

# PROCEEDINGS OF THE 3<sup>RD</sup> CMAS South America Air Quality Conference Brazil 2017

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## Summary

Session 1	3
Session 2	33
Session 3	41
Session 4	63
Session 5	82
Session 6	118
Session 7	137
Session 8	141
Session 9	169
Session 10	219

## Session 1 Air Quality Modeling Applications



### EFFECTS ON MANAUS CO CONCENTRATIONS BY POWER PLANT FUEL SWITCHING

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Abstract: The study below show how a changing energetic matrix that burns fossil fuel impacts air quality in a tropical environment. To do so, WRF-Chem were used to simulate CO concentrations in Manaus urban zone. CO emissions of the three scenarios considered has decreased by 25% between a pre-change scenario (100% fuel oil and diesel) to an actual scenario (65% natural gas and 35% fuel oil + diesel), and decreased by 55% from the same pre-change scenario to a future scenario (100% natural gas). The results show that the complete change in energetic matrix reduces CO maximun values significatedly on most polluted days, improving air quality. It also leads CO values to close-to-background values on simulated month (February 2014).

Keywords: Carbon Monoxide, Air quality, WRF-Chem, Amazon, Manaus.

#### **INTRODUCTION**

It is known that anthropogenic influence modifies the environment around it, including atmospheric composition. Emissions of pollutant gases in land use change, biomass burning, power generation and automobiles increases of polluting gases concentration the troposphere, interfering with air quality and, consequently, on human health in urban environment. In this context, can be cited Manaus as a large city (2 million inhabitants) located in Brazilian Amazon (largest tropical forest in the world), as an important source of pollutant gases in an environment with little anthropogenic influence like Amazon forest. In addition, Manaus, unlike what happens in Brazil that has the main form of energy the hydroelectric power plant, has 75% of its energy generated from the burning of fossil fuels.

According to Medeiros et al. (2017), a fuel change is being carried out in this energy matrix originally from fuel oil and diesel to natural gas. Currently, this matrix of thermoelectric power plants works using 65% natural gas and 35% of a composition between fuel oil and diesel. This constitutes important change an unprecedented scenario of energy matrix change in a tropical forest environment and its effects on air quality. The pollutant to be evaluated in this work is carbon monoxide, an important indicator of air quality and public health, as well as the effects of this fuel change in urban concentrations of CO. To study these effects, this work was developed using the atmospheric model coupled to the chemical module WRF-Chem. Figure 1 shows the area considered in this study.

#### **METHODS**

To study the effects of fuel switching in CO values, were carried out simulations using the model WRF fully coupled to a chemical module (WRF-Chem version 3.6.1) (Grell et al., 2005). Were used the same parameterizations as Medeiros et al. (2017), described in Table 1.

Table 1. Configuration of the modelling

Cloud Microphysics	Lin et al. (1983)
Land Surface	(Chen et al., 1997)
Boundary Layer	(Hong et al., 2006)
Short-wave radiation	(Chou and Suarez, 1999)
Long-wave radiation	(Mlawer et al., 1997)
Cumumus	Grell and Freitas (2013)
Meteorological data	(Saha et al., 2011)
Land cover	MODIS
Chemical mechanism	(Stockwell et al., 1990;Chang, 1991)
chemical Initial and	(Emmons et al.,
boundary conditions	2010)
Biogenic emissions	(Guenther et al., 2012)
Mobile emissions	(Martins et al. (2010))

Reference: Medeiros et al. (2017)



Were used two nested domains of 1050 km x 800 km (Domain 1 in Figure 1) and 302 km x 232 km (Domain 2 in Figure 1. That domains had 10 km and 2 km of resolution, respectively. The simulations were performed for February of 2014 (entire month), with each run of 96h and 24h of spin-up.

Emissions by forest, vehicles, power plant, and refinery were inserted methodology described in Medeiros et al. (2017). Power plants and refinery locations are shown at Figure 1. There are 11 locations that generates energy for Manaus urban region to supply both industrial and residential demands. Further details like energy production by each power plant and emissions by refinery can be found at Medeiros et al. (2017). They also show that th parcial change in energy matrix reduces total CO emissions by 25%, and total switch reduces thus emissions by 55%



Figure 1. Sattelite image of the region. Manaus is located at the center, with power plants (red dots) and refinery (blue dots) also indicated. The white box at Manaus indicate the area used to evaluate CO concentrations. At top left the domains employied are represented. Figure obtained from Medeiros et al. (2017).

Three scenarios were simulated to evaluate the effects on Carbon Monoxide's concentrations (Cases A, B, and C). Case A considers the emissons by power plants before the change in the matrix, when only fuel oil and diesel were used to generate energy. The Case B considers 2014 emissions, when 65% of the power generation were done by burning natural gas, while the remaining 35% used fuel oil and diese. In the end, Case C considers the future case with 100% of the energy generated from power plants in Manaus region done by burning natural gas.

#### FINDINGS AND ARGUMENT

From the methodology described, Figure 2 show box-whisker plot the urban CO concentrations over Manaus (area correspondent to the white box

in Figure 1). There are significant differences of maximum CO values among Cases A, B, and C. In Case C (Figure 2), the values of CO are very similar through February, all ranging from 110 ppb to 140 ppb. That values corresponds to a clean atmosphere at the region, indicating that the change reduces significatedly CO concentratons in Manaus. From Cases A and B (Figure 2), there are significant increase in relation to C, specialy in polluted days (stands out days between February 12 to 18, where didn't rained in Manaus region according to Medeiros et al. (2017)).

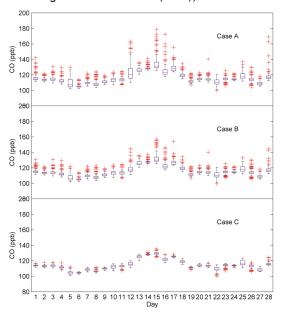


Figure 2. Box-whisker plot of carbon monoxide concentrations over manaus region. Both botton and top of the blue boxes are the first and the third quartiles, while red line inside the box represents the median value. The whiskers are the outliers.

For Case A, maximun CO values reached 180 ppb (around 34% increase from a mean value of 120 ppb in Case C), while the same maximun CO reached 160 ppb in Case B (an increase of 25% from case C). It also can be seen a slight variability for the considered month due to meteorological conditions, and this variability is present among the three cases, as expected once the meteorological data are the same. The differences among cases stands out in most polluted days (i.e. days 12 to 18 and 28). For the rest of the days, there are no significant differences between Cases A, B, and C.

#### CONCLUSIONS

In summary, the present study show the benefits of change fuel oil and diesel to natural gas in a tropical air quality context. It is indicated that the fuel switch in Manaus power plants brings CO values close to background conditions after the total switch. It is shown that a decrease in 25% and



55% on CO emissions leads to decreases of 11% and 22% in maximun CO concentrations on the most polluted days. In mostly clean days, the concentrations are simmilar among cases, indicating that the improve in ir quality are intensified on polluted days.

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## Evaluating BRAMS forecasts of carbon monoxide for Tijuca and Irajá stations during the 2016 Olympic Games

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Abstract: Rio de Janeiro was the hosting city of the Olympic Games in 2016. Monitoring and forecasting the air quality in the Metropolitan Area of Rio de Janeiro (MARJ) became a priority in order to support government agencies and population during this period. For that, the air quality forecast system for MARJ (AQFS-MARJ) in high resolution (1km of grid space) was implemented in 2016 using the Brazilian developments on the Regional Atmospheric Modeling System (BRAMS) version 5.2 in the Center for Weather Forecasting and Climate Research of the National Institute for Space Research (CPTEC/INPE). In this work, we analyze the performance of BRAMS forecasts for carbon monoxide comparing to observation data from Irajá and Tijuca ground stations provided by the local government agency (Secretaria Municipal do Meio Ambiente - SMAC). It was used 3 different versions during the games: 20km (operational version), 5km and 1km dedicated to the Olympic period. The results indicated BRAMS model forecasts better represent the observed concentrations during the morning and early afternoon, clearly underestimating the observed nighttime behavior.

### *Keywords*: BRAMS, air quality forecast, Olympic Games 2016 INTRODUCTION

The city of Rio de Janeiro in Brazil welcomed the Olympic and Paralympic Games during August and September 2016, respectively. Rio is one of the biggest cities in Brazil, located in a complex terrain beside the sea, which experiences poor air quality due to high concentrations of vehicular pollution, specially in densely populated areas. In this city with about 7 million inhabitants, air pollution levels are high enough to pose a threat to public health (Gouveia et al., 2003; Junger et al., 2005).

To support government agencies and population during the Olympic Games, the Center for Weather Forecasting and Climate Studies of the National Institute for Space Research (CPTEC/INPE) implemented in 2016 the air quality forecast system (AQFS) for the Metropolitan Area of Rio de janeiro (MARJ) in high resolution (1km of grid space) using the Brazilian developments on the Regional Atmospheric Modeling System (BRAMS) version 5.2 (Frassoni et al., 2016). BRAMS model has been used for operational forecasts and also for research in weather and air quality modelling since 2003, in a limited area domain for South America (Freitas et al., 2009, Longo et al., 2010, Freitas et al., 2017). This model simulates the transport, removal and chemical transformations of gases and aerosols, as well as the atmospheric

physics, dynamics and surface feedbacks in an integrated way (Freitas et al., 2017).

The spatial and temporal distribution of emissions has a strong role in the air quality forecast and better emission representation in local scale helps improving the numerical model results as well as the global inventories commonly used in air quality models. Since 2003, many improvements have been applied to the BRAMS model to better represent emission sources, resulting in successful forecasts for South America.

To quantify the improvements of the AQFS-MARJ compared to the operational version of BRAMS for air quality forecasts, we performed objective evaluation for CO in 24h and 48h forecast lengths for Irajá and Tijuca air quality monitoring ground stations in the Rio de Janeiro City during the period August 01 to September 30 in 2016.

#### **METHODS**

The AQFS-MARJ consisted in forecasts in three spatial resolutions: the operational version with a 20km grid resolution over the limited area domain of South America (47°S, 12°N/25°W, 87°W), a 5km grid resolution in a limited area domain over part of Southeast Brazil (25,5°S, 18,5°S/37°W, 49°W) and a 1km grid space limited area domain over MARJ (24°S, 21,5°S/45°W, 41,5°W). The 20km version has been used as initial (IC) and boundary



conditions (BC) for dynamically downscaling 5km model domain and 1km model has been dynamically downscaled from IC and BC from 5km domain. Each version has been performed for up to 48h forecast length. Since 1km grid space modeling requires a better representation of the land surface due to urban characterization in the MARJ, the urban parameterization 2T (Silva et al., 2016) from the surface model Joint UK Land Environment Simulator (JULES) of BRAMS has been used with a better characterization of the emissivity, LAI (leaf area index) and albedo of each class of land use and cover from the International Geosphere-Biosphere Program according to the JULES classes (Belem and Peres, 2016). To better represent emissions in MARJ, vehicle emissions were updated within the PREP-CHEM-SRC emissions preprocessor used to generate BRAMS emissions (Chovert et al., 2016). The PREP-CHEM-SRC is a tool that provides emissions fields of trace gases and aerosols for regional and global atmospheric chemistry models (Freitas et al., 2011).

Georeferenced emissions for five different types of roads in the MARJ were included. The emission percentage for each road was computed using the most recent traffic information available. To include the industrial contributions to the emissions, the global datasets RETRO (REanalysis of TROpospheric chemical composition) and EDGAR-HTAP (Emission Database for Global Atmospheric Research) were used. Biogenic contributions took into account information from the MEGAN (Model of Emissions of Gases and Aerosols from Nature) model.

To analyze the performance of the model to forecast CO, Tijuca and Irajá Air quality monitoring ground stations managed by the local government agency (Secretaria Municipal do Meio Ambiente - SMAC) were used. The stations and their locations are shown in Table 1.

Tijuca station is characterized by steeper and higher terrain (above 500 m) from the Tijuca Range. Prevailing land use is urban. It is characterized by an important residential middleclass area with high population density and intense verticalization. This monitoring ground station is located in an area surrounded by high-rise buildings which act as barriers for natural air flow, hindering pollutants dispersion. It is also near a locally important secondary arterial road with intense vehicle traffic and so, under the direct impact of mobile sources of pollution (Nacaratti, 2013). Given this configuration, direct sea breeze influence is not perceived and the mountain breeze becomes the main force driving wind direction in this location, due to the proximity to the Tijuca Range highlands.

Irajá station is located in a smooth terrain area, with elevations not higher than 70m. A mixed land cover with urban area, shrubland and grassland is present. This station is also subject to intense vehicle flux in its vicinity, which constitute the main emission sources. The Estrada da Água Grande highway is considered a primary arterial road and is located at approximately 112m from the monitoring site (Nacaratti, 2013).

We computed a 2-days moving average in the temporal evolution of the forecasts and observations for each ground station. We also computed the mean diurnal cycle and correlated it with CO observations for the aforementioned stations.

Table 1: Municipality and geographical coordinates of the CO measuring stations.

Municipality	Geographical Coordinates
Irajá	43°19'36,89"W/22°49'53,89"S
Tijuca	43°13'57,27"W/22°55'30,03"S

#### FINDINGS AND ARGUMENT

According to the SMAC, winter is the season with highest CO concentrations in Tijuca station, followed by autumn and spring, with main peaks occurring around 9h local time and secondary peaks around 20h local time, with concentrations around 0.3 ppm for both peaks. Analysis of the observed diurnal cycle during August-September 2016 indicate a main peak at 10h local time and a secondary peak with the same magnitude at 18h, in accordance with previous studies (Fig. 1a).

Irajá has the highest CO concentration during autumn, followed by winter, summer and spring, with main peaks at 8h and secondary peaks at 20h local time (Nacaratti, 2013). The mean diurnal cycle for August-September 2016 indicates a main peak at 20h local time and the secondary peak in the morning, between 7h-8h local time (Fig.1b). Both concentration peaks in the ground stations coincide with the increase of vehicular activity during the morning and also during early night rush hours.

The mean diurnal cycle of 24h CO forecasts (Fig. 1) indicates BRAMS better simulated the diurnal behavior for both stations, specially in the morning hours. Clearly the higher resolution model versions lacks in the representation of nighttime concentrations. For Irajá, while the 20km operational version represents better the diurnal cycle including secondary peak during nighttime even with overestimation in most of the diurnal cycle, 5km and 1km versions have negative bias, underestimating the observed concentrations with



limitations in the concentration forecast during nighttime. In Tijuca station, both versions delayed the morning peak, with overestimation in the 1km resolution, while 5km and 20km underestimated the peak. Also, both versions had limitations to forecast the secondary peak in the evening, possibly associated with limitations in the model to represent local circulations during the nighttime. The 48h forecast length (Fig. 2) fitted better with observations for Irajá station (Fig 2b), with a good representation of the morning peak mainly by 1km version. The secondary peak was indicated by both versions, but underestimated by higher resolution versions. The 48h forecast had better skill compared with 24h forecast also for Tijuca station, with decrease of the bias (Fig. 2a), but the same characteristics with 24h simulation were observed. The computed correlation between mean diurnal cycle observations and 24h and 48h forecasts was low for both stations, mainly due to the poor skill of the model after midday.

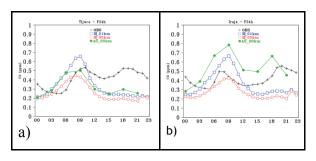


Figure 1: CO average diurnal cycle of BRAMS 24h forecasts for 20km horizontal resolution (dotted green line), 5km horizontal resolution (circle red circle line) and 1km horizontal resolution (squared blue line), and observation (cross black line) for: a) Tijuca and b) Irajá ground stations.

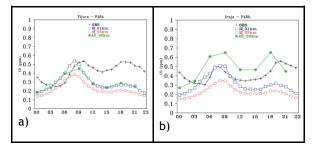


Figure 2: The same as Fig. 1, except for 48h forecast length.

#### **CONCLUSIONS**

The observed diurnal cycle of CO concentrations for August-September 2016 indicate highest concentrations during the morning and early evening hours, associated to the increase in vehicular traffic, the main emission sources of CO in the analyzed regions. The BRAMS model

forecasts better represent the observed concentrations during the morning and early afternoon, clearly underestimating the observed nighttime behavior. Future investigation will be conducted to identify the model limitations in representing CO concentrations during nighttime.

#### **ACKNOWLEDGMENTS**

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## TRANSPORT OF POLLUTANTS IN THE REGION OF THE METROPOLITAN AREA OF SÃO PAULO AND CUBATÃO INDUSTRIAL CITY IN A HIGH WINTER SEASON

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Abstract: In the present work, we investigated the Transport of pollutants from Metropolitan Area of São Paulo (MASP) (CO) and Cubatão ( $PM_{10}$ ) to nearby areas from August 23 till 26, 2006, a high winter season period. Simulations provided by the system of models BRAMS (meteorological model) and SPRAY (lagrangian diffusion model) were validated with observed values measured in station monitoring meteorological and air pollution data in this area. They enabled the discussion of the pollutants transport map between MASP, Cubatão and nearby areas, during the studied period.

Keywords: Atmospheric pollution, Dispersion modeling, Pollutants Transport, São Paulo, Cubatão

#### INTRODUCTION

Mesoscale model BRAMS (Fazenda et al., 2013) was used to provide meteorological variables needed by the Lagrangian dispersion model SPRAY (Tinarelli et al., 1994), to simulate 3D concentration fields in the Metropolitan Area of São Paulo (MASP), and in Cubatão, the main Brazilian industrial city. CO is the major pollutant emitted by the more than 7 million vehicles fleet of the MASP, directly affecting the life of more than 20 million inhabitants. At the same time the particulate matter  $(PM_{10})$  is the worse air pollution problem in the industrial area of Vila Parisi and Vale do Mogi, at Cubatão. Therefore, the dispersion of CO and  $PM_{10}$ , from each of these places, respectively, were taken to study the transport of pollutants emitted in this area, from August 23 till 26, 2006, in the high winter season, when pollutants concentration usually increase. Their impacts on nearby areas could cause problems for vegetation and human beings. Comparisons between simulated and observed data obtained in 16 stations (measuring meteorology, and/or CO and/or PM, by CETESB and IAG-USP), showed that simulations are reliable. Concentrations field showed transport of CO to areas of the shoreline (near to Cubatão) and of PM from industrial plants at Cubatão to MASP during two episodes observed in these areas, on August 25 and 26, 2006.

