design in buses and operational restrictions in trucks). The results suggest a small rise in VKT for motorcycles (2%). New highways will reduce travel times, so motorcycle traffic in these new highways increases at the expense of longer trajectories for some trips. For the Scenario-2, VKT increase only for private vehicles for which we assumed a 13% increase in vehicle trips. This increased demand assigned to the new highways results in a 4% increase in VKT for private vehicles with respect to the baseline.

Table 2 Traffic operation results for Base line and two infrastructure scenarios

Mode	Avg. Travel Time [min]			Daily VKT [thousands]		
	Base line	Scen-1	Scen-2	Baseline	Scen-1	Scen-2
Private Vehicle	46	39	46	34,45	32,124	35,98
Bus	67	56	67	4,348	4,247	4,247
Bus Rapid Transit	59	59	59	422	422	422
Motorcycle	40	32	38	18,666	19,107	19,11
Taxis	36	30	37	10,487	8,294	9,206
Trucks	50	45	50	1,695	1,604	1,604

Not surprisingly, the results suggest lower average travel time per trip for all modes in Scenario-1 with respect to the baseline. In Scenario-2, motorcycles and taxis have a slight reduction in average travel time compared to the Baseline, while average travel time for other vehicles types remains the same as in the Baseline.

Table 3 summarizes annual values of traffic-related emissions of the five criteria air pollutants for the Baseline, Scenario-1, and Scenario-2. These results suggest a reduction on emissions after adding capacity on highways and assuming inelastic demand (Scenario-1). Specifically, Scenario-1 results in a 15% reduction in PM₁₀ emissions and a 10% reduction in NO_x emissions (Figure 2). Such emissions reductions are a result of reductions in VKT in Scenario-1. In contrast, the Scenario-2

results in increased emissions for all criteria air pollutants. For example, VOC and CO emissions increase by 21% and 22% compared to the Baseline scenario, respectively. Increased emissions are a result on increased VKT and lower speeds than the Baseline in the network.

Table 3. Traffic operation results for Baseline and two infrastructure scenarios

Pollutants	Baseline	Scen-1	Scen-2
	[Metric ton/yr]	[Metric ton /yr]	[Metric ton /yr]
CO	433,536	412,768	526,593
NO _x	35,943	33,948	40,991
PM ₁₀	2,044	1,735	2,071
SO ₂	1,126	1,008	1,266
VOC	55,196	53,093	67,239



Figure 2. Percent change of traffic-related emissions of five criteria pollutants for Scenario-1 and Scenario-2 with respect to the baseline.

CONCLUSIONS

Policy makers often assume that alleviating traffic congestion reduces noise and air pollution. However, evidence from transportation research strongly suggests that failure to take into account induced traffic (new demand) when assessing highway expansion plans could lead to poor transportation policy [10]. In this article, we examine the impact on traffic-related emissions on five criteria pollutants in Bogotá from a transport supply change. We have thus investigated how expanding highway capacity affects traffic-related emissions of CO, NO_x, PM₁₀, SO₂, and VOC in Bogotá. Taken together, these results can lead to some points of discussion. First is the obvious, yet important fact, that adding additional capacity to the heavily congested road network of Bogotá could reduce traffic-related emissions immediately after they start operating while induced demand is low (without accounting for congestion caused during construction). Transportation researchers have noted, however, that increased highway capacity increases vehicle demand until congestion levels in the network reach or exceed pre-expansion levels

[11]. In the model for Bogotá, a 13% increase in personal vehicle trips in the expanded highway network would result in the same travel times as in the baseline conditions (without the additional highway capacity). Such increased demand in the Scenario-2 results in reduced speed and increased distance travelled, which in turn eliminates the initial emissions reductions from increased highway capacity. The combined effect of lower speeds and increased VKT in this scenario is a 22% increase in VOC emissions and 21% increase in CO emissions, compared to the baseline (without additional highway capacity). The increase in NO_x and SO₂ emissions is not negligible. Previous studies in Bogotá state that ozone peaks can be mainly attributed to the summed contribution of VOC and NO_x [12]. Therefore, the new traffic demand would eliminate the emissions savings observed in the Scenario-1, and could potentially further degrade air quality in Bogotá. While an exact estimate of induced demand that may result from highway expansion in Bogotá is not available, this analysis highlights that such projects could lead to an increase in emissions unless there is a combined effort to limit growth in vehicle demand.