#### **METHODS**

BRAMS was used to generate 3-D wind, temperature and diffusion coefficient fields, and the 2-D topography and surface layer parameter (roughness length, Monin-Obukhov length, friction velocity) fields needed to run SPRAY. BRAMS was initialized with CPTEC (Weather Forecast and Climate Studies Center) global files for days 23 to

29 August 2006 (12h and 0.9375°, time and spatial resolutions, respectively, covering a 90°S to 40°N latitude and 120°W to 80°E longitude area with 28 vertical levels). Full microphysics and 3 nested grids covering MASP, Cubatão and nearby areas were set (Silva, 2017). SPRAY was fed with BRAMS simulated data through GAP (Grid Adaptor - used to convert and interpolating lat/lon to UTM coordinates) and SurfPRO that, with the addition of land-use data, provides turbulence scaling parameters, 2-D mixing height field, horizontal and vertical diffusivities, deposition velocities. The MASP CO's Sources (5kmX5km resolution) followed Kerr et al. (2005) updated to 2006 emissions, and overall Cubatão's industrial sources for PM as in CETESB (2007). BRAMS's grid 2 (3kmX3km resolution) were used for CO simulations and grid 3 (1kmX1km resolution) for the PM ones. Probability Density Function for dispersion modeling was a  $3^{rd}$  order Gram-Charlier, and the Ground Boundary Conditions for Velocity fluctuations was set as Normal Reflection Over Bilinear.

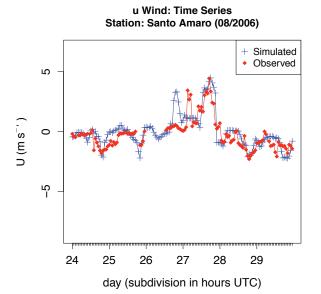
Simulation results were compared with the measures made in the CETESB's monitoring stations, following Hanna & Chang (2012), but using some other performance parameters, like correlation (R), with significance level lesser than  $\alpha = 0.05$ , NRMSE (Normalized Root Mean Square Error)< 300%, FB (Fractional BIAS) < 0.67, FAC2 (Factor of two) > 0.3, NMSE (Normalized Mean Square Error) < 6 and  $\sigma_{sim} \approx \sigma_{obs}$ . Simulation results are said to be acceptable for one station when it hits the criteria for at least 50% of parameters, but P-value < 0.05 was mandatory, hence if P-value > 0.05, the simulation has failed for that station. According to Hanna & Chang (2012), criteria for urban simulations must be relaxed due to buildings, uncertainty of sources etc. In previous works this



modeling system has been shown ability to simulate pollutant dispersion in this complex region Kerr et al. (2005).

#### FINDINGS AND ARGUMENT

Figures 1 and 2 shows time series for zonal wind in Santo Amaro and Cubatão's stations, the worst simulated wind component. The worse result for Cubatão may be due to the complexity of the regional terrain.



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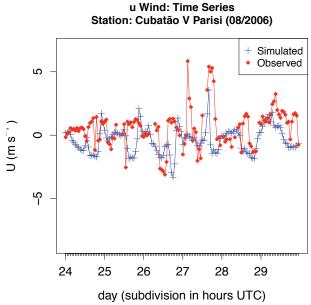


Figure 2: Cubatão - Vila Parisi's Station:Time Series for zonal wind

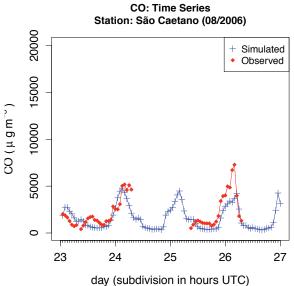


Figure 3: São Caetano's Station: Time Series for CO

Figure 3 shows time series for CO in São Caetano's station. The simulations at the major part of the stations satisfied the performance criteria. Nevertheless, at São Paulo downtown we observed over prediction, likely due to the high intensity of the emissions in this area, and the inability of the coarse source resolution represent local emission contrasts. São Caetano, like other more peripheral zones, shows more homogeneous emissions, assimilating the low source resolution.

#### **CO Concentration for MASP and Nearby Areas**

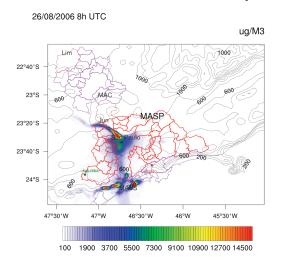


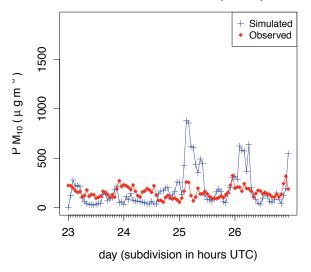
Figure 4: CO transport from MASP to MABS

Figure 4 shows CO transport from MASP to MABS (Metropolitan area of Baixada Santista), were is noticeable some areas wit concentrations exceeding  $10000 \mu gm^{-3}$ , the WHO standards for CO (World



Health Organization, 1999).

#### PM10: Time Series Station: Cubatão V Parisi (08/2006)



 ${\rm Figure}~5:~{\rm Cubat\~ao}$  - Vila Parisi's Station:Time Series for  $PM_{10}$ 

Figure 5 shows the time series for  $MP_{10}$  in Cubatão Vila Parisi's station. The performance criteria were filled only there. Other stations were influenced by sources related to vehicular fleet, or by bad zonal wind simulation for this area, that relies on a complex terrain, not well captured by the meteorological model. Figure 6 shows significant amount of PM transported to the eastern borders of São Paulo and nearby areas - up to  $20\mu gm^{-3}$ .

#### PM10 Concentration for MASP and Nearby Areas

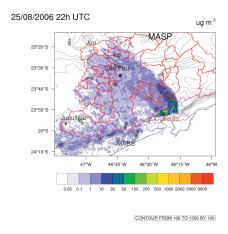


Figure 6:  $PM_{10}$  Transport from Cubatão to MASP

#### **CONCLUSIONS**

The Couple BRAMS/SPRAY meteorological and diffusion simulation modeling systems was able to simulate reliable concentration fields for vehicular CO emitted in the MASP, as well as the PM emitted by industrial plants at Cubatão. Significant transport of CO could be observed from MASP to shoreline in the Baixada Santista on August 26, after 5 UTC, and PM transport from Cubatão to the MASP in the August 25 evening. Better results should be reached for CO simulation if increasing the CO source resolution. The complex topography at Cubatão indicates the necessity of improve the local topographic resolution. Non-industrial sources should also be included there, specially for better define the local  $PM_{10}$  concentrations.

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## PARAMETERIZATION OF MASS TRANSFER OF POLLUTANT AT THE TOP OF THE URBAN CANOPY

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Abstract: The objective of this work was to investigate the mass exchange process through the top of the urban canopy by large-eddy simulation (LES). The LES simulation was performed over a staggered array of buildings with different heights and with different source locations. It was found that for a more realistic array of buildings (buildings with different heights) the flow and dispersion of pollutants become more complex than they are in the case of buildings with uniform heights. It was conclude that the vertical scalar transfer through a surface located at a mean height of the obstacles is influenced by both effects turbulent and advective, whereas the turbulent component dominates the vertical flux through the top of the array of buildings with uniform heights. Thus, the parameterization of the transfer velocity on the top of the urban canopy will be strongly influenced by different transfer process occurring on it, depending on the configuration used.

Keywords: mass exchange, transfer velocity, urban canopy, buildings with different heights.

#### **INTRODUCTION**

The threat of deliberate or accidental releases of harmful substances in urban areas makes understanding atmospheric flow and dispersion important. When the source is located within the urban canopy the highest concentrations are in the short-range, i.e. less than 1km, where the dispersion is strongly affected by the presence of buildings. Understanding the processes that govern point source dispersion in the short range is important in order to develop a dispersion model for the use of emergency responders.

The general objective of this work is to understand the mass transport processes of pollutants at the top of an urban canopy with buildings with different heights using large eddy simulation (LES).

#### **METHODS**

The LES data were obtained from a single configuration of buildings, a matrix of staggered buildings with different heights (configuration used by Cheng and Castro (2002) in an experimental study). The direction of the wind was equal to 0° and it was considered three different source locations that were punctual and continuous. Figure 1 show the configuration used.

The sources were located near the ground, at a height of  $z=0.001h_m$ . Two sources are located between two buildings and the other was located in front of the highest building in the domain. The domain consists of 64 buildings with heights varying

from 2.8 mm to 17.2 mm. In this way, the average height of the buildings is  $h_m$  =10mm. The spacing between buildings in the y direction is 10 mm and the distance between rows of buildings in the x direction is also 10 mm. The dimensions of the domain are  $16h_m$ x1 $6h_m$ x8 $h_m$ . Validation of the methodology is presented in Cezana(2015).

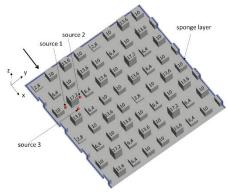


Figure 1: Computational domain for the LES simulation, showing a matrix of staggered buildings, with different heights and wind direction equal to  $0^{\circ}$ . The sources are indicated in the figure and are located at a height of z=0.001 $h_m$ . The numbers at the top of each building indicate the heights of buildings in millimeters.

FINDINGS AND ARGUMENT



The transfer velocity was calculated in repeated units as shown in Figure 2. Repeated units were chosen according to the location of the pollutant plume. Each repeated unit is composed of four boxes: a building, a box behind a building, a box in front of a building and a box between two buildings.

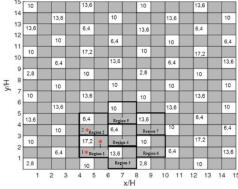


Figure 2. Repeated units where the transfer velocity was calculated. (\*) Represents the location of the sources and the numbers at the top of the white squares indicate their heights in millimeters.

In order to analyze the accuracy of the parameterizations available in the literature for the transfer velocity, Figure 3 and Figure 4 present the comparisons of the LES data with the parametrizations from literature employed. Table 1 summarizes the analyzed parameters.

In general, it is possible to identify that in the region between the buildings the parametrizations give better results regardless of the source. On the other hand, in the region behind the buildings, the values of the transfer velocity are higher and thus the parameterizations do not agree satisfactorily with the values obtained from the LES data. In the boxes located behind a building are found high values of the transfer velocity that can be explained due to the intense vertical movement that happens in these regions. The pollutant is taken to the top of the canopy and thus the difference of concentration between the interior and above the canopy will be small, leading to high values of transfer velocity.

It is important to emphasize that in the parameterization formulation of Soulhac et al. (2011) one of the hypotheses is that the flow at the top of the urban canopy is dominated by turbulent effects. However, for this configuration of buildings of different heights, both advective and turbulent effects are important. Therefore, it is not possible to say if this parameterization performs well because the physical phenomena that it considers are not the same.

Table 1. Parameters for the transfer velocity.

Parametrization	Equation for $U_T$
SOULHAC01 (SOULHAC et al., 2011)	$\label{eq:UT} \textbf{U}_T = \frac{\sigma_w}{\sqrt{2}\pi} \text{, where } \sigma_w \text{ was}$ calculated with LES data.
SOULHAC02 (SOULHAC et al., 2011)	$U_T=rac{\sigma_w}{\sqrt{2}\pi},$ where $\sigma_w$ was calculated by $\sigma_w=1.3u_*(1-0.8z/h)$
B&B01 (BENTHAM; BRITTER, 2003)	$\frac{\textbf{U}_{T}}{\textbf{u}^{*}} = \left(\frac{\textbf{U}_{ref} - \textbf{U}_{c}}{\textbf{u}^{*}}\right)^{-1} \text{, where } \textbf{U}_{ref} \in \textbf{U}_{c}$ were calculated with LES data.
B&B02 (BENTHAM; BRITTER, 2003)	$\frac{U_T}{u^*} = \left(\frac{U_{ref} - U_c}{u^*}\right)^{-1}$ , where $U_{ref}$ was calculated with LES data and $U_c$ was calculated by $\frac{U_c}{u^*} = \left[\frac{\lambda_f}{2}\right]^{-1/2}$ .

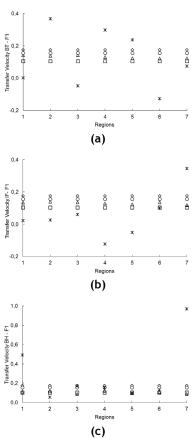


Figure 3: Transfer velocity calculated at regions (a) between buildings (BT); (b) in front of a building (IF) and (c) behind a building (BH) at a height of  $z/h_m=1$  for source 1. (\*) represents the average transfer velocity on repeated units using LES data; represents the parametrization of ( $\Delta$ ) SOULHACO1; ( $\diamond$ )SOULHACO2; ( $\Box$ ) B&BO1 and (o) B & BO2



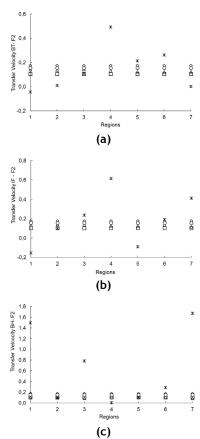


Figure 4: Transfer velocity calculated at regions (a) between buildings (BT); (b) in front of a building (IF) and (c) behind a building (BH) at a height of  $z/h_m$ =1 for source 2. (\*) represents the average transfer velocity on repeated units using LES data; represents the parametrization of ( $\Delta$ ) SOULHAC01; ( $\diamond$ )SOULHAC02; ( $\Box$ ) B&B01 and (o) B & B02

In general, the parameterizations do not present significant deviations if the averages of  $U_T$  for the entire canopy are considered. However, the deviations are occasionally considerable especially in regions where the advective flow is important. This can lead to a considerable overestimation or underestimation of the concentration values within the urban canopy predicted by practical models, such as the street network models (SOULHAC et al., 2011).

#### **CONCLUSIONS**

The parametrizations produce results closer to the velocities calculated using the LES data for the region between buildings. In the region behind the buildings, the values are the ones that are more distant from the parametrizations. It is important to note that the parameterization of Soulhac et al. (2011) has certain limitations as to formulation. One

is the hypothesis that canopy flows are dominated by turbulent effects and that advective effects can be neglected. However, in this work it was verified that for a group of buildings with different heights, the mass flow of the scalar through the surface located at a mean height of the buildings, both advective and turbulent effects, are important. It can be concluded that this parameterization should be used with caveats in the cases of urban regions with buildings with different heights.

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## BUILDING AN INTEGRATED MANAGEMENT SYSTEM FOR AIR QUALITY IN BOGOTA, COLOMBIA

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Abstract: Bogota is one of the most polluted cities in Latin America. Of particular concern is air pollution because of its impact on public health and ecosystem deterioration. The cause of the problem is the dense industrial, commercial, and vehicular activity necessary to support a population of nine million. With the objective of abating air pollution in the city, Bogota's environmental agency, SDA, teamed up with academic researchers and implemented an air quality modeling system in 2012. The model was able to characterize spatial and temporal gradients of pollutants, but model estimates were relatively high biased for PM10, CO, NOx, and SO2. In a subsequent exercise in 2014, emission levels were adjusted and modeling parameters were optimized. An adjustment factor for resuspended particulate matter was applied considering precipitation, humidity, land use, and a transport factor. As a result of these changes, modeling results in 2014 performed better than 2012. Spatial and temporal fields for PM10 were used to assess health outcomes and economic costs. The air quality model is widely used by SDA to understand air pollution in the city and design abatement plans. The emission-concentration-health impact management system is unique in the country.

Keywords: air quality modeling, emission sources, health outcomes, Bogota.



### SIMULATION OF GAS DISPERSION RELEASED BY THE ACCIDENT WITH THE SPACEX FALCON 9 ROCKET AT CAPE CANAVERAL

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#### Abstract:

This study consists of a qualitative analysis of the accident with the SpaceX Falcon 9 rocket during a test on a launch pad at Cape Canaveral Air Force Station on Thursday, Sept. 1<sup>st</sup>, 2016. This kind of event does not occur very frequently, therefore, it is important to verify the impact on the environment through weather and air quality modeling. Thus, the main objective was to apply Weather Research and Forecasting (WRF), Model for Simulating the Rocket Exhaust Dispersion (MSRED), Community Multi-scale Air Quality (CMAQ) modeling system to simulate the dispersion of the contaminants emitted during a situation of explosion of rocket launching for environmental management. The results showed that the modeling system captured the phenomena well.

Keywords: MSRED, CMAQ, WRF, air quality modeling, explosion of rocket launching.

#### **INTRODUCTION**

SpaceX's Falcon 9 rocket exploded on the launch pad at Cape Canaveral, Florida, around 13:07 GMT, Sept. 1st, 2016. The explosion occurred during the preparation for the static fire test of the rocket's engines. This kind of event does not occur very frequently, therefore, it is important to verify the impact on the environment through weather and air quality modeling. Thus, this study simulated the launch of a rocket in an explosion situation in the Cape Canaveral region, through the application of the MSRED and CMAQ models.

The MSRED is based on a semi analytical three dimensional solution of the advection-diffusion equation, incorporating a modern three dimensional parameterization of the atmospheric turbulence, designed to simulate the formation, rise, expansion, stabilization and dispersion of rocket exhaust clouds for short range assessment, being able to directly read meteorological data from the *Weather Research* and *Forecasting* (WRF) model output. And, for the long range and chemical transport modeling, the MSRED was built to be integrated to the CMAQ model, by generating a ready-to-use initial conditions file to be input to CMAQ (Nascimento, 2016; Skamarock *et al.*, 2008; Byun and Schere, 2006).

#### **METHODS**

This study was divided in two parts. In the first part, the meteorological modeling of the event was performed using the WRF model for a domain configuration with 3 domains with horizontal resolution of 9km, 3km and 1km, and horizontal dimensions in grid cells of 63x63, 96x96 and 144x144, for domains 1 to 3, respectively (see Figure 1). The innermost domain was used to

model a hypothetical aborted rocket launch event in Cape Canaveral Air Force Station (CCAFS), in an explosion situation. These domains were modeled in a one-day simulation (Sept. 1<sup>st</sup>, 2016). For WRF initialization, data from the National Centers for Environmental Prediction (NCEP) Final Analysis (FNL) with 0.25° resolution was used.

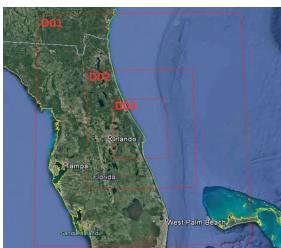


Figure 1. Localization and distribution of the domains in the WRF modeling

Regarding the physical parameterizations of the model, the National Aeronautics and Space Administration (NASA) uses the WRF model with the Lin microphysical scheme and the Yonsei University planetary boundary layer scheme, with a triple-nested grid configuration over KSC/CCAFS (Shafer and Watson, 2015). Therefore, these settings were also used in this work.



In the second part, after the meteorological modeling stage has been performed, the formation, dispersion and chemical transport modeling of the pollutant exhaust cloud were carried out using the MSRED for the short-range evaluation and the CMAQ for the long-range assessment of the impact of the exhaust cloud released by the explosion of the rocket during the accident episode.

The WRF model output data were analyzed by the Integrated Data Viewer (IDV), version 5.3, while the CMAQ output data were analyzed by the R software package (IDV, 2016; R Core Team, 2017).

For the accomplishment of this case study, information and data about the rocket and the accident were sought, such as, amount of material burned, time of burning, compounds present in the explosion effluents etc., but without success. Thus, it was decided to carry out this study using data from the launching of the *Veículo Lançador de Satélites* (VLS, which in Portuguese means *Satellite Launcher Vehicle*), derived from the work of Nascimento (2016), for the location of Cape Canaveral, in an explosion situation. As there is no monitoring data available to confront the modeling results, a qualitative evaluation of the event was carried out.

#### FINDINGS AND ARGUMENT

Figure 2 illustrates the vertical profile of the wind direction at 14:00h GMT, one hour after the explosion. The red line corresponds to planetary boundary layer height (PBLH).

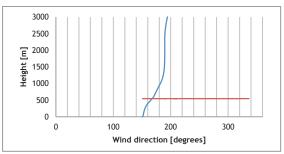


Figure 2. Wind direction vertical profile [degrees] at 14:00h GMT. The red line corresponds to PBLH.

Figure 3 illustrates a frame of the explosion event at Cape Canaveral captured by RadarScope Pro and Figure 4 shows the concentration of CO at 9m height, in an interval of 20 min after the first hour of the launch.



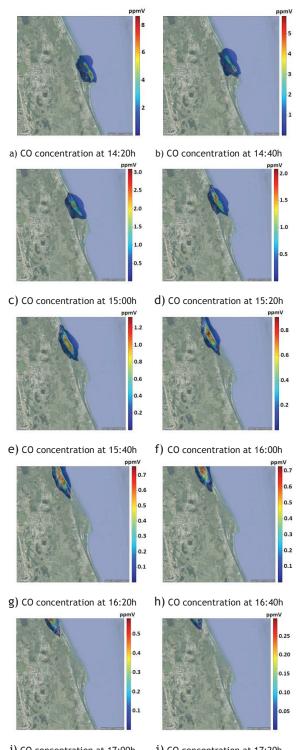
Figure 3. Event of explosion captured by RadarScope Pro (one hour after launch)

The atmospheric stability evaluated at the time of the explosion as well as during the burning time (1 hour), using the Monin-Obukhov similarity theory, was neutral. After completion of the burning time at 2:00 p.m., the atmospheric stability has changed to unstable, which provides a strong vertical mixture of pollutants, high levels of turbulence and an intense dispersion of the contaminants in the atmosphere, which is consistent with the behavior of the plume presented in Figure 4.

By comparing the behavior of the simulated plume (Figure 4) with that of the RadarScope Pro video (Figure 3), it was observed that the MSRED/CMAQ model captured the phenomenon well, however, it was possible to identify some differences.

First, the simulated plume followed along the coast, while the video portrayed by RadarScope Pro showed that, after following the coast line for one hour after launch, while there is still burning, it turned right to the ocean. This can be explained due to two factors. First, the radar did not record the entire duration of the simulated event. Second, the radar is only capable of recording the entire column of clouds, i.e. the curve that the cloud makes may have occurred at higher levels. This can be observed in Figure 2, which shows that the wind near the surface blows from the southeast direction, changing its direction to southwest as it rises above the boundary layer. Therefore, the WRF model was able to simulate the vertical profile of the wind direction accordingly. The MSRED model takes into account all the portion of the exhaust cloud that is inside the boundary layer, since it is the region where there is the greatest atmospheric turbulence and the greatest interest in studying, because it is where human beings live. Thus, this behavior of the vertical profile of the wind direction, and consequently of the plume, would only be noticed if it would happened inside the boundary layer.





i) CO concentration at 17:20h
 j) CO concentration at 17:20h
 Figure 4. CO concentration at 9m for each time step after the first hour of the launch

Second, the plume's shape presents a tail extension, which does not appear in the simulation. As at 14:00 GMT there is no more burning and the pollutant cloud is being scattered

and transported along the coast, which is consistent with the observed and simulated wind direction, the concentration of CO decreases as the cloud is transported.

#### **CONCLUSIONS**

In this work, the main objective was to apply WRF/MSRED/CMAQ modeling system to simulate the dispersion of the contaminants emitted during a situation of explosion of rocket launching for environmental management. Comparing the behavior of the simulated plume (Figure 4) with that of the RadarScope Pro video (Figure 3), it was concluded that the modeling system captured the phenomena well.

#### **ACKNOWLEDGEMENTS**

The authors acknowledge the Supercomputing Center for Industrial Innovation (Yemoja), the Foundation for Research Support of the State of Bahia (FAPESB) and also to the Coordination for the Improvement of Higher Education Personnel (CAPES) for granting the doctoral scholarship to the first author.

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## ESTIMATE OF PM<sub>10</sub> EMISSIONS DUE TO WIND OVER CONSTRUCTION SITE OF VITORIA AIRPORT-ES AND SIMULATION OF THE IMPACTS ON AIR QUALITY THROUGH MATHEMATICAL MODELING

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Abstract: Heavy civil construction has a potential to deteriorate air quality and wind incidence over construction sites can generate significant  $PM_{10}$  emissions, which indicates a necessity for emission control to minimize particle dispersion (wind dragging). In order to estimate  $PM_{10}$  emissions from Eurico de Aguiar Salles Airport expansion construction and evaluate their impacts on air quality, particulate emissions were estimated by using a methodology proposed by United States Environmental Protection Agency in 2006. Three different scenarios were defined: one in which no emission control was considered; second scenario with application of water every 3.2-hour to disturbed areas and a third scenario with 2.1-hour watering interval. Using AERMOD dispersion modeling, each emission scenario was simulated to analyze evolution of pollution plume over Vitoria and compare to Air Quality Standards (120  $\mu g/m^3$  - 24-hour mean) established in the State Decree 3463-R/2013 which is the current legislation in the study area. Both Scenario 1 and 2 infringed the threshold determinated by the Decree reaching  $PM_{10}$  concentrations of  $436\mu g/m^3$  e  $169~\mu g/m^3$ , respectively, whereas maximum modeled concentration in the Scenario 3 presented lower than  $120\mu g/m^3$ , meeting concentration of  $113~\mu g/m^3$ . Therefore, environmental benefits promoted by improving air quality in the regions close to the construction site when the use of emission control was intensified have noticed.

Keywords: Wind Erosion, Air quality, PM<sub>10</sub>, Wet supression, Vitoria.

#### **INTRODUCTION**

Heavy civil construction is a dust emission source which can cause a temporary impact, nonetheless significant on the local air quality that could be associated with deforestation, drilling, blast, land excavation and earthmoving operations (USEPA, 1995). The main impacts on the air quality which may occur during construction activities are visible dust plumes, promoting inconvenience as sedimentable dust, besides the health hazards due to increments of  $PM_{10}$  in the atmosphere. (Cheminfo, 2005). The amount of dust emitted from construction activities is related to exposure areas to wind and precipitation. Owing to weather variability, it is impossible to predict what climate conditions will take place when specific construction activity is being performed (Holman et al, 2014).

Thus, this paper aims evaluate the different impacts caused by emission sources, located in the Vitoria airport expansion construction and subject to wind erosion, through air quality modeling by considering distinct PM<sub>10</sub> emission control.

#### METHODS Study Area

The study area includes Vitória city, capital of the Espírito Santo state, where airport expansion construction are located. Figure 1 illustrates the study area as well as typical wind rose for Vitória,

which presents prevalence of north-northeast winds.

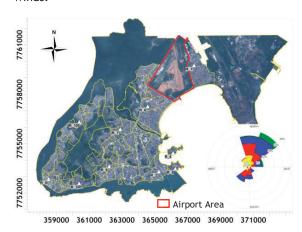


Figure 1. Study Area

#### **Wind Data**

Particle emission from exposure areas subject to wind erosion is strongly influenced by predominant wind velocity and direction. Calm wind tends to cause zero or low emission while strong winds leads to high emissions, which can affect air quality in surroundings areas to the source negatively. Therefore, according to the calculation approach, hourly gust wind speeds recorded during the period September 1<sup>st</sup>, 2016 to September, 30<sup>th</sup>, 2016 at the meteorological station Vitória-A612



owned by National Institute of Meteorology were considered.

#### **Emission Inventory**

Particle emissions induced by wind over mixtures erodible and non-erodible surface materials subject to disturbances can be expressed in unit of grams per meter square (g/m²) per hour (USEPA, 2006) by the following equation:

Emission factor = 
$$k \sum_{i=1}^{N} Pi$$
 (Eq.1)

#### Where:

k = particle size multiplier (0.5 for PM10) N = number of disturbances per hour Pi = erosion potential corresponding to the observed (or probable) fastest mile of wind for the i<sub>th</sub> period between disturbances, g/m<sup>2</sup>.

A field study from Midwest Research Institute (MRI) contracted by USEPA (2001) noticed that application of water, in various intervals, over exposure areas inside construction sites, results in high efficiency level of  $PM_{10}$  control. These watering intervals were used in this paper.

#### Air Quality Model

Emission rates as well as physical features of the sources were entered into an air quality model, AERMOD View® version 9.1.0. Three 24-hour simulations were run:

- Scenario 1: No emission control in disturbed areas within construction site was considered:
- Scenario 2: Application of water every 3.2hour to disturbed areas within construction site;
- Scenario 3: Application of water every 2.1hour to disturbed areas within construction

#### **RESULTS**

After usage of Equation 1 in order to quantify emission rates for each scenario, average efficiency of  $PM_{10}$  emission control can reach 61% for 3.2-hour watering interval and 74% for 2.1-hour watering interval (Table 1).

Table 1. Calculated PM<sub>10</sub> Emission Data

Exposure area	1,458,153.3 m <sup>2</sup>	
Number of disturbances in the month	37 hours	
PM <sub>10</sub> Emission considering no Control	94.4 t/month	
PM <sub>10</sub> Emission considering 3.2-hour watering interval	36.8 t/month	
PM <sub>10</sub> Emissions considering 2.1-hour watering interval	24.5 t/month	

Figures 2, 3 and 4 present modeled concentrations by using AERMOD for the scenarios 1, 2 and 3, respectively. All scenarios were compared to Air Quality Standards (AQS) for 24-hour (120  $\mu g/m^3$ ), current standard established by the State Decree 3463-R/2013.

Considering the airport as reference, southwestern region of study area is always more affected by emissions from all three scenarios analyzed. The greatest impact is noticed in the scenario 1 (no control), following by scenario 2. Both scenarios reported infringements of AQS.

Scenario 3 is a single in which no infringements of  $120 \,\mu\text{g/m}^3$  occurred.

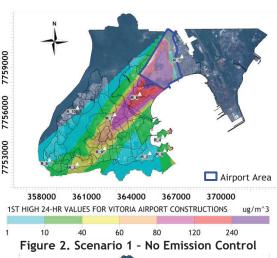


Figure 2. Scenario 1 - No Emission Control

Airport Area

358000 361000 364000 367000 370000

1ST HIGH 24-HR VALUES FOR VITORIA AIRPORT CONSTRUCTIONS ug/m^3

Figure 3. Scenario 2 - 3.2-hour Watering Interval



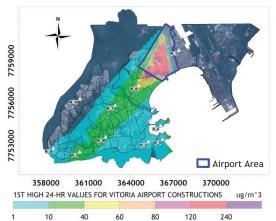


Figure 4. Scenario 3 - 2.1-hour Watering Interval

In addition, 10 points were selected in the study region (Figure 5) in order to analyze the intercomparison in each point of mitigatory effects due to water application on exposure areas in the Vitoria airport construction site. Especially over R6, lack of mitigation of dust emissions causing deterioration of air quality is evident.

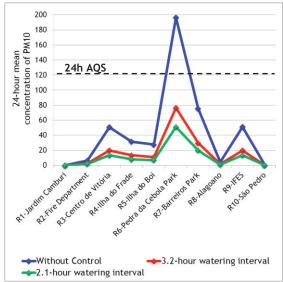


Figure 5. Effects of Water Application on Air Quality

#### CONCLUSIONS

Regarding to the acquisition of efficiency of  $PM_{10}$  emission control due to application of water on exposure areas located in the civil construction site. This study determined a significant decrease in the  $PM_{10}$  emissions, above 50%, and, consequently, a high positive impact on air quality, mainly for the scenario considering 2.1 hour watering interval, for which modeled concentrations by AERMOD did not exceed the Air Quality Standard of 120  $\mu g/m^3$  for 24-hour mean, established by the State Decree 3463-R/2013.

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## Modeling the Air Quality and Public Health Benefits of Increased Residential InsulationImpacts of Multiple Source Sectors in the United States through Sensitivity Approaches

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To address the continuous lowering of the health-based air quality standards and identify efficient emissions control measures, there is a need to understand the relative contributions to air quality and health from individual source sectors. We used the Community Multiscale Air Quality (CMAQ) model instrumented with the Decoupled Direct Method (DDM), an advanced sensitivity analysis technique that allows us to estimate the influence of individual pollutants from individual sources or regions. We specifically focused on three individual source sectors – residential combustion, electric generating units and aircraft emissions. We considered direct residential combustion by state, leveraging Census and housing start data to determine spatial patterns of emissions within states, and modeled individual power plants in geographic groupings using a design of experiments that allow us to estimate the impacts for all major power plants on the grid. In addition, we also modeled each of the major airports in the U.S. We then estimated sensitivities of state-specific O3 and PM2.5 – key drivers of monetized health impacts - to individual precursor emissions. As CMAQ provides concentration estimates by grid cell, we were able to determine total public health benefits in terms of avoided mortality and morbidity (using BenMAP-CE) as well as the distribution of those benefits for directly modeled facilities and locations. A key outcome of this study was assessing the carbon reductions and health cobenefits from increased residential energy efficiency measures. We will present results from this study focusing on CMAQ and BenMAP-CE results quantifying the air quality and health benefits associated with reduced residential heating and electricity generation from individual states and/or regions in the U.S. and further illustrate how the results from this approach can be used to develop damage functions across various emissions sectors for individual precursors for developing policy options.



# POLLUTANTS DISPERSION SIMULATION CONSIDERING DATA SIMULATED BY WRF MODEL USING MELLOR-YAMADA-JANJIC SCHEME AND BY LES-PALM MODEL, CONSIDERING THE WIND MEANDERING PHENOMENON

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Abstract: The aim of this work is evaluate the behavior of the pollutant plume in the region where the INEL (USA) experiment was released considering the wind meandering phenomenon. We utilize the WRF and LES models and 3D-GILTT Technique. The INEL experiment consists of a diffusive test series that was conducted in a flat and uniform terrain under stable and low wind atmospheric conditions. The physics option of the Planetary Boundary Layer (PBL) used in WRF model was Mellor-Yamada-Janjic Scheme (MYJ). The potential temperature profiles and heat fluxes generated by the WRF (Weather Research and Forecasting) model will be used as initial conditions to the LES-PALM (Large-Eddy Simulation-Parallelized) model. PALM is referred as a model to Large Eddy Simulation (LES) to atmospheric and oceanic fluxes that is destined to parallel computer architectures. The horizontal wind generated by LES-PALM model will be used as initial conditions to the dispersion model based in the 3D-GILTT (3D Generalized Integral Laplace Transform Technique) technique that analytically solve the advection-diffusion equation. This technique of the integral transform combines a series expansion with an integration. In the expansion, is used a trigonometric base determined with the help of a Sturm- Liouville auxiliary problem. The integration is made in all range of the transformed variable, making use of the orthogonality property of the base used in the expansion. The resultant ordinary differential equations system is analytically solved using the Laplace transform and diagonalization. The pollutant plume is simulated of satisfactory way, with maximum concentration in the source, decreasing radially to away.

Keywords: Air Pollution, WRF, LES, Advection-diffusion equation, 3D-GILTT Technique.

#### **INTRODUCTION**

In many times, in stable conditions in the Planetary Boundary Layer (PBL), in such situations that the mean wind velocity present low magnitude (V < 1.5 m/s), are observed low frequency oscillations of the horizontal wind [Anfossi et al., 2005]. These directional oscillations of the horizontal wind are known as wind meandering phenomenon. In general we observe two criterias to consider the occurrence of the wind meandering. The first is to verify the existence of negative lobules in autocorrelation function and the second one is the ratio (in module) between the adjustment parameters is greater than or equal to one.

In general, the eulerian dispersion models consider that the mean wind is dominant in the x direction and not consider the v wind component [Buske et al., 2007]. In situations where the wind meandering is present, the u and v wind component must be considered.

The INEL experiment [Sagendorf and Dickson, 1974] consists of a diffusive test series that was conducted in a flat and uniform terrain under stable and low wind atmospheric conditions.

#### **METHODS**

We made simulations with WRF (Weather Research and Forecasting Model) model to the region were the INEL experiment was realized to each test (Table 1). The potential temperature profiles and heat fluxes generated by WRF model were utilized to run the LES-PALM (Large-Eddy Simulation-Parallelized) model [Raasch, 2017]. The horizontal wind field simulated by LES-PALM model was used to run the dispersion model based in the solution of the advection-diffusion equation.

The data used to run the WRF model are reanalysis 1 of the NCEP/NCAR. We are working with 3 nested grids and we will to consider data of the domain 3 to run the LES-PALM model. In the Figure 1 we can see the grids configuration that we are using in the WRF model.