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AIR QUALITY AND URBAN PLANNING: ANALYSIS OF POLLUTANT DISPERSION IN DIFFERENT URBAN CONFIGURATIONS

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Abstract: The study of pollutant dispersion in urbanized cities is of great importance due to the proximity between polluting sources and the population. The impact of different urban parameters on the dispersion pattern becomes necessary in order to achieve a planned and sustainable urban development. The objective of this work was to investigate and to increase the understanding on the influence of different Floor Area Ratio (FAR) and Floor Space Index (FSI) using URANS with $k-\epsilon$ turbulence model. The parameter FAR is the relation between the total built area and the total area of the lot, while the parameter FSI is the ratio between the total useful constructed area (built area multiplied by the number of floors) by the total area of the lot. The unsteady solver method was chosen in order to simulate the transient effects of the turbulent structures of the atmospheric flow. The simulations were performed using the commercial code Ansys Fluent for three different urban configurations (Case 1 - FAR = 70.4% and FSI = 8.45, Case 2 - FAR = 70.4% and FSI = 4.20, Case 3 - FAR = 45.6% and FSI = 4.20). The results demonstrated that the concentration in urban configurations with taller buildings have a great interference in the dispersion of pollutants, which act promoting higher concentrations zones behind the buildings compared the shorter building arrays. In addition, the effect of the street width between the buildings showed to be even more significant to determine how pollutants are spread throughout the urban matrix, where the configuration with longer street widths produced lower concentration levels near the ground.

Keywords: Urban matrix, Pollutant dispersion, CFD, URANS

INTRODUCTION

Urban areas are characterized by a wide range of air pollution sources, such as traffic, industries, ventilation and air conditioning systems, among others. The impact of air pollution on urban environment has become an important topic (OKE, 1988), leading to several modelling studies with the main concern to assess the influence of buildings and other urban structures on pollutant accumulation and dispersion patterns (VAROULAKIS et al., 2003).

The urban typology of high-density populated areas of the cities, usually the central areas with huge buildings, may contribute to a poor atmospheric dispersion (VARDOULAKIS et al., 2003), since these type of constructions can affect the wind flow. In fact, the natural ventilation in urban environments is related to urban morphology, which is a combination of urban density, arrangement of the buildings along with the geometry and dimensions of these buildings.

It is important to study the impact of different urban parameters on the wind flow, especially at the transeunt level, since its parameters varies from city to city. So, the simulated scenarios consider the relationship between parameters such as height and spacing, built density, architectural

types, dimensions of the lot and the geometry of the buildings. Therefore, the aim of this work is to simulate scenarios that resemble existing cities in order to be able to extract data that can be translated into urban public policies.

METHODS

This work is divided into 2 steps:

(i) Validation of the simulation by comparisons between the numerical results and experimental data obtained by BOPPANA et al. (2010). Figure 1 was the geometry used in the validation.

(ii) Numerical simulations of different configurations of interest in order to analyse the influence of the building height and the distance of the buildings on the air quality inside an urban matrix. Figure 2 shows the geometries that were used for the simulation, where

Case 1 - building height = 36m, distance between buildings = 4m;

Case 2 - building height = 18m, distance between buildings = 4m;

Case 3 - building height = 18m, distance between buildings of 8 meters.

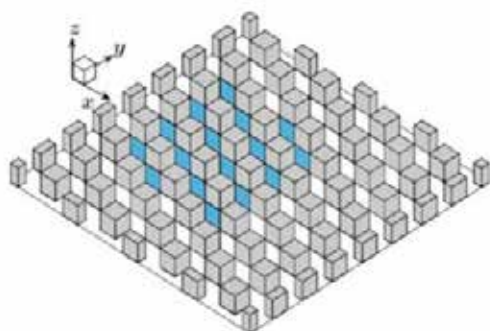


Figure 1: Geometry used for validation (BOPPANA et al., 2010).