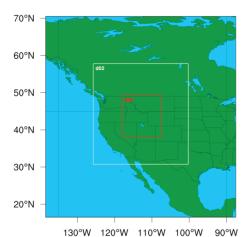


Figure 1. The grids configuration used in the WRF model

In the Table 1 we can see all tests of the INEL experiment with the date of realization. The physics option of the PBL used in WRF model was Mellor-Yamada-Janjic Scheme (MYJ) [Janjic, 1994].

Table 1. Tests of the INEL experiment

Table 1, Tests of the INCL experiment		
Time/MST(-7)	Date	
0642-0742	02/07/1974	
0630-0730	02/08/1974	
0646-0746	02/09/1974	
0630-0730	02/12/1974	
0630-0730	02/21/1974	
0530-0630	03/21/1974	
0458-0547	04/17/1974	
0146-0246	04/30/1974	
0411-0511	04/30/1974	
0422-0522	05/03/1974	
0345-0445	05/22/1974	
	Time/MST(-7) 0642-0742 0630-0730 0646-0746 0630-0730 0630-0730 0530-0630 0458-0547 0146-0246 0411-0511 0422-0522	

The parameterized advection-diffusion equation

[Blackadar, 1997] can be written as
$$\bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z}$$

$$= \frac{\partial}{\partial x} \left( K_x \frac{\partial \bar{c}}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial \bar{c}}{\partial y} \right)$$

$$+ \frac{\partial}{\partial z} \left( K_z \frac{\partial \bar{c}}{\partial z} \right) \tag{1}$$

Assuming that the velocity w is zero and that the eddy diffusivity has only dependence in the z

direction 
$$(K'_{y} = 0)$$
, the equation (1) is written as
$$-\bar{u}\frac{\partial \bar{c}(x,y,z)}{\partial x} - \bar{v}\frac{\partial \bar{c}(x,y,z)}{\partial y} + \frac{\partial}{\partial x}\left(K_{x}\frac{\partial \bar{c}(x,y,z)}{\partial x}\right) + K_{y}\frac{\partial^{2}\bar{c}(x,y,z)}{\partial y^{2}} + \frac{\partial}{\partial z}\left(K_{z}\frac{\partial \bar{c}(x,y,z)}{\partial z}\right) = 0$$
(2)

The equation (2) is solved by 3D-GILTT technique (3D-Generalized Integral Laplace Transform Technique) [Buske et al., 2007, Moreira et al., 2009]. This technique of the integral transform combines a serial expansion with one integration. In the expansion, is used a trigonometric base determined with the help of an auxiliary problem of Sturm-Liouville. The integration is made in all range of the transformed variable, by to make use of the orthogonality property of the base used in the expansion. The resultant ordinary differential equation system is analytically solved using the Laplace transform and diagonalization. The eddy diffusivities were parameterized following [Degrazia et al., 1996].

#### FINDINGS AND ARGUMENT

The Figure 2 shown the vertical profiles of potential temperature simulated by WRF model to the domain 3 for each tests of the Table 1. These profiles are typical of stable atmospheric conditions.

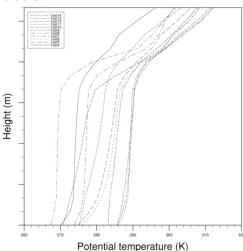


Figure 2. Vertical profiles of potential temperature simulated by WRF model.

For simplicity reason only results to the test 14 are shown. The results to the others tests are similarly to these. The Figures 3 and 4 shown the autocorrelation function calculated with base in the u and v wind components simulated by LES model, where we can observe the negative lobule. The rate (in module) between the adjustment parameters of the u wind component proposed by Frankiel is 2.169583 and the proposed by Degrazia is 2.786426 and the adjustment parameters of the v wind component proposed by Frankiel is 2.323922 and the proposed by Degrazia is 3.199611.

The pollutants concentration determined trough the techniques describes above is showed in the Figure 5 and we can see the opening of the plume pollutants. Therefore, the hierarchy of the models



above is able to simulate the pollutants plume in a satisfactory way.

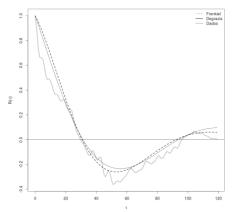


Figure 3. Autocorrelation function calculated with the u wind component simulated by LES model.

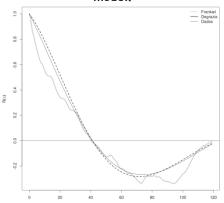


Figure 4. Autocorrelation function calculated with the v wind component simulated by LES model.

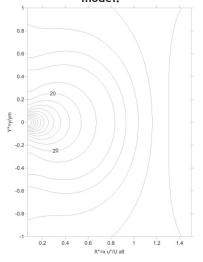


Figure 5. The simulated pollutant plume by applying the 3D-GILTT technique in the advection-diffusion equation.

#### **CONCLUSIONS**

The pollutants plume was simulated in a satisfactory way, the potential temperature profiles simulated by WRF present the stability condition of the INEL experiment.

The autocorrelation function shows the characteristics to the occurrence of the wind meandering phenomenon, through the negative lobules and the ratio of the adjustment parameters greater than or equal to one.

The pollutants plume shown the expected results, with the maximum concentration in the source, decreasing radially to away. To use the potential temperature profiles from of mesoscale models is a very useful tool in the evaluation of the air quality of a determined region.

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## ASSESSMENT OF THE IMPACT OF NO<sub>X</sub> AND SO<sub>2</sub> EMISSIONS FROM STACKS IN CAMAÇARI INDUSTRIAL COMPLEX OVER THE METROPOLITAN REGION OF SALVADOR CITY.

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Abstract: Considering the fact that the exposure to polluted air has been associated with adverse health effects (WHO, 2016), it is important to look into the air pollution in urban areas. To evaluate the impact of emissions on the air quality in the Metropolitan Region of Salvador (RMS) in the Northeast region of Brazil, simulations using the Weather Research and Forecasting-Community Multiscale Air Quality (WRF-CMAQ) model were applied. The region's choice was due to the lack of scientific studies about air quality and air pollution dispersion, especially using WRF-CMAQ. The aim of this work was to assess the impact of atmospheric pollutants (NO<sub>x</sub> and SO<sub>2</sub>) from stacks held in Camaçari Industrial Complex over the RMS. The emissions rates were based on another study since there is no inventory made for the region. Since there were no pollutant measurement data to be compared, a qualitative analysis was done. The stacks emissions rates were considered constant, hence the variation in the pollutant concentration were due uniquely to the meteorological conditions. The highest concentrations occurred near the sources, and when the atmospheric stability changed, which influenced in the concentration, regardless of the pollutant. Further, the change in the wind direction led the plume of contaminants reach different regions around the RMS.

Keywords: air quality, dispersion, modelling, Salvador, Bahia, WRF, CMAQ.

#### **INTRODUCTION**

The RMS is an urban-industrial area, and is formed by 13 cities, being Salvador the major city and also the capital of the state of Bahia (Figure 1). The economic activities are based on tourism, commerce and a huge petrochemical complex, including a Petrobrás refinery. The choice of this region was due to its growing industrialization and urbanization, leading to potential transformations in the environmental conditions, besides the fact that there is no previous work performing any assessment in this area using WRF-CMAQ modeling system.

The petroleum industry converts crude oil into more than 2500 refined products, employing a wide variety of processes (US EPA, 2017). In each of these processes, air pollution emissions are involved. The volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs), nitrogen oxides (NO $_{\rm x}$ ), sulfur dioxide (SO $_{\rm z}$ ), methane (CH $_{\rm 4}$ ), and particulate matter (PM) are considered as the common contaminants from oil-gas sector emissions (Xu and Chen, 2016).

Therefore, this work presents a hypothetical case study which aims to evaluate the impact of atmospheric pollutants ( $NO_x$  and  $SO_2$ ) from stacks held in Camaçari Industrial Complex over the RMS, in order to provide some scientific background about the impact of local anthropogenic emissions.

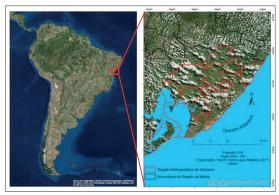


Figure 1: The location of the RMS in Brazil (left) and in Bahia State (right).

#### **METHODS**

The study was carried out using the Weather Research and Forecasting (WRF) model (Skamarock et al., 2008) v3.6.1 to simulate the meteorological fields and the Community Multiscale Air Quality (CMAQ) model (Byun and Schere, 2006) v5.0.2 to simulate the chemical transport of the target pollutants.

The WRF model was configured with 3 nested domains with grid resolutions of 9, 3 and 1 km, respectively. WRF meteorological input data came from National Centers for Environmental Prediction (NCEP) Final Analysis (FNL) at 0.25° resolution while the land use data were provided by United States Geological Survey (USGS) at 5 min, 2 min and 30 s resolutions. The physics options are listed in Table 1.



Table 1. Major physics options.

Options		
Boundary Layer	MYNN2.5	
Microphysics	Kessler scheme	
Longwave radiation	RRTM scheme	
Shortwave radiation	Dudhia scheme	
Land-surface option	Noah scheme	

24h spin-up time was used to obtain realistic initial conditions. Simulations were performed during March 20<sup>th</sup> to 26<sup>th</sup> 2016. Overall this period was the end of summer and the beginning of autumn, characterized by hot and dry weather conditions, wherein temperatures ranged between 24°C-33°C.

Emissions inventory has not yet been developed for RMS, for this reason this work was built on Lyra (2008) who estimated the emission rates of  $\mathrm{SO}_2$  and  $\mathrm{NO}_x$  based on the amount of fuel consumed in the industrial complex of Camaçari and the US EPA emission factors, considering just some emissions sources located in the region

Carpenter and Nokleby (2012) carried out  $NO_x$  instack measurements for various combustion sources and showed that the  $NO_2$  average was of 0.05 (5%). AP-42 (US EPA, 2017) also revealed that for most external fossil fuel combustion systems, over 95% of the emitted  $NO_x$  is in the form of NO. Thereby the chemical speciation of  $NO_x$  in this work was of: 95% NO and 5%  $NO_2$ .

The emissions rates calculated by Lyra (2008) were processed by SMOKE. No initial and boundary conditions were applied. The CMAQ plots were made using R software packages (R Core Team, 2017), the wind rose plots were generated by VSQA software (Vitória Software, 2017), and are shown in the next section

#### FINDINGS AND ARGUMENT

The results of the air quality simulations are closely related to WRF performance. Since the stacks emissions rates were considered constant, the changes in the concentrations over time are primarily due to meteorological conditions.

In this way, to evaluate the chemical transport of NO,  $NO_2$  and  $SO_2$ , the planetary boundary layer height (PBLH) (Figure 2), and the Monin-Obukhov length were checked in order to observe the hourly variation generated by the atmospheric turbulence, which was responsible for the pollutants diffusion.

Temperature at 2 m and the wind speed and direction at 10 m are also presented in Figure 3 and 4 for the purpose of comparing the observed and simulated data. One can note that the simulation were underestimated, and the observed wind direction came chiefly from the southeast (Figure

4-a), while the simulated data had some variations coming from east (Figure 4-b).

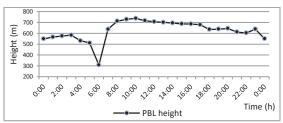


Figure 2: Hourly variation of the PBLH simulated by WRF.

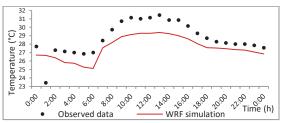


Figure 3: Mean hourly temperature at 2 m above surface at Airport station.

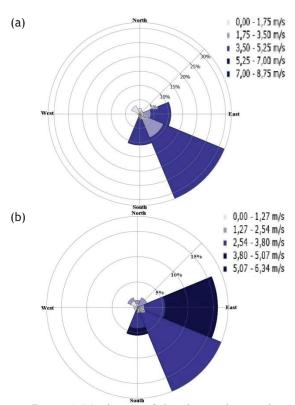


Figure 4: Wind roses of the observed (a) and simulated (b) data at Airport station.

Figure 5 shows NO,  $NO_2$  and  $SO_2$  concentrations at first level (approximately 10 m), on March  $22^{nd}$  and  $23^{rd}$ , at 10:00 GMT (7 a.m. local time). The time selection was made by examining the PBLH (shown



in Figure 2) and the Monin-Obukhov length, which revealed when occurred the changing in the atmospheric stability, passing from stable to unstable condition. The choice of these both dates is related to the fact that for the other simulated days the behavior of the plume was similar to day 22<sup>nd</sup>, changing only the concentration values, except on 23<sup>rd</sup> when there was a change in the wind direction. It can be noticed in Figure 5 that the change in the wind direction impacted in different regions of the State of Bahia. Most of the days (20-22 and 24-26), the plume reached Dias d'Ávila e São Sebastião do Passé cities. However, on March 23<sup>rd</sup>, the wind direction changed and got cities like Camaçari, Simões Filho, Salvador, Vera Cruz and Itaparica.

Figure 5 also indicated that the highest concentrations occurred near the sources. And, regardless of the pollutant, the plume presented the same behavior.

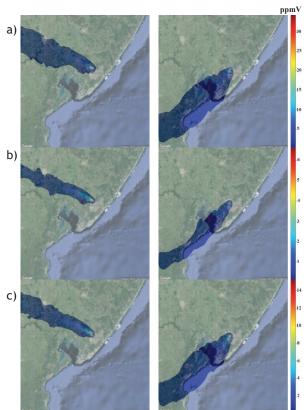


Figure 5: NO (a), NO<sub>2</sub> (b) and SO<sub>2</sub> (c) concentrations on  $22^{nd}$  March (left) and on  $23^{rd}$  March (right) at 10 meters at 10:00 GMT.

#### **CONCLUSIONS**

The main purpose of this work was to apply WRF-CMAQ to assess qualitatively the dispersion of the atmospheric pollutants ( $NO_x$  and  $SO_2$ ) from stacks located at Camaçari Industrial Complex in the RMS. Notwithstanding it was an hypothetical case study,

this work was a first step towards providing background to new studies about the impact of local anthropogenic emissions on the air quality. It is evident that the construction of a proper emissions inventory is needed since some difficulties were faced due to the lack of information about the emissions sources of the region. For future works it is recommended the development of a full inventory for the whole region in order to allow an analysis of the local air quality, and moreover to relate the air pollution with adverse population health events.

#### **ACKNOWLEDGMENTS**

The authors thank the Supercomputing Center for Industrial Innovation (Yemoja), the Fundação de Amparo à Pesquisa do Estado da Bahia (FAPESB) and also to the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for granting the master scholarship to the first author.

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## CONTRIBUTION OF CAPUAVA PETROCHEMICAL COMPLEX EMISSIONS TO OZONE AIR QUALITY IN THE METROPOLITAN AREA OF SÃO PAULO AND GREAT ABC REGION

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Abstract: The aim of this work is to study how emissions from mobile and industrial sources are influencing the formation and dispersion of tropospheric ozone in the Great ABC Region and in neighboring regions, through the use of photochemical model of air quality CIT (Caltech Institute Technology), simulating three scenarios: (i) Scenario 1: mobile sources; (ii) Scenario 2: industrial sources; (iii) Scenario 3: both sources, enabling a separate analysis of the contribution of each source. Results demonstrated that breeze circulation of the Great ABC Region causing the region to export its pollutants and precursors to the northwest region of the Metropolitan Area of São Paulo.

Keywords: tropospheric ozone, photochemical model, air pollution, Great ABC Region.

#### INTRODUCTION

The problem of air pollution by ozone  $(O_3)$  is recurrent around the world, Molina et al. (2006) analysed the air quality situation in nine urban centers around the world (Beijing, China, Bogotá, Colombia, Cairo, Egypt, Delhi, India, Metropolitan Region of Los Angeles, United States, Central Region of Ontario, Canada, Region Metropolitan of Mexico, Mexico, Santiago, Chile and São Paulo, Brazil), considering cities of developed and/or developing countries. Most of the urban centers studied have exceeded the standard adopted for maximum concentrations of  $O_3$ , Beijing for example, reached a maximum concentration greater than double the standard.

According to the air quality monitoring data held by CETESB (Environmental Company of São Paulo State), even with the National Program for Control of Air Pollution from Motor Vehicles (PROCONVE), the  $O_3$  concentrations in the Metropolitan Area of São Paulo (MASP) and Great ABC Region have shown a growing annual increase in the number of standard exceedances of air quality (160  $\mu$ g/m³ or 80 ppb of  $O_3$  in 1 hour) and attention level (200  $\mu$ g/m³ or 100 ppb of  $O_3$  in 1 hour), established by Resolution CONAMA n° 3/1990. According the State Decree n° 52469/07 which defines concepts of saturation of atmospheric pollutants in a given region and instructs the environmental licensing the study area has severe saturation of  $O_3$ .

In complex areas, such as urban areas, with a variety of industrial and mobile sources, the use of atmospheric modelling is recommended to describe and predict the effect of pollution. Photochemical models are used to describe the formation chemistry of secondary pollutants, specifically  $O_3$  and fine particles, it is also possible to predict air

quality, to characterize advection and diffusion transport, to analyze impacts and strategies to control emissions in the atmosphere to develop reliable emission inventories

In this context, the main objective of this work was to simulate the contribution to Capuava Petrochemical Complex to  $O_3$  air quality in the MASP and Great ABC Region using the photochemical model of air quality Caltech Institute Technology (CIT). In order to reach the objective of this work, simulation scenarios were made, considering: (i) Scenario 1: mobile sources; (ii) Scenario 2: industrial sources; (iii) Scenario 3: both sources.

The chosen period for simulation was from September, 28 to October 1, 2011. The criteria for selection were: (i) period between annual increases in the quality standard for  $O_3$  in the Grande ABC Region; (ii) high temperatures; (iii) low relative humidity; (iv) high concentrations of  $O_3$  in the Great ABC Region measured by CETESB monitoring stations; (v) availability of data from CETESB monitoring stations.

#### METHODS Study area

The Great ABC Region is located in the southeast sub-region of the MASP. It has regional boundaries with the municipalities of Mogi das Cruzes, Suzano, Ferraz de Vasconcelos, São Paulo and the cities of Baixada Santista (Figure 1). With a population of about 2.7 million inhabitants in an area of 828 km².

The Great ABC Region comprises the cities of Santo André, São Bernardo do Campo, São Caetano do Sul (although they are not part of the original acronym, the municipalities of Mauá, Ribeirão



Pires, Rio Grande da Serra and Diadema are also part of the region).

In the city of São Paulo, a large part of the emissions of air pollutants is due to the immense fleet of motor vehicles (of different ages), running with the most diverse types of fuels (ethanol, gasoline, diesel, NGV, diesel/biodiesel mixture). In 2011 there were around 12 million vehicles, the car fleet was responsible for 97% of the emissions of carbon monoxide (CO), 77% of hydrocarbon (HC), 80% of nitrogen oxides (NO<sub>x</sub>), 37% of sulfur dioxide (SO<sub>2</sub>) and 40% of particulate material (PM).

Figura 1. MASP, with emphasis on Great ABC Region.



The Great ABC Region has singularities because in addition to a significant vehicular fleet, it also has a strong industrial character, with the presence of the Capuava Petrochemical Complex on the border of the municipalities of Mauá and Santo André. This complex is made up of the Capuava Refinery installed with an capacity approximately 53 thousand barrels of oil, plus 14 other industries, located in an industrial plant of petroleum by-products, producing polyethylene and polypropylene, from the distillation of naphtha and various intermediate substances that are used as feedstock for the manufacture of other products. The Capuava Petrochemical Complex presents a peculiarity in relation to the others distributed in Brazil, it is the only one located in the surroundings of a densely occupied residential

#### Photochemical model

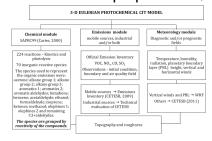
In this study it was used the 3-D Eulerian photochemical CIT model to simulate the air pollution dynamics for O<sub>3</sub> in the Great ABC Region and MASP, which is a photochemical model developed jointly by the California Institute of Technology and Carnegie Mellon University, see McRae and Senfeild (1983). The model consists of three basic modules (chemistry mechanism, meteorology and emissions), which simulates, respectively, dispersion in the planetary boundary layer (PBL), chemistry and emission inventories, including spatial and temporal distribution. The CIT airshed model is based on the numerical solution of the atmospheric diffusion equation. The input data for the model used to solve the atmospheric diffusion equation meteorological variables (temperature, absolute humidity, solar and ultraviolet radiation, mixinglayer height and three-dimensional wind fields), topographical characteristics (including surface roughness), and the rate of emission of the chemical species, and air-quality data for initial and boundary conditions. The model employs the 1999 California Statewide Air Pollution Research Center (SAPRC99) photochemical mechanism. More details can be seen in Boian and Andrade (2012). The vertical resolution of the model has five levels (1-5 levels, see Table 1) to represent all the boundary layer and the top of the model for these simulations is 3575 m. The top of the model was determined with basis in the simulations of mixing-layer height with Weather Research and Forecasting Model (WRF).

Table 1. Specifications of the vertical layers of the model: thickness and height of the top (m).

Layer	Fraction	Thickness (m)	Top (m)
1	0,010	35,8	35,8
2	0,105	375,4	411,1
3	0,165	589,9	1001,0
4	0,330	1179,8	2180,8
5	0,390	1394,3	3575,0

Figure 2 summarizes the air quality and meteorological input parameters and the source of the data.

Figure 2. Modules of the CIT photochemical model and the input parameters.



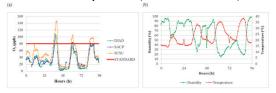
#### FINDINGS AND ARGUMENT

For the analysis of the air quality for  $O_3$  in relation to the meteorological conditions (temperature and humidity), the data of the CETESB monitoring stations of Diadema (DIAD), Santo André Capuava (SACP) and São Caetano do Sul (SCSU) were used. These stations are, respectively, distance of 13.7 km, 760 m and 7.5 km in relation to the Capuava Petrochemical Complex. For the meteorological variables temperature and humidity there were only data for the SCSU station. Due to the unavailability of data in the Great ABC Region monitoring stations, wind direction and speed data were obtained from the IAGU Meteorological Station, which is about 14 km west of the Capuava Petrochemical Complex.

Figure 3 (a-b) shows the air quality and meteorological conditions (temperature and humidity) for the period of simulation, respectively.



Figure 3. Hourly O<sub>3</sub> concentrations (ppb), temperature (°C) and humitidy (%) measured by CETESB from September, 28 to October 1, 2011.



As expected, a directly proportional relationship of  $O_3$  concentrations and temperatures was observed, since  $O_3$  is a secondary pollutant formed by photochemical reactions and an inverse relationship with the humidity. Higher levels of humidity are associated with higher cloud occurrence and atmospheric instability, which results in slower photochemical processes and greater dispersion of pollutants, making it difficult to form  $O_3$ , explaining the inverse relationship between them.

With the evolution of time, O<sub>3</sub> concentrations were increased, with exceedances of the air quality standard at the measurement stations, accompanied by an increase in temperature and a significant reduction of relative humidity. The maximum concentrations of O3 were measured in the period from 11 am to 5 pm, ranging from 81 to 145 ppb. During this period, no nocturnal peaks of O<sub>3</sub> were observed, indicating that there was no transport effect at the time. The analysis of direction and speed of the winds in the simulation period, for the IAGU Weather Station, showed that main direction of the winds was southeast, with speeds varying between 0 - 5.8 m/s.

Comparison between hourly  $O_3$  concentrations measured and simulated for the Great ABC Region for the three scenarios is showed in Figure 4 (a-d). The better agreement between measured and simulated  $O_3$  concentrations were obtained for the days September, 30 and October 1, 2011. It is emphasized that first days of simulations corresponds of the spin up of the model. Thus, for the discussion of the results were chosen the day of better agreement (September, 30).

Figure 5 (a-c) shows a comparison between the three scenarios for September, 30 at 4:00 pm. The predominance of the southeast winds in the  $O_3$  formation period causes the plume to be transported to the northwest region of MASP, where the highest  $O_3$  concentrations where observed (scenario 1: 130 - 140 ppb and scenario 2: 180 - 200 ppb). Due to the transport effects of  $O_3$  and precursors, the Great ABC Region shows lower concentrations of  $O_3$  (Scenario 1: 100 - 110 ppb and Scenario 2: 100 - 120 ppb). The analysis of the contribution of the emissions of only the Petrochemical Complex of Capuava shows an increase of about 30 ppb in the source area.

Figure 4. Compared between O<sub>3</sub> concentrations measured and simulated (first level of the model - 36m) for the Great ABC Region for the three scenarios, (a) mobile sources; (b) industrial sources; (c) mobile + industrial sources and (d) three scenarios.

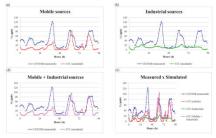
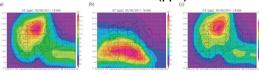


Figure 5. Comparison between the three scenarios for September, 30 at 4:00 pm, (a) mobile sources, (b) industrial sources and (c) mobile + industrial sources. The bar shows O<sub>3</sub> concentrations (ppb).



#### **CONCLUSIONS**

The results showed that the breeze circulation plays an important role in the dispersion of the pollutants and precursors of the Great ABC Region causing the region to export its pollutants and precursors to the northwest region of the MASP. Thus, of great importance to assess the contribution of emissions from mobile and industrial sources, since the pollutants emitted and generated will have impacts not only at local level.

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## Session 2 Model Development



### THE SHORT-RANGE TRANSPORT AND REACTION OF EFFLUENTS FROM ROCKETS AT THE BRAZILIAN SPACE RANGE CENTER

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One of the risks associated with the rocket launching activity is the inhalation of exhaust gases, that can occur either in the vicinity of the launch center or, depending on the way these gases are transported and dispersed through the atmosphere, in locations far from launch. Immediately after ignition of the rocket motors, it is formed a large hot cloud near the ground, composed of monoxide and carbon dioxide (CO and CO2), hydrogen chloride (HCl) and also particulate material composed of oxide of Aluminum (Al2O3) for the case of rockets driven by solid propellant. The atmospheric model Weather Research and Forecasting Model (WRF) has been modified to simulate the transport, dispersion and chemistry (with the addition of reactions involving HCl and other chlorinated compounds) of these gases released during a launching. Simulations of the dispersion of effluents were performed for different rainfall regimes (dry and rainy period) as well as atmospheric thermal stability (daytime and nighttime) for a specific launching (Satellite Launcher Vehicle (VLS)) at the Brazilian Launching Center (CLA). The results show that the most critical levels of HCl and CO occurred in the meteorology sector (SMT) from the time of launch (Ho) up to 10 minutes. The city of Alcântara (distant 10 km from the launching pad) can be affected according to the direction of the wind, although the concentrations are smaller than those presented in the CT, due to a longer exposure time. The HCl concentration reached a level of 3768 ppmv in the wet period and 2214 ppmv in the dry period (está certo isto, maior valor na estacao chuvosa?), as daytime releases for these same periods presented significant lower concentrations (2045 and 1540 ppmy, to rainfall and dry period, respectively).



### TOWARDS A COUPLED AEROSOL-CHEMISTRY-ATMOSPHERE INTERACTIONS IN BRAZILIAN GLOBAL MODEL: DESIGN & PROGRESS

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Abstract: Atmospheric aerosols and trace gases have been increasingly recognized as a key component of the highly dynamic and complex global system. The two-way feedback between meteorology and chemistry are important and is a strongly coupled process. The new version of the CPTEC global model, Brazilian Atmospheric Model (BAM), has new dynamics and state-of-the-art physical processes. However, it does not yet have a model of aerosols and chemistry. In this work, we propose a design for the implementation of aerosol-chemistry-atmosphere interactions in BAM with the objective of improving the forecast of weather and seasonal climate in Brazil. The design comprises of three phases: initialization phase, computational phase, and the validation phase. The initialization phase is being completed and the computational phase is in progress.

Keywords: aerosol-chemistry-atmosphere interactions, Brazilian Global Model.

#### **INTRODUCTION**

The representation of the trace gases and aerosols has become imperative in current numerical models for weather, air quality and climate prediction. The two-way feedback between the atmosphere and its chemistry is a strongly coupled process that has remained a challenge to the modeling community. The existing state-of-thescience global aerosol-chemistry climate models were developed using lab/field data mostly from the Northern Hemisphere, they may not necessarily represent the chemistry and aerosol formation for Brazil where the meteorological/climate conditions and emission sources are quite different. For example, studies indicate large disagreements among models over Northern Hemisphere and Southern Hemisphere for black carbon burden and deposition fluxes (Lee et al., 2013). Most of the models indicate deficiencies with O<sub>3</sub> precursor emissions resulting in low bias in the Southern Hemisphere (Young et al., 2013). Apart from this, the Southern Hemisphere has different but fewer, and more localized sources of anthropogenic emissions.

Brazilian Global Atmospheric Model (BAM, Figueroa et al., 2016, & references therein) is the new operational model of the Center for Weather Forecasting (CPTEC/INPE) and a first step towards developing the next generation non-hydrostatic/hydrostatic global dynamic core, which can be used for a wide range of horizontal resolution O(1-200 km). Double-moment microphysics scheme with predicted droplet concentration is used. The vertical diffusion is a modified version of the local PBL Mellor-Yamada Level 2.0 closure scheme. Shallow convection scheme is from Park and

Bretherton and modified Grell Devenyi developed at CPTEC/INPE is for deep convection. The radiation scheme for short wave and long wave is the Rapid Radiative Transfer Model for GCMs. There is no representation of aerosols or chemistry in BAM.

The aforementioned factors in addition to the presence of rich Amazonian biosphere and its influence over the continent justify the need for the implementation of the aerosol-chemistry-atmosphere interactions in BAM. The strategy is to first port the aerosol-chemistry modules from one of the existing state-of-the-science global aerosol-chemistry numerical models in BAM followed by improvement of its performance over Brazil against the factors stated above. In this work, we propose the design for this implementation, its progress and challenges therein. In addition, we contemplate to have remarks & suggestions on our design and a possible collaboration at the CMAS conference.

#### **METHODS**

A prime task in the implementation includes the evaluation of the global aerosol-chemistry models for their performance over Brazil (see Alvim et al., 2017 for one such assessment). The design for the implementation is enumerated below:

- Develop a pre-run configuration in BAM to facilitate compiling external modules and performing short test runs
- Identify dependencies in the module and map them to BAM environment
- Identify the necessary meteorological inputs



- 4. Build a driver/ interface in BAM to includes routines from the modules
- 5. Define trace gases & aerosols in BAM
- Read the emissions in BAM parallel environment
- Develop routines for outputs and restarts, if any
- 8. Introduce computational calls in BAM through the interface
- Perform short simulations to evaluate the new parameterization and compare
- Improve discrepancies in the new parameterization, if any

#### FINDINGS AND ARGUMENT

The implementation is categorized into 3 phases: initialization phase, computational phase and validation phase. The Initialization phase is completed. It includes:

- Understanding the workflow of aerosolchemistry modules in their respective climate models.
- Developing a pre-run setup to facilitate the inclusion of subroutines in BAM and perform short runs
- Introducing trace gases and aerosol species in BAM
- Identifying the input meteorological variables required for the computational phase
- e. Reading the emissions in BAM parallel environment

The computational phase is ongoing and includes passing or referencing the meteorological fields through the interface into the chemistry modules, introduce modules routines pertaining to chemistry calculations and preparing outputs and restarts. The validation phase will include designing short and long simulations to check the performance of BAM with the new parameterization and improve further.

#### **CONCLUSIONS**

Implementing the aerosol and chemistry parameterization in BAM is different compared to coupling of the other Earth system components like ocean, land, sea ice requiring only a coupler that facilitates exchange of variables across it at a preset time. The modules here must not only integrate with the atmospheric model, their output and restart variables must be accommodated in the host climate model. The module poses strict requirements on:

- the attributes (shape, dimensionality, global/local scope) of the variables,
- arguments in a subroutine call,
- place where a function or subroutine is called in the model,

- updating, referencing and dereferencing variables
- accommodating restart and output variables etc.

The biggest challenge is the presence of atmospheric variables those are required for aerosol-chemistry interactions. In some instances, the host model undergoes critical changes that may reflect adversely on other processes; lay dormant until long simulations etc. The implementation work is ongoing and the group is looking for helpful suggestions and collaboration with a model-developing group.

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# Challenges of modelling multi-scale flows in Wind Engineering applications

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**Abstract:** Numerical environmental wind tunnel technique is increasingly attractive because of its fast increasing capability and decreasing cost, in particular for the interaction between weather scale and street scale flows. We briefly review our recently developed Numerical Environmental Wind Tunnel Of Newtonian fluid (NEWTON) and present a couple of case studies to demonstrate its capability for modelling multi-scale flows in Wind Engineering applications.

*Keywords*: coupling of mesoscale and microscale modelling, NEWTON, large-eddy simulation.

#### INTRODUCTION

Owing to the rapidly increasing computer power and decreasing cost, along with the recently developed new technology, Computational Fluid Dynamics (CFD) is becoming increasingly attractive in modelling environmental flows. However, some challenging issues remain to be tackled. One among these is modelling multi-scale physical/chemical processes in the urban atmospheric boundary layer. The time scale of transport/dispersion/reaction of gas particulate matter (PM) pollutant in urban environments varies from micro-seconds (10<sup>-6</sup> s) to days (10<sup>5</sup> s). It is not feasible to resolve all of these scales in the foreseeable future. One option perhaps is to segment the full spectrum of these scales (such as the inertial sublayer of turbulence) and resolve one or more segments, whereas the other scales are to be modelled or to be synthetically generated using a sort of stochastic procedure [Xie & Castro, 2008; Xie et al, 2015].

### **CASE STUDIES**

In the first part of the talk, we will use case studies to demonstrate the importance of modelling muti-scale flows using our recently developed Numerical Environmental Wind Tunnel Of Newtonian fluid (NEWTON) [Xie, 2014], which is a comprehensive tool using Computational Fluid Dynamics (CFD) primarily to model physical wind tunnel scale, i.e. O(1m) problems, but not limited to, such as considering the effects of weather-scale wind variations. The case studies are: a) the effect of unsteadiness of weather scale variation of wind on point/line source dispersion in the DAPPLE site - central London; b) locally generated large-scale motions by tall buildings (- O(100m)) which could have a significant impact on the urban

environments in cities primarily consisting of low rise buildings.

In the second part of the talk, we will aim to identify some key issues, such as how to assess and reduce the modelling uncertainties due to the coupling of the weather scales and street scale motions. At the end of the talk, we will suggest one solution to address these, i.e. by adding correlated fluctuations at the nest interface of the two domains.

### **ACKNOWLEDGEMENT**

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## SEMI-ANALYTICAL DISPERSION MODEL IN THE FORMATION OF SECONDARY POLLUTANTS IN THE ATMOSPHERIC BOUNDARY LAYER

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#### Abstract:

One interesting problem regarding dispersion in the atmosphere is how to estimate the concentration of primary and secondary pollutants, like  $SO_2$  and sulfate. If there is a continuous wind from a point with high concentration of  $SO_2$ , this is transformed through chemical reactions to sulfate aerosol, and both the  $SO_2$  and sulfate-containing particles are removed by means of wet and dry deposition. The equation used to estimate the dispersion of  $SO_2$  in the atmosphere is linear and its solution is easily obtained for specific situations. On the other hand, the equation to calculate the sulfate concentration is coupled to that of  $SO_2$ , thus making its resolution more difficult. To solve this problem, we decoupled the system governing the concentration of secondary pollutants (in this case the sulfate) and thus obtained a linear transformation involving the concentration of primary pollutant and an auxiliary equation that could be solved in a manner similar to that of the primary pollutant. To solve these simpler equations, we used the ADMM method (Advection Diffusion Multilayer Model), which consists of a semi-analytical solution based on discretization of atmospheric boundary layer (ABL) in sub-layers, such that the advection equation could be solved by means of the Laplace transform technique. The ability of the model to predict the concentration of primary and secondary pollutants is demonstrated qualitatively.

Keywords: Mathematical modeling; Air pollution modeling; Secondary pollutants; Sulfate; Laplace transform.