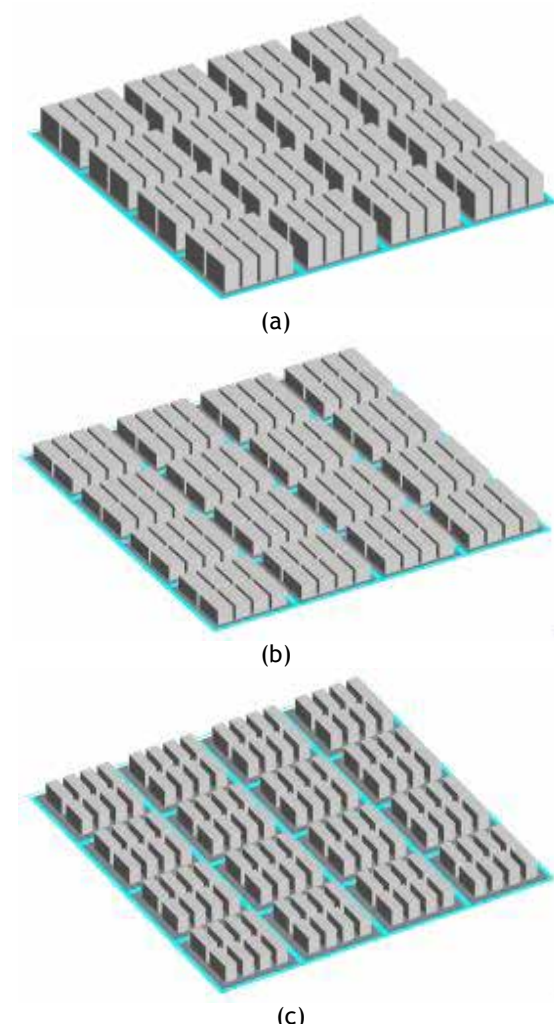


Figure 2: Schematic representation of the configurations studied: (a) case 1, (b) case 2 and (c) case 3.

The conservation equations of mass, momentum and mass of the chemical species describing the atmospheric flow and the dispersion of contaminants were solved numerically using commercial software FLUENT (Ansys Inc., 2011),

which employs the finite volume method. The effects of atmospheric turbulence were modelled using the unsteady $k-\varepsilon$ turbulence model. The methodology described was used for both validation and studied scenarios.

Instead of using the traditional solution form of the turbulent equations based on a RANS (Reynolds Averaged Navier-Stokes) approach, the transient solution of the governing equations was used to simulate the effects of turbulent flow structures (Unsteady RANS). The URANS simulation is expected to improve significantly in the predicting the dispersion of pollutants around buildings, according to Tominaga and Stathopoulos (2013).

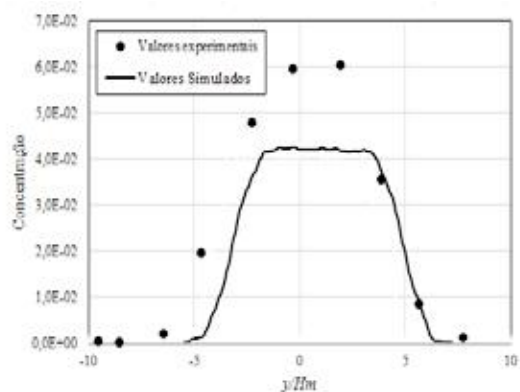
FINDINGS AND ARGUMENT

The results are also divided into 2 steps:

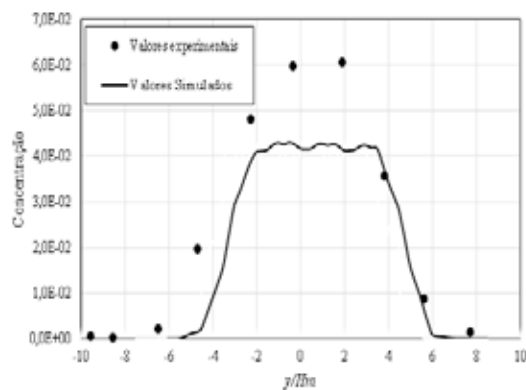
(i) Validation: Figure 3 shows a comparison between the results obtained in the present work and the wind tunnel results (Pasccheke 2008) in 03 cross-flow profiles $x/H = 5.5$, $x/H = 7.5$ ex $H = 9.5$. It is possible to observe that the values obtained numerically capture the transversal cross-sectional profiles, since in spite of predicting approximately a Gaussian profile, but the maximum concentration values are underestimated. Such behaviour may indicate a greater trend of vertical pollutant diffusion when compared to the observed experimentally. However, with increasing distance from the source, numerical and experimental profiles tend to present better agreement.