## **INTRODUCTION**

The dispersion of the air pollutant into the atmosphere from a point source is ruled by the molecular diffusion process and it considers some factors, such as stack heights, wind velocity, temperature inversion, dry deposition, and rainout/washout. A primary air pollutant, such as sulfur dioxide, undergoes chemical transformations in the atmosphere to form secondary pollutants, such as sulfates and sulfuric acid (Seinfeld and Pandis, 1997, Shukla et al., 2012). Therefore, a relevant problem is to estimate the dispersion of secondary pollutants. However, the transformation of a primary contaminant into a secondary one brings up equations that are coupled, making the problem harder to solve analytically.

Astarita et al. (1979), Alam and Seinfeld (1981) and Shukla and Chauhan (1988) proposed a methodology to decouple the system, resulting in a linear transformation involving the concentrations of the primary pollutant and an auxiliary equation whose resolution is similar to the primary pollutant one. For that matter, the aim of this work is to find the secondary pollutant concentration through this methodology, also using the ADMM method (Advection Diffusion Multilayer Model) (Moreira et al., 2010).

The innovation is to applicate the ADMM method in order to solve these equations. To invert the Laplace transform, an updated version of the fixed Talbot (FT) algorithm (Talbot, 1979) was used, which was based on deformation of the outline of

the Bromwich inversion integral. From the solution found, it was possible to calculate the solution of the equation governing the secondary pollutant, and it was validated using data provided in Alam and Seinfeld (1981), but with an up to date parameterizations for eddy diffusivity and wind profile (Degrazia et al., 1997).

The ADMM method is based on a discretization of the ABL in N sub-layers, where in each sub-layers the advection-diffusion equation is solved by the Laplace transform technique, considering an average value for eddy diffusivity and the wind speed. The main feature of this method relies on the following steps: stepwise approximation of the eddy diffusivity and wind speed, Laplace transform application to the advection-diffusion equation in the x variable, semi-analytical solution of the set of linear ordinary equation resulting for the Laplace transform application and construction of the pollutant concentration by the Laplace transform inversion using the FT scheme (semi-analytical due to the numeric inversion).

At this point, it is important to mention that the analytical solutions are useful for a variety of applications, such as: providing approximate analyses of alternative pollution scenarios, conducting sensitivity analyses to investigate the effects of various parameters or processes involved in contaminant transport, extrapolation over large times and distances where numerical solutions may be impractical, serving as screening models or benchmark solutions for more complex transport processes that cannot be solved exactly, and for



validating more comprehensive numerical solutions of the governing transport equations.

### **METHODS**

Following the ADMM method, the average concentration C(x,z) of the primary pollutant, considering a Cartesian coordinate system in which the x-axis coincides with the average wind, and in which a first-order removal process exists, can be described by the atmospheric diffusion equation (Alam and Seinfeld, 1981):

$$u \frac{\partial C}{\partial x} = K_Z \frac{\partial^2 C}{\partial z^2} - (k + k_g)C \tag{1}$$

where  $K_z$  is the Cartesian component of eddy diffusivity in the vertical direction, u is the longitudinal wind speed, k is the rate of conversion of primary pollutant and  $k_g$  is the removal rate.

The source and boundary conditions to equation (1) are:

$$C(0,z) = \frac{Q}{R}\delta(z - H_S), \quad x = 0$$
 (1a)

$$K_Z \frac{\partial c}{\partial z} = 0$$
, at  $z = h$  (1b)

$$C(0,z) = \frac{Q}{U}\delta(z - H_s)$$
,  $x = 0$  (1a)  
 $K_Z \frac{\partial C}{\partial z} = 0$ , at  $z = h$  (1b)  
 $K_Z \frac{\partial C}{\partial z} = v_d c$ , at  $z = 0$  (1c)

where Q is the emission rate,  $\delta(.)$  is the Dirac delta function,  $H_s$  is the source height, h is the ABL height and  $v_d$  is deposition velocity of the gaseous pollutant.

Similarly, the differential equation ruling the concentration  $C_{D}(x,z)$  of the secondary pollutant can be written as:

$$u\frac{\partial C_p}{\partial x} = K_Z \frac{\partial^2 C_p}{\partial z^2} + kC - k_p C_p \tag{2}$$

The source and boundary conditions for Eq. (2) are:

$$C_p(0,z) = 0$$
, at  $x = 0$  (2a)

$$K_Z \frac{\partial C_p}{\partial z} = 0$$
, at  $z = h$  (2b)

$$K_{Z} \frac{\partial c_{p}}{\partial z} = 0$$
, at  $z = 0$  (2d)  
 $K_{Z} \frac{\partial c_{p}}{\partial z} = 0$ , at  $z = h$  (2b)  
 $K_{Z} \frac{\partial c_{p}}{\partial z} = v_{dp}C_{p}$ , at  $z = 0$  (2c)

where  $k_p$  is the removal rate and  $v_{dp}$  is the deposition velocity of secondary pollutant.

It could be seen that Eq. (2) was coupled to Eq. (1), and so we could rewrite them in a compact manner as follows:

$$L\begin{bmatrix} C \\ C_p \end{bmatrix} - \begin{bmatrix} k + k_g & 0 \\ -k & k_p \end{bmatrix} \begin{bmatrix} C \\ C_p \end{bmatrix} = 0$$
 (3)

where  $L=-u\; \frac{\partial}{\partial x}+\; K_Z\; \frac{\partial^2}{\partial z^2}$  is an operator. Using the same transform as Astarita et al. (1979)

and Alam and Seinfeld (1981), the uncoupled system appears as follows:

$$LC - (k + k_g)C = 0$$
 (4a)  

$$LB - k_pB = 0$$
 (4b)

$$LB - k_p B = 0 (4b)$$

where,

$$B = C_p - \frac{kC}{k_p - k - k_q} \tag{5}$$

Thus, B(x,z) could be written as follows, with the appropriate source and boundary conditions:

$$u\frac{\partial B}{\partial x} = K_Z \frac{\partial^2 B}{\partial z^2} - k_p B \tag{6}$$

$$B(0,z) = \frac{-k}{(k_x - k_z)_{II}} C(0,z)$$
, at  $x = 0$  (6a)

$$K_Z \frac{\partial B}{\partial z}$$
, at  $z = h$  (6b)

$$u\frac{\partial B}{\partial x} = K_Z \frac{\partial^2 B}{\partial z^2} - k_p B$$
 (6)  

$$B(0,z) = \frac{-k}{(k_p - k - k_g)U} C(0,z), \text{ at } x = 0$$
 (6a)  

$$K_Z \frac{\partial B}{\partial z}, \text{ at } z = h$$
 (6b)  

$$K_Z \frac{\partial B}{\partial z} = v_{dp} B - \frac{k(v_{dp} - v_d)}{k_p - k - k_g} C, \text{ at } z = 0$$
 (6c)

To solve Eqs. (1) and (6), the ADMM method were applied. Then, the secondary concentration reads like:

$$C_p = B + \frac{k}{k_p - k - k_q} C \tag{7}$$

Finally, an inversion method of the Laplace transform had been applied, the Fixed Talbot (FT) algorithm (Talbot, 1979), and the concentrations C and B were obtained with the expressions:

$$C(x,z) = \frac{r}{M} \left[ \frac{1}{2} \hat{C}(r,z) e^{rx} + \sum_{j=1}^{M-1} Re \left[ e^{xs(\theta_j)} \hat{C}(s(\theta_j),z) \left(1 + i\tau(\theta_k)\right) \right] \right]$$
(8)

$$B(x,z) = \frac{r}{M} \left[ \frac{1}{2} \hat{B}(r,z) e^{rx} + \sum_{j=1}^{M-1} Re \left[ e^{xs(\theta_j)} \hat{B}(s(\theta_j),z) \left( 1 + i\tau(\theta_k) \right) \right] \right]$$
(9)

where,

$$\hat{C}(s,z) = \mathcal{E}\{C(x,z); x \to s\}$$

$$\hat{B}(s,z) = \mathcal{E}\{B(x,z); x \to s\}$$

$$s(\theta_j) = r\theta(\cot\theta + i), -\pi < \theta < +\pi$$

$$\tau(\theta_j) = \theta_j + (\theta_j\cot\theta - 1)\cot\theta_k$$

$$\theta_j = \frac{k\pi}{M}$$

r is a parameter based on numerical experiments, M is the number of terms in the summation and £ indicates the application of the Laplace transform.

The fixed Talbot (FT) method is based on the contour deformation of the Bromwich inversion integral and requires complex arithmetic.

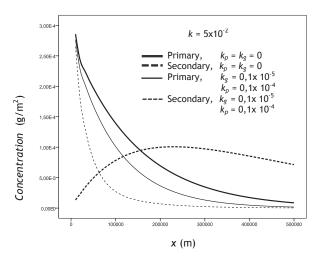
Then, the Eq. (7) was used to find the concentration of the secondary pollutant.

## FINDINGS AND ARGUMENT



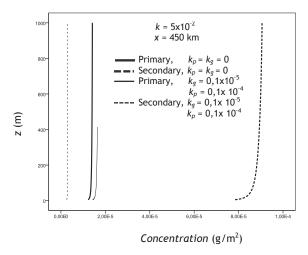
The solutions were implemented for the values of k,  $k_p$ ,  $k_g$ ,  $v_d$  and  $v_{dp}$ , which are available in Alam and Seinfield (1981).

In Figure 1, the ground level concentrations of the primary and secondary pollutants are shown as functions of the longitudinal distance x, which assumes a maximum value of 500 km. It is possible to see the effect of wet deposition. There is an abrupt decay of the secondary pollutant. This condition is due to the fact that, when it comes to wet deposition, the secondary pollutant rate is higher than the primary pollutant rate. Also, the wet deposition is more effective than the dry deposition.



**Figure 1.**Ground-level of C (primary) and  $C_p$  (secondary) as a function of source distance.

Figure 2 shows the vertical profile. It is interesting to note that secondary pollution accumulated at ground level, due to the slow rate of dry deposition.



**Figure 2.** Vertical profile of C (primary) and  $C_p$  (secondary) as a function of height z.

### **CONCLUSIONS**

In this work, was presented a semi-analytical solution of the two-dimensional steady state advection-diffusion equation for primary and secondary pollutants, which considers dry and wet deposition, sedimentation velocity and first-order chemical reactions. Linear algebra was used to decouple the system from the secondary pollutant, then, it was found an auxiliary equation. It was possible to determine the concentration of the secondary pollutant from the solutions of the primary pollutant and the auxiliary equation.

The study showed results with similar behavior of previous works from the literature. The analytical nature and simplicity of the solution emphasize that the proposed method is a robust and promising method for simulating the dispersion of primary and secondary pollutants in the atmosphere.

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# Session 3 Emissions Inventories



# SÃO PAULO MUNICIPALITY ON-ROAD PASSENGER TRANSPORTATION EMISSIONS INVENTORY

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Abstract: This work aimed at developing an emissions inventory for the municipality of São Paulo with space and time resolution suitable for air quality studies. Methods applied followed a common emissions inventorying practice, where activity rates are combined with specific emission factors. Transport modelling for private transportation modes (passenger cars and motorcycles) and GPS tracking for public buses were the two main utilized sets of activity data. Emission factors applied represent the local fleet and traffic conditions (speed). The work resulted in estimated emissions from on-road passenger transportation for a 1 km per 1 km geographic grid in the São Paulo municipality, covering an hourly basis for a typical day in 2015. Since activity data and emission factors applied are specific for São Paulo, emission results provides elements to better understand and propose solutions to the air pollution problem in the city, such as feeding dispersion models and promoting studies that explore the relationships among human activity, meterology, air quality and human health.

Keywords: local-scale emissions inventory, transportation, air pollution, greenhouse gases, spatial emission mapping

#### INTRODUCTION

Air quality, as measured through the concentrations of atmospheric pollutants during a given moment, is a complex environmental aspect. It changes daily and seasonally as human activities generate emissions and varied climate impacts, interacting with the natural dynamics of the atmosphere. Therefore, managing the urban environment's air quality requires the adoption of technically sophisticated instruments and the production of specialized information (IEMA, 2014).

Emissions inventories are one of the most important strategic instruments for air quality management. Nevertheless, in Brazil, few are the examples of emissions inventories related to local scales, those of a city or metropolitan region, that can be directly linked to local air quality.

Worldwide, the geographic representation of emissions estimates in urban scales are improving and becoming more common (Sidiropoulos et al, 2009). These estimates can be used as input data for dispersion modelling and the results of these models can be used to formulate policies to improve air quality and human health (Cook et al, 2008).

The population of São Paulo municipality has been suffering with air pollution for decades. Today, as the São Paulo State Environmental Agency reports (CETESB, 2015), the main pollutants that degrade the air quality in the city are particulate matter and ozone gas, with ambient standards stablished by the state systematically being exceeded. Also according

to the Agency, transportation is the main source of pollution in the metropolitan region of São Paulo.

The present work aims at developing an emissions inventory for the municipality of São Paulo with space and time resolution suitable for air quality studies. Besides estimating criteria pollutants (carbon monoxide, non-methane hydrocarbons, nitrogen oxides, aldehydes and particulate matter), this work also estimated greenhouse gas emissions (carbon dioxide, methane and nitrous oxide).

Hence, the specific objectives of this work include representing transportation emissions in a high-resolution geographic grid, detailed in daily profiles for a typical day and identifying source participation, by vehicle type and fuel.

## **METHODS AND DATA**

In order to estimate emissions, the general equation was applied:

 $E = A \times EF (1)$ 

Where E is emissions (g), A is activity rates, and EF is emission factors.

For this study, activity rates are expressed in distance travelled (km) and emission factors are expressed in quantity of emissions per distance travelled (g/km).

Mainly, data for activity rates were provided by public agents: (i) transport modelling results from Companhia de Engenharia de Tráfego (CET), for



passenger cars, and (ii) urban buses GPS data from São Paulo Transportes (SPTrans). Other data sets were also used such as origin-destination surveys, coach buses departures and arrivals records, vehicle registration and fuel sales.

Emission factors applied for passenger cars and motorcycles where those published by CETESB (2016), based on type-approval tests, but adapted to reflect the influence of urban traffic. Curves relating emissions and vehicle speed where assumed as similar to those from the European Environment Agency Air Pollutant Emissions Inventory Guidebook 2016 (EEA/EMEP, 2016).

For buses, emission factors applied where those from EEA/EMEP, since Brazilian buses are mostly manufactured by European companies.

### FINDINGS AND ARGUMENT

The work resulted in estimated emissions from onroad passenger transportation for a 1 km per 1 km geographic grid in the São Paulo municipality, covering an hourly basis for a typical day in 2015.

The inventory was capable of presenting analytical framing such as:

- Daily emissions profile, hour by hour, by transport mode (an example is presented in Figure 1):
- (ii) Daily emissions maps, on 1 km<sup>2</sup> grid, hour by hour, by source transport mode (an example is presented in Figure 2);
- (iii) Comparisons of total emissions by source transport mode;
- (iv) Comparisons of emissions intensity by source transport mode (example in Table 1).

These results will soon be available on an online platform developed within this inventory containing user interactive graphs and maps.

For most pollutants and greenhouse gases, passenger cars were found to be the main responsible for passenger transportation related emissions. Nitrogen oxides  $(NO_x)$  and combustion generated particles have buses as major sources.

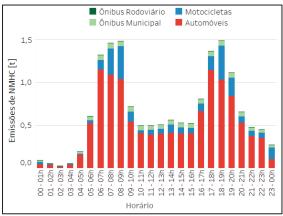


Figure 1. Illustration graph: Daily profile of NMHC emissions estimates from passenger cars, motorcycles and buses for a typical day in 2015

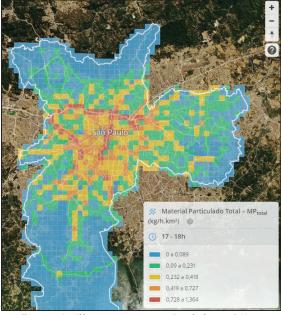


Figure 2. Illustration map: Peak-hour PM<sub>10</sub> emissions estimates from passenger cars, motorcycles and buses for a typical day in 2015, calculated at 1 km<sup>2</sup> grid

Table 1. Daily GHG emissions by transport mode for a typical day in 2015

Transport mode	Emissions intensity [tCO2e/passenger-km, GWP IPCC AR2]
Passenger cars	65,8
Motorcycles	35,6
Buses	17,0



## **CONCLUSIONS AND RECOMMENDATIONS**

The São Paulo Municipality On-Road Passenger Transportation Emissions Inventory presented here provides elements to better understand and propose solutions to the air pollution problem in the city. It was built aiming to feed dispersion models and promoting studies that explore the relationships among human activity, meterology, air quality and human health.

Besides improvements that can be conducted regarding passenger transportation activity data and emissions factors, this inventory needs still to be complemented by emissions estimations from freight transportation and other sources (e.g. industrial, commercial and residential). Furthermore, expanding the spatial coverage to include all metropolitan region would be necessary from a dispersion perspective.

Although the study was based on one single municipality, the procedures developed can be applied on an amplified manner where transport modelling data or vehicle tracking by GPS are available.

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# UPDATE OF THE INDUSTRIAL ATMOSPHERIC EMISSION INVENTORY FOR BELO HORIZONTE, MINAS GERAIS - BRAZIL

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Abstract: The aim of this study was to do an update on the 2003 Emission Inventory, provided by the local Environmental Agency for the city of Belo Horizonte, Minas Gerais, Brazil, once many changes in the industrial activities occurred over the last 12 years (with reference to the baseline year 2015). The quantification of emissions was preferably performed based on the chimneys monitoring data, through consultations on the environmental licensing processes and emission monitoring reports of companies with significant polluting potential in the study area. The focus of this study was on regulated pollutants: particulate matter (PM), oxides of sulfur (SOx) and nitrogen (NOx), carbon monoxide (CO) and volatile organic compounds (VOC). As preliminary results, 72 point sources of significant impact on atmospheric emissions in the study area were identified. It was observed that CO, among the five pollutants evaluated, was the most emitted, followed by PM, NOx, SOx and, finally, COV. As these preliminary results considered only data from chimneys reports, where not all the pollutants that could be emitted were quantified, estimates and complements should be made according to the AP-42 for a better understanding of the emissions of pollutants by industrial and other point sources in Belo Horizonte.

Keywords: Atmospheric emissions, point source, industry, air pollution, Belo Horizonte.