Figure 4 shows the concentration distribution for the three simulated cases. It can be observed that cross streets have a flow behaviour in urban canyons, where there is a perception of higher concentrations behind the buildings, this behaviour is expected in these places because it is a low pressure area with recirculation, making it difficult to disperse the pollutants. It can be observed that in Case 1, Figure 6a, the corners are more representative in their higher concentrations, compared to Case 2 (Figure 6b), because Case 1 has a height 2 times greater than Case 2.

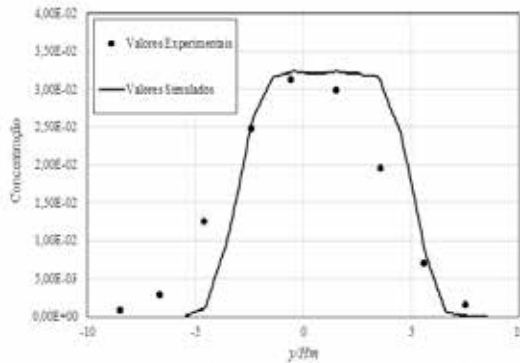
The concentrations obtained in Cases 2 and 3 are significantly lower than those obtained in Case 1. This effect is probably related to the lower flow velocities inside the urban canopy in Case 1, since the higher heights of the buildings tend to decelerate the flow.



(a)



(b)

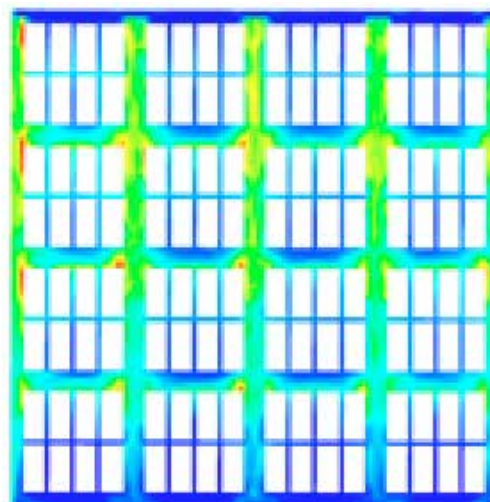


(c)

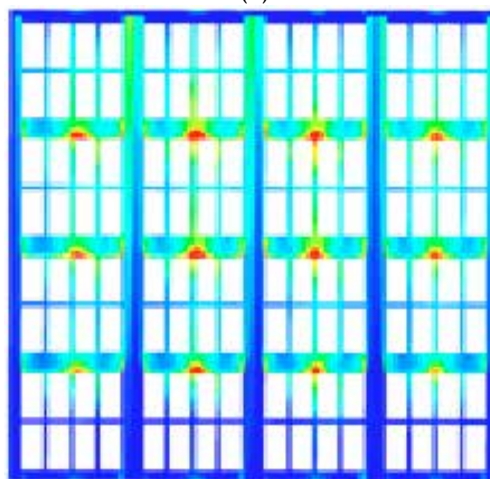
Figure 3: Comparison between results obtained experimentally (BOPANA et al., 2010) and by simulation: (a) at $x / H_m = 5.5$, (b) at $x / H = 7.5$, and (c) at $x / H = 9.5$.

(ii) Numerical simulations of different urban configurations: In Figure 4c, it is important to note that the smaller distances between the buildings reduces the volumetric flow passing through it, and consequently reduces the wind speed between them, causing a reduction of urban canyon phenomenon effect. In fact, the concentrations obtained for Case 3 are much smaller than the others, demonstrating the effect of the spacing of the buildings on the natural ventilation of the city.

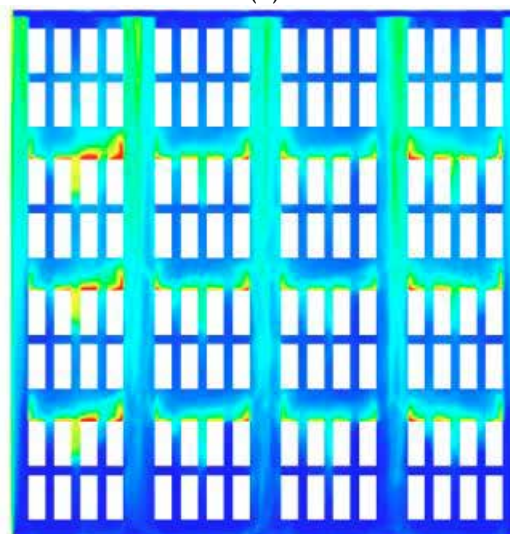
This behaviour can best be observed by means of vertical concentration profiles.