## **INTRODUCTION**

Belo Horizonte is a highly urbanized city in the state of Minas Gerais, Brazil, with a population of more than 2.5 million inhabitants. In addition, it has an area of 331 km² and a population density of 7,167 inhabitants/km². Its Human Development Index (HDI) is 0.810 and the Gross Domestic Product (GDP) of 25.84 billion dollars, which represents 16.7% of the state GDP and 1.53% of the national GDP, being one of the most important cities in the country (IBGE, 2016).

Belo Horizonte has several potential atmospheric pollutants emission sources due to the development of diverse economic activities such as metallurgical, food and pharmaceutical industry, and the vehicular fleet (1,760,978 vehicles in 2016). This can affect its air quality and, consequently, it could impact the population health (Freitas *et al.*, 2013; Radicchi, 2012).

Despite this critical scenario, few studies have been developed with the objective of evaluating the air quality in this city, especially with regard to the identification of pollutant emission sources and their processes of dispersion and environmental contamination. The identification of sources, atmospheric emission especially industrial, together with their emission profiles (quantification of pollutants emitted over time), and physical data, such as geographic location and sources characteristics, could provide better answers regarding the industrial sector contribution to the emissions in the region nowadavs.

The quantification of the pollutant emissions in the inventoried sources constitutes a fundamental subsidy for feeding and use of emission models, such as SMOKE, which are essential tools for air quality evaluation in the study area through the photochemical models, such as CMAQ (Borge et al., 2008; 2014; Kim et al., 2008). Thus, the aim of this study was to do a preliminary update on the 2003 Emission Inventory, provided by the local Environmental Agency (FEAM, 2003), once many changes in the industrial activities occurred over the last 12 years (with reference to the year 2015).



#### **METHODS**

The survey of industrial emissions was done through consultations on the environmental licensing processes and emission monitoring reports of companies with significant polluting potential in the study area, according to the local legislations (DN COPAM 74/2004; DN COMAM 74/2012). The focus of this study was on regulated pollutants: particulate matter (PM), oxides of sulfur (SOx) and nitrogen (NOx), carbon monoxide (CO) and volatile organic compounds (VOC). The baseline year was 2015.

The quantification of emissions was preferably performed based on the chimneys monitoring data. On the emission monitoring reports the following information was collected: emission source physical data, such as location, diameter and height, and emitted pollutants data, such as flow, speed, temperature, concentration, and emission rate. From these data, a preliminary estimate of the total emission of the regulated pollutants emitted in the city of Belo Horizonte was made.

#### FINDINGS AND ARGUMENT

As preliminary results, 72 point sources of significant impact on atmospheric emissions in the study area were identified. These sources are distributed among 24 companies from various sectors, including the metallurgical and food industries, thermoelectric plants, painting booths, and the service sectors, such as hospitals, laundries and crematorium (Figure 1).

Compared with the Emission Inventory of the year 2003, the number of identified chimneys and companies, which contribute to air pollutant emissions, incresed by 24.1 and 100%, respectively (Figure 1). This increase was mainly due to the emergence of new companies, such as some painting booths and crematorium. Furthermore, in this study, some domestic boilers such as from hospitals and laundries, was considered, which were not evaluated in the 2003 inventory.

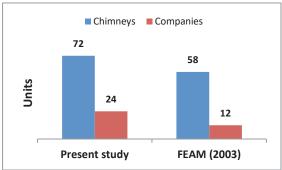


Figure 1. Number of identified chimneys and companies contributing to the atmospheric pollutants emission.

In this preliminary study, it was observed that carbon monoxide, among the five pollutants evaluated, was the most emitted by the chimneys in Belo Horizonte. It was followed by particulate matter, nitrogen oxide, sulfur oxide and, finally, by volatile organic compounds (Figure 2).

Compared to the results obtained in the 2003 inventory, emission rates were very similar for particulate matter. There was also a considerable increase in emissions of sulfur oxides and carbon monoxide. However, for nitrogen oxides an expressive reduction was observed (Figure 2 and 3).

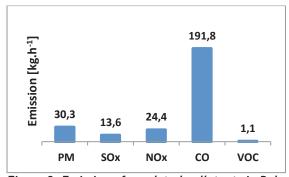


Figure 2. Emission of regulated pollutants in Belo Horizonte in the year of 2015 - preliminary results of this study.

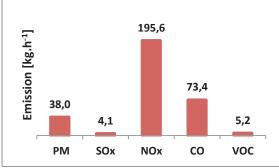


Figure 3. Emission of regulated pollutants in Belo Horizonte in the year of 2003 (FEAM, 2003).

However, as these preliminary results only considered monitoring data from chimneys reports, where not all the pollutants that could be emitted were quantified, precise conclusions about thte increase or the reduction in emissions rates can not be yet taken. Also, there are domestic boilers in some companies, but there is no monitoring reports of their emissions.

Thus, for a better understanding of the pollutants emissions from industrial and other point sources in Belo Horizonte, estimates and complements should be made based on AP-42 (Compilation of Air Pollutant Emission Factors from the USEPA - United



States Environmental Protection Agency) (US EPA, 1995) guidelines, as suggested by González et al. (2017) and Sadavarte and Venkataraman (2014). Thus, based on production process data, such as daily operating time, raw materials used, fuel consumption rates, types of emission control system, it will be possible to complement already identified emissions and understand better the atmospheric emissions in Belo Horizonte.

#### **CONCLUSIONS**

Seventy two point sources of significant impact on atmospheric emissions in the study area were identified. It was observed that CO, among the five pollutants evaluated, was the most emitted, followed by PM, NOx, SOx and, finally, COV. As these preliminary results only considered monitoring data for chimneys reports, where not all the pollutants that could be emitted, were quantified, estimates and complements should be made according to the AP-42 for a better understanding of the emissions of pollutants by industrial and other point sources in Belo Horizonte.

### **ACKNOWLEDGMENTS**

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# APPLICATION OF TWO METHODOLOGIES FOR ESTIMATES VEHICULAR EMISSIONS IN AIR QUALITY MODELING USING CMAQ MODEL

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Abstract: : The Metropolitan Region of Greater Vitória (RMGV) is located in the state of Espírito Santo (Brazil) and is a region that has many industrial emissions such as mining-steel, logistics, etc and still has large vehicular emissions (IEMA, 2011). The emissions of atmospheric pollutants of RMGV were inventoried and made available by the IEMA for the population. With this information, pollutant dispersion researches were developed, such as Loriato (2015), which identified that vehicular emissions could be overestimated, mainly for particulate matter, results that were also observed in studies of Santiago (2015) and Pedruzzi (2016). In 2013 the Brazilian Ministry of the Environment (MMA) released the National Inventory of Atmospheric Emissions by Road Automotive Vehicles together with its methodology and emission factors for Brazilian vehicles and fuels. Based on the MMA methodology, Araújo (2016) developed an inventory of vehicular emissions for the RMGV, applying the emission factors from MMA methodology for fleet of 2010 in the study region. From the new inventory and with the intention to apply it in air quality models such as CMAQ, the spatial and temporal allocation and chemical speciation of the emissions were performed using the SMOKE model version 3.5.1. Based on studies in the RMGV and mainly on the possible overestimation of pollutant emissions, the objective of this work is to apply the emission inventory developed by Araújo (2016) in the CMAQ model, comparing the results with those found by Pedruzzi (2016). For generation of meteorological fields, the WRF model version 3.6.1 was applied and for dispersion of pollutants it was used the CMAQ v. 5.01.

Keywords: RMGV, MMA, Vitória, Vehicular emissions, WRF, SMOKE, CMAQ.

### INTRODUCTION

The air quality of a region is the result of complex interactions involving the emission of air pollutants from stationary and mobile sources, local and remote, natural and anthropogenic, which together with the weather and topography of the region determine concentration of pollutants. Thus, it is crucial understand the emission inventory of pollutants aiming effective management of air quality in a region.

Large industrial facilities were installed in the metropolitan region of Vitoria (RMGV), Espírito Santo, Brazil (Fig.1), but unfortunately, the main wind direction in the area carry the gases and particles emitted to the most populated sector of the city. (Loriato et. Al., 2013), and because of this quantity of pollutant emissions and complains about air pollution, the Local Environmental Protection Agency (IEMA) released the current local inventory for RMGV with emissions coming from facilities like mineral and metallurgical industries, thermoelectric, ports, airports, vehicles, dust resuspension, etc.

The inventory provided has been adapted and tested with the air quality model (AQM), Chemistry Model Air Quality (CMAQ) in studies of Loriato (2015), Santiago (2015) and Pedruzzi et al. (2015) that used CMAQ over RMGV using the local

inventory and found that it could be overpredicted.

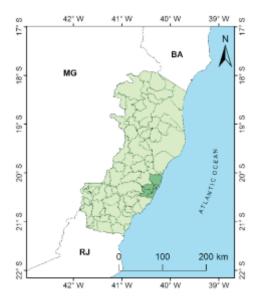


Fig. 1. Metropolitan Region of Great Vitoria - RMGV (study area in dark green).

Loriato (2015) and Santiago (2015) in their research explain that the emission inventory created needs some upgrades in future versions, more explicit in its chemical speciation, temporal



and spatial allocation and, mainly, choice of emission factors. It was concluded that particulate matter resuspension values in RMGV roads were likely overestimated, claiming an improvement in IEMA's inventory.

The present work conducted the spatial and temporal modeling of the emissions of traffic routes in the metropolitan region of Vitoria, through the SMOKE emissions model, using data from the 2010 emission inventory, new emission factors and actual composition of the current vehicle fleet, proposed by the Ministry of Environment of Brazil, which had sources georeferenced and temporally allocated, emissions chemically speciated and subsequently included in the SMOKE model

#### **METHODS**

Due to the factors above exposed, an intensive and deep analysis was promoted in the IEMA's original emission inventory, identifying some methodological deviations, but two principal:

- Simplified use of just one value (emission factor) to represent all ages of vehicles;
- Overestimation of ressuspension fraction, and double counting of emissions from vehicles in the form of exhaust, brake wear, and tire wear due to use of outdated AP-42 section 13.2.1 Paved Roads, from October, 2002.

Vehicle atmospheric emissions of RMGV were recompiled and the emissions rates were recalculated using the new methodology according Brasil (2014). The principal goal were to identify the different parts between the two, estimate the emissions rate according current national methods and apply it in Sparse Matrix Operator Kernel Emissions (SMOKE) v3.5.1 using time (hourly) and space variation and chemical nature (speciation) for performing the preparation of the inventory for use it in air quality models.

After the change of emissions rates in vecular emissions, the sources were divided in two types: point and area sources, as IEMA's inventory do. Sources, whose features required them to be classified as point sources (\$PTINV) by the model such as font height, diameter of the chimney, emitted gases temperature, stack gas exit velocity, etc., were so classified. Area sources (\$ARINV) were composed of regions exposed to various materials and urban roads, commercial, residential emissions and the new emissions from vehicular emissions.

From the perspective of emissions inventory, the chemical speciation implies the use of the chemical mechanism (ex: CB05) that is the mapping of pollutants for emissions inventory, for species of interest required in AQM. Therefore, the percentage of each chemical component of the CB05 chemical mechanism for all types of emissions of PM2.5 and VOC were performed according SPECIATE V4.2 database (USEPA, 2009) adapted to local emissions and regional experimental measurements.

The spatially allocating of regional emission inventories into grid cells depends on the source characteristics and resolution size (Zheng et al, 2009. For large industrial plants, emissions from chimneys were treated as point sources and allocated directly to grid cell based on their geographic coordinates (latitude and longitude). For allocating area sources and vehicular source emissions, Geographic Information System (GIS)-based road network information as spatial surrogates was adopted. This approach has been shown to provide more reasonable spatial allocations of regional mobile source emissions, especially at higher resolutions (Zheng et al, 2009c).

To compare the SMOKE and CMAQ results with Pedruzzi (2016) that used in this work the current IEMA's inventory emissions, were simulated meteorological fields for August 2010, same period of Pedruzzi (2016) using the Weather Research and Forecasting model WRFv3.6.1. It used four nested domains starting at 27-km grid resolution with nests at 9-km, 3-km and the 1-km finest resolution with 120 x 120 km, centered on 20.251°S, 40.285°W, all domains with 21 vertical layers. The initial and boundary conditions were provided from NCEP Global Forecast System (GFS) with 0.5° x 0.5° horizontal resolution and MCIP was used to extract 61x79 1-km grid cells were used from the inner WRF domain (120x120km).

The CMAQ v.5.0.1 were used to simulate the pollutant dispersion over RMGV, using CB05 for chemical mechanism and AERO-06 aerosol.

## FINDINGS AND ARGUMENT

Preliminary simulations in SMOKES reveal large differences between the two inventories methodologies for vehicular emissions. The Fig.3 and Fig.4 shows this discrepancy, in principal vehicular emissions, because the highest emissions cell of the domains is located in an industrial area and it is possible to see this cell in both scenarios but the vehicular emissions are smaller when the MMA methodology is applied, as we can see by the figures.



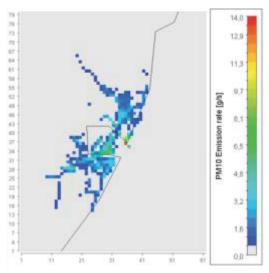


Fig. 3. IEMA's current inventory for PM10.

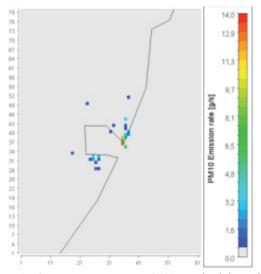


Fig. 4. New inventory using MMA methodology for PM10.

## **EXPECTED RESULTS AND CONCLUSIONS**

For CMAQ simulations is expected the same discrepancies between the two dispersions scenarios, because one inventory is overestimating the emissions and the other is probably underestimating the emissions. These differences in both situations implies that the RMGV emissions inventory needs a huge review.

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# TRAFFIC AND AIR POLLUTANT EMISSIONS MODELLING IN BELO HORIZONTE AT LOCAL SCALE

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Abstract: The identification of vehicle pollutants contribution to air quality, as well as the estimation of the main effects of these pollutants emissions through the use of computational modeling, presents as an important research opportunity for the more densely populated urban areas with a representative vehicle fleet. A Brazilian example of these areas is the city of Belo Horizonte, capital of the State of Minas Gerais, with the third largest metropolitan region of the country. Belo Horizonte is located in a territorial area of 331 km<sup>2</sup> with a population of approximately 2.5 million inhabitants. The city vehicle fleet is mostly made up of cars (69.5%), followed by light commercial vehicles (14.6%), motorcycles (13.2%), trucks (2.2%) and buses (0.5%). Regarding fuel consumption, flex fuel vehicles are the majority (54.2%), and the other fuels are distributed as follows: gasoline (34.9%), diesel (5.7%), alcohol (2.9%), NGV (0.6%) and others (1.7%). With respect to vehicular sources, specifically, emission and air quality models do not have emission inventories in their internal data structure, and the user is responsible for entering such information. In this context, this work consisted in the integration of the atmospheric emission model PREP-CHEM-SRC (A processor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models) with the macroscopic traffic model EMME/2 (Equilibre Multimodal/Multimodal Equilibrium), which has as one of the results the road network of the selected study region and its respective vehicle flows, from the modeling and calibration of the results of an OD (Origin/Destination) research. The input data of the integrated model are emissions inventory data, for example emission factors, and variables such as vehicle type, fuel type, fleet age and daily flow behavior (day cycle), in addition the emissions model information. These data were incorporated into the integrated model with the objective of identifying the real contribution of road vehicles use in the emission of pollutants in an urban center. As preliminary results it was possible to model emissions of pollutants CO, NOx, HC (hydrocarbons), HCHO (aldehydes) and PM (particulate matter) to Belo Horizonte due to the vehicle flows in the roads which make up the city's road network.

Keywords: Emission Model, traffic model, road vehicles, pollutants emissions, air pollution.

### **INTRODUCTION**

Air pollution can be defined as the presence in the atmosphere of one or more contaminants in quantity and duration that are or are likely to be harmful to their properties, to humans, plants, animal life, or interfere with the comfort of life or in the use of properties (Vianello e Alves, 2012).

The increase of urban air pollution due to the installation of industries near the big cities and the increase of the number of vehicles circulating in the urban centers is a great environmental problem in current days, directly affecting the population health, especially children and elderly people, besides the fauna, flora and materials. Growing concern about the environment and human health has led to a significant increase in scientific interest in issues related to meteorology and air quality. The scientific interest in particulate matter in the atmosphere is related to its effects on the climate,

environment, visibility and risk to human health. In 2012, a study by the World Health Organization (WHO) estimated that 12.6 million deaths worldwide, accounting for 23% of all deaths, were attributed to environmental changes. In children younger than five years, up to 26% of all deaths could be avoided if environmental risks were removed (Prüss-Ustün et al., 2012). In addition, WHO has shown that more than two million premature deaths can be attributed to the effects of air pollution in urban areas (WHO, 2005).

In urban areas, the main sources of air pollution are the vehicular sources, mainly due to the burning of fuels such as ethanol, gasohol (gasoline and ethanol) and diesel (Sbayti et al., 2001; Alonso et al., 2010; Albuquerque et al., 2012; Andrade et al., 2012; Mahmod et al., 2013; Uddin, 2013).

Brazil has become an example for studies of air pollution by vehicular emissions due to the diversity of its fleet, the different types of fuels and various



emission control technologies (Kumar et al., 2016). According to Pacheco et al. (2017) by the end of 2015, the country had approximately 42.6 million vehicles in its vehicle fleet. Among the three main metropolitan regions of the country, São Paulo (RMSP), Rio de Janeiro (RMRJ) and Belo Horizonte (RMBH), RMSP had more than 7 million vehicles, followed by RMRJ with 2.7 million and RMBH with 1.7 million vehicles (SINDIPEÇAS, 2016; IBGE, 2015). The Southeast region stands out when it comes to the increase in the number of vehicles, since its fleet corresponds to 52% of the national fleet and had an average growth of approximately 43%, from 2012 to 2015. The state of Minas Gerais represents 21% of the fleet in the southeast region and grew by approximately 37% in the last 13 years (CNT, 2016).

The identification of vehicle pollutants contribution to air quality, as well as the estimation of the main effects of these pollutants emissions through the use of computational modeling, presents as an important research opportunity for the more areas denselv populated urban with representative vehicle fleet. In this context, this work consisted in the integration of the atmospheric emission model PREP-CHEM-SRC (A processor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models) with the macroscopic traffic model EMME/2 (Equilibre Multimodal/Multimodal Equilibrium), which has as one of the results the road network of the selected study region and its respective vehicle flows, from the modeling and calibration of the results of an OD (Origin/Destination) research.