(a)



(b)



(c)

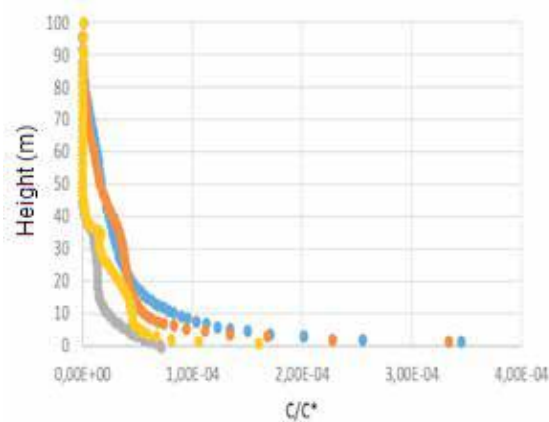
Figure 4: Concentration distribution in a horizontal plane 2 meters height, for the 3 configurations studied: (a) Case 1, (b) Case 2 and (c) Case 3.

Figure 5 indicates the positions used to plot vertical concentration profiles for each configuration, which are shown in Figure 6. The point 1 represents an intersection between paths, the point 2 represents a location in a path aligned with the main flow, the point 3 represents a location in the middle of the courtyard, while the point 4 represents a location in a not aligned path with the main flow.

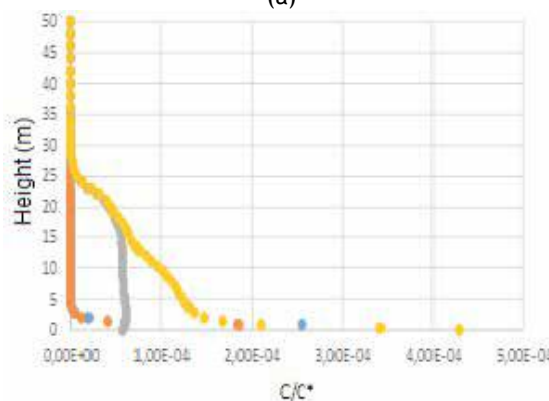


Figure 5: Location of vertical concentration profiles.

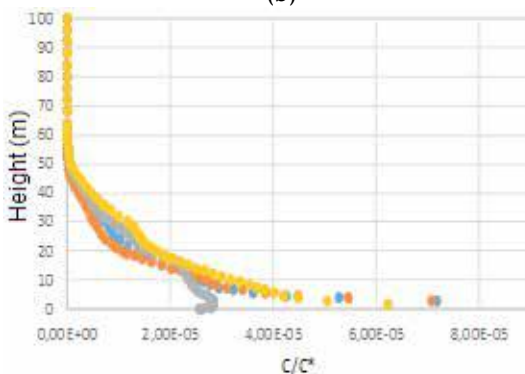
it is possible to observe in Figure 6 that the concentration inside the courtyard (point 3) is slightly lower in Case 2 than in Case 1. On the other hand, the concentration inside the courtyard (Point 3) is significantly lower in Case 3 compared to Cases 1 and 2. This trend may indicate that the effect of the remoteness of the buildings on the concentration in this region is more significant than the height of the buildings. It can also be observed that the concentrations in the streets aligned with the flow and at the intersections are significantly higher in Case 1, indicating that higher buildings heights contribute to the increases residence time of the pollutant inside the canopy.



(a)



(b)



(c)

Figure 6: Vertical Profiles of concentration at the points indicated in Figure 5: (a) Case1, (b) Case 2, (c) Case 3.

CONCLUSIONS

It is concluded that the concentration in urban configurations with greater buildings heights have a great interference in the dispersion of pollutants increasing the concentrations of pollutants. This response is consistent with the literature, since it creates a zone of lower pressure in urban configurations due to the lower verticalization.

However, the effect of spacing between buildings was even more significant within the urban matrix. The configuration with greater distance between the buildings produced much lower concentration than those with the less distance. Such behaviour indicates the need to test the effect of spacing variations in conjunction with height variations, in order to maintain the coefficient of utilization constant, increasing the height of the buildings and the distance between them.

The observation of this change in concentrations can be used in PDU (Plano Diretor Urbano) of developing cities and can be a parameter for the buildings influencing the air quality of this place.

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