## **METHODS**

### • Characterization of the study area

Belo Horizonte, capital of the State of Minas Gerais, with the third largest metropolitan region of the country was chosed for this study. Belo Horizonte is located in a territorial area of 331 km<sup>2</sup> with a population of approximately 2.5 million inhabitants.

The city vehicle fleet is mostly made up of cars (69.5%), followed by light commercial vehicles (14.6%), motorcycles (13.2%), trucks (2.2%) and buses (0.5%). Regarding fuel consumption, flex fuel vehicles are the majority (54.2%), and the other fuels are distributed as follows: gasoline (34.9%), diesel (5.7%), alcohol (2.9%), NGV (0.6%) and others (1.7%). The age of the fleet is also a relevant data for this research and is characterized by vehicles aged 0 to 5 years (40.6%), 5 to 10 years (25.4%), 11 to 15 years (9.8), 16 to 20 years (7.5%), 21 to 25 years (5.7%), 26 to 30 years (3.1%), 31 to 35 years (2.9%), 36 to 40 Years (2.8%) and over 40 years (2.6%) (DETRANMG, 2016).

### Transport Model EMME/2

The EMME / 2 macroscopic transport model (Equilibre Multimodal / Multimodal Equilibrium), whose input data is the OD (Origin / Destination) research whose basic objective is to identify the origins and destinations of the trips performed by the different types of vehicles in a given track system (DNIT, 2006).

The OD research is introduced in the EMME / 2 matrix format and information such as traffic zones, centroids, links, regular nodes and lines are also registered. The elements of the road network used in this research are shown in table 1.

Table 1:Elements of the road network

Elements	Amount
Modes	11
Centroids	1.916
Nodes	12.469
Links	37.395
Types of vehicles	18
Routes	4.062
Routes segments	181.198

#### • Emission Model PREP - CHEM - SRC

It is known that for a good quality of the results obtained by the numerical models of emissions and air quality it is necessary a better knowledge about the sources of emission and also the measurement of aerosols and their precursors. The input data of the integrated model are emissions inventory data, such as emission factors, and variables such as vehicle type, fuel type, fleet age and daily flow behavior (day cycle). These data were incorporated into the emissions model with the objective of identifying the real contribution of the use of road vehicles in the emission of pollutants in an urban center. It is worth mentioning that it will be necessary to improve the representation of the sources of the current emissions inventory, by updating the city's emissions inventory.

#### FINDINGS AND ARGUMENT

Preliminary flow data from the EMME / 2 model provided by BHTrans were coupled to the PREP-CHEM-SRC emission model. The result of the EMME / 2 model that contains the flow of vehicles traveling in Belo Horizonte was converted into a LAT (Latitude), LON (Longitude), FLUX (flow) file and interpolated into the grid of the national emissions model. The FLUX was partitioned into vehicle types and age according to data provided by DETRAN of Minas Gerais; The emission factors were extracted from the CETESB Emissions Inventory and the National Vehicle Emissions Inventory (MMA, 2014; Cetesb, 2016) for pollutants CO, NOx, HC (hydrocarbons), HCHO (aldehydes)



(particulate material). The coupled modules were written in the Fortran90 language within the PREP-CHEM-SRC emissions model code and were defined as emme\_parameters and emissions\_factors\_cetesb. The preliminary results of this model are the emissions of vehicular pollutants in kg.m<sup>-2</sup>day<sup>-1</sup> according to the flow of vehicles that travel in the urban roads of the Belo Horizonte road network. The preliminary results of the emission of CO in the RMBH as shown in figure 1.

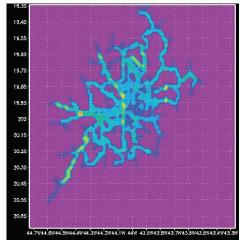


Fig. 1. CO Emission in RMBH

## **EXPECTED RESULTS AND CONCLUSIONS**

The results of this project are expected to assist managers and decision makers in planning vehicle emissions control actions, implementing improvements to the transportation infrastructure, and adopting regulatory measures for the use of the private vehicle. The research for improvements in vehicular technologies and the increase in fuel quality are also actions that may be based on the result of this work.

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# ANALYSIS OF THE IMPACT OF EURICO DE AGUIAR SALLES-ES AIRPORT EXPANSION PROJECT IN AIR QUALITY IN THE GREAT VITÓRIA REGION

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Abstract: Air pollutant emissions from aircrafts during landing and take-off procedures have a potential to deteriorate air quality. Eurico de Aguiar Salles airport, located in Vitória-ES, has been expanded and its annual transportation capacity of will be extended from the current 3.5 million to 6.2 million of passengers in 2025. In order to predict the impact in air quality due to airport expansion and verify modeled results when emission source is treated as two distinct types (area and volume),  $SO_x$  emission rates for two different scenarios (current and future) were quantified by using Tier 2 methodology available in 1.A.3.a Aviation do Emission Inventory Guidebook 2016 elaborated by European Environmental Agency (EEA). These emission rates were placed into AERMOD modeling system. Besides, three different heights of release (2 m, 250 m e) which has the same emission rate were considered. Results indicated that maximum 24-hour and annual  $SO_x$  concentrations are higher when emission source is represented as area than when it is a volume source for the current scenario. In case of future scenario, concentrations generated due to volume source are highest. Finally,  $SO_x$  emissions from Vitoria airport expansion will lead to impacts in the air quality higher than current scenario.

Keywords: Vitoria airport, air quality, Great Vitoria Region, SO<sub>X</sub>

## **INTRODUCTION**

In 2015, the Vitoria airport expansion project was restarted. This construction will contribute to state economic development due to possibility to receive international flights as well as increase of cargo shipping to other Federal States (ANAC, 2017).

However, the new airport can results in significant effects to air quality. According to IEMA, the ports and airports segment is the third highest pollutant emitter source in the Great Vitória Region (2013). Mainly for  $SO_2$  emissions, this sector contributes to 22% of the total emissions (IEMA, 2013).

In this context, this study aims to demonstrate the impact of Vitoria airport (current) and its expansion (future) in air quality in Great Vitória. Additionally, modeling results are compared to two different types of source: area and volume.

Besides, in order to simulate aircraft performance during take-off and landing, emissions from these sources were split into distinct heights: 2m, 250m and 500m.

## METHODS Study Area

The study area (Figure 1) contains the following cities: Serra, Vila Velha, Cariacica, Viana, Santa Leopoldina and Vitória, totalizing 1,600km² (40x40 km) with grid cell 500x500m.

Figure 1 also presents seven receptor points (RP) distributed across the study area, where pollutant concentrations were analyzed.

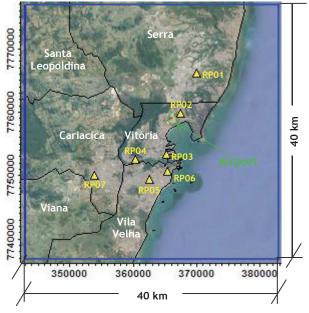


Figure 1. Study area and receptor points (RP).

## **Emission scenarios**

This study compares current and future scenarios. For the current scenario,  $SO_X$  emissions were quantified for 2015 when roughly 3.5 million of passengers flew. Future scenario was defined based on emissions caused by 6.2 million passengers traveling in 2025. This estimate was determined by National Agency of Civil Aviation (ANAC) in 2005.



Figure 2 exhibits the growth of the operational capacity and LTO (landing and take-off) in Vitória airport through the years (2010, 2015-current scenario and 2025-future scenario).

In addition to the increment in  $SO_X$  emission rates, modifications on the airport runway (area and location) in the future scenario were considered.

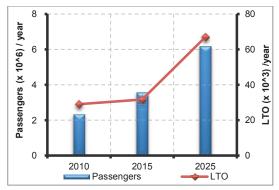


Figure 2. Operational capacity through years for Vitória airport

#### Aircraft Data

Aircraft types were defined based on consultations on the airlines companies website which work at the Eurico de Aguiar Salles airport. These aircrafts were classified regarding to their number of seats as contained in the ANAC document.

### **Emission inventory**

In order to quantify emissions from aircrafts in the Vitoria airport, Tier 2 methodology available in 1.A.3.a Aviation do Emission Inventory Guidebook 2016 elaborated by European Environmental Agency (EEA) in 2016 was used for operations which involves LTO cycle. In this study, only regular domestic flights were considered. The following equation was applied to calculate emission rate per aircraft:

$$ER = \sum LTO x EF$$
 (Eq.1) Where:

ER = pollutant emission rate [kg/year]

 $\sum LTO$  = number of LTO cycles per aircraft type [year<sup>-1</sup>]

EF = pollutant emission factor [kg/LTO]

LTO data were obtained from Brazilian Company of Airport Infrastructure (INFRAERO) for 2015 and from National Agency of Civil Aviation (2005) for 2025. Besides, fleet composition for both study scenarios was acquired from ANAC document, utilized to allocate LTO per aircraft type.

The  $SO_X$  emissions factors were extracted from EEA (2013). In case of aircrafts not listed, a similar aircraft type was used.

## Air quality modeling

Emission rates as well as physical features of the sources were placed into an air quality model, AERMOD View® version 9.1.0. Two distinct scenarios were run: one considering maximum 24 hour and another with annual average.

Moreover, surface meteorological data recorded in the surface station located in the Vitória airport, for the entire year (2014) were utilized.

Simulations were performed assuming emissions as area or volume sources and  $SO_X$  emissions (current and future scenario) were split into three different heights along the airport runway length (Figure 3). This procedure attempts to reproduce aircraft performance during take-off and landing operations phase (LTO).

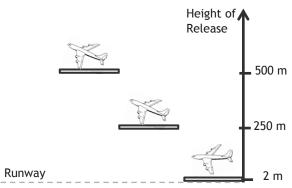


Figure 3. Schema of Variation of Height of Release

## **RESULTS**

Table 1 exhibits calculated emission rates by applying the EEA methodology as well as area size considered as emission source in the simulation with AERMOD.

Table 1. Emission Rates

Scenario	Area	Volume	Source Area
Scenario	[g/s*m <sup>2</sup> ]	[g/s]	[m²]
Current	0.000006	0.542	86,750
Future	0.000015	1.904	125,000

In the Table 2, maximum 24-h  $SO_X$  concentrations (short-term) and annual (long-term) are presented. These concentrations from simulations, in which area and volume sources were considered, were compared with each other.

For the current scenario, modeled concentrations when source is defined as area are higher. In case of short-term, modeled concentrations when volume source emits  $SO_X$  represent 60% of the concentrations obtained from an area source. For the long-term, this difference is more significant. Modeled concentrations for area source are roughly 4 times greater than modeled concentrations for volume source.



However, for the future scenario, this pattern is not noticed. For volume sources, concentrations were higher than concentrations due to area source for both temporal references considered (24-hour and annual averages). It would be also emphasized that, besides the emission rate is higher in the future scenario, airport runway location will be altered.

Table 2. SO<sub>x</sub> Modeled Concentrations

	rable 2: 50 modeled concentrations					
Scenario	24 hours [µg/m³]		Annual [µg/m³]			
Scenario		Area Volume Area		Area	Volume	
	Current	62,21	37,59	17,09	4,22	
	Future	116,58	176,40	23,43	24,84	

To exemplify, in the Figure 4, maximum 24-hour  $SO_X$  concentrations for each receptor point considering area and volume sources for the current scenario are compared.

Among the receptor points analyzed, concentrations at the RP02 are highest, independent of physical features of the emission source and how they were considered in the simulation (area or volume).

In all of the other 6 receptor points considered, concentrations caused area source are higher than  $SO_X$  concentrations as results of a volume source.

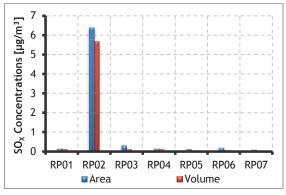


Figure 4. Maximum 24-houras [SO<sub>X</sub>] per RP -Current Scenario [µg/m³]

## **CONCLUSIONS**

This study demonstrated that emission sources modeled for the Vitoria airport in the current scenario when defined as area source leads to a higher impact in the air quality, if compared to volume source, considering  $SO_\chi$  24-hour and annual concentrations.

Nonetheless, for the future scenario, sources simulated as volume generated concentrations

higher than those caused by area source, in both temporal references analyzed.

Over all receptor points, maximum  $SO_\chi$  24-hour concentrations for area source were higher than when volume source was considered.

Finally, independent of the type of emission source, the prediction for the future scenario indicates a greater impact in air quality than the current scenario.

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# EMISSIONS INVENTORY FOR SOUTHEAST OF BRAZIL: THE INFLUENCE OF THE METROPOLITAN AREAS ON THE REGIONAL AIR QUALITY

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Abstract: Actually more people are living in urban centers and the air pollution of these large urban centers is caused by a variety of sources, with major emissions coming from vehicular sources, followed by industrial sources and also there are biogenic emissions, biomass burning and influence from other cities emissions. Emissions of pollutants, especially in large urban centers, affect air quality negatively, not only on a local scale, but also on larger scales. Pollutant dispersion studies applying emissions inventories are important for understanding the processes of transport, chemical reactions and pollutants transformations in the atmosphere, but good emissions inventories for regional scales are difficult, even more for local scales.

Brazilian Southeast has large metropolitan areas, like in the states of São Paulo, Rio de Janeiro, Minas Gerais and Espírito Santo and there are no inventories for all these regions, only a few urban areas. Thus, it is a great challenge to study atmospheric dynamics, especially at large scales, and the influence of large urban centers on each other, since the scarcity of local emissions inventories makes it difficult to apply in air quality models. Therefore, the objective of this work is to apply PREP-CHEM-SRC v.1.5 (a processor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models) to create an emissions inventory of pollutants for Brazilian Southeast from global emissions database and with Alonso et al.(2010) update for these emissions for Brazilian Southeast, both implemented in PREP-CHEM-SRC.

Keywords: Urban areas, global inventory, CMAQ, PREP-CHEM, Brazil.

## **INTRODUCTION**

Worldwide, more people live in urban areas than in rural areas, with 54 percent of the world's population residing in urban areas in 2014 and by 2050, 66 per cent of the world's population is projected to be urban (UN, 2014).

Population growth in large cities leads to air quality degradation at local and regional scale, among other problems. Toxic trace gases emitted to the troposphere and their oxidation products represent a direct human health risk (Alonso et al., 2010). However, the emissions from large cities do not affect only local scale and the population of these cities, but reach large distances and can degrade air quality in "clean" regions or intensify the air pollution in other locations.

The necessity of good information for air quality modeling is mandatory. Emissions estimates are generally difficult to build, because of the complexity of the emissions and the variables that should be consider in estimation, like in case of mobile sources, which should consider fuel type and consumption, vehicle technology and the fleets condition and use (Gallardo et al., 2012).

In addition to vehicle emissions, there are air pollutants and greenhouse gases emissions from fossil fuel, biofuel and biomass burning, agricultural activities, biogenic emissions, industrial emissions

and human energy (Freitas et al., 2011; Dang and Unger, 2015).

With the increasing use of numerical atmospheric chemistry modeling on local, regional and global scales, the creation of inventories with wider coverage and analysis of the interaction among the various scales have become essential (Alonso et al., 2010)

In this context, Freitas et al. (2011) developed PREP-CHEN-SRC a tool that allows the build of emissions inventories from local to global scale and contemplates most recent emissions database for gases and particles for urban/industrial (RETRO/EDGAR), biogenic emissions (GEIA/MEGAN), biomass burning (3BEM/GFEDv2), volcanic, biofuels use and burning of agricultural waste sources.

In general, the global scale emissions inventories are lacking in detailed representation of local scale emissions, like in South America, where information for emission inventories are scarce. Thus Alonso et al. (2010), in order to update emissions for South America from global inventory of PREP-CHEM-SRC, developed a consolidation of regional urban emissions that integrates information from local inventories of vehicle emissions into existing global databases.

The construction of a emissions inventory for Brazilian southeast is part of a project that aims to simulate this region in CMAQ model to evaluate the



simulations and describes the influence of great urban centers in each other and try to understand the dynamics of pollutant dispersion. Thus, the goal of this preliminary work is to apply the PREP-CHEM-SRC to create emissions scenarios.

## **METHODS**

It were set a domain the covers the entire area ou Brazilian Southeast, so was build a modeling domain that is centered at coordinates 43.969°S, 19.816°W, with 2061km by 1737km and 9km grid resolution, Fig.1 shows the domain covering the study area. The cases were analyzed for July 2015 during winter season in Brazil when the pollutant concentration increases.

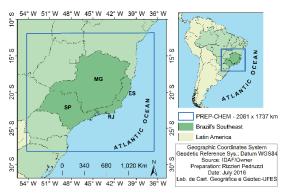


Fig. 1. Brazil's southeast domain.

It was applied the PREP-CHEM-SRC v.1.5 to generate emissions and were built two scenarios. The first used the "default" global emissions inventories available:

- RETRO/EDGAR anthropogenic emissions:
- · biomass burning emissions;
- MEGAN for biogenic emissions; and
- GOCART for aerosol.

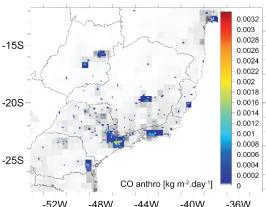
The second scenario considered the same global database but using, the updated made by Alonso et al. (2010) to improve the emissions resolution.

## FINDINGS AND ARGUMENT

The preliminary results are for July 01 and the emissions for CO are shown in Fig. 2 and Fig. 3. A significant difference is observed between the two databases, not only for the emission resolution, but also for the emission points and total pollutants emitted per km². The scenarios with updated emissions show more significant emission points and great urban centers like São Paulo, Rio de Janeiro, Belo Horizonte, Curitiba and Vitória are with higher peaks of emissions. Likewise great urban centers, inland cities are more prominent with higher emissions peaks.

This difference may be due to the methodology applied by Alonso et al. (2010), which extrapolated

the available emissions information to municipalities without inventories. Furthermore, Alonso et al. (2010) also emphasize the considerable differences between the two inventories.



-52W -48W -44W -40W -36W Fig. 2. Emissions of anthropogenic CO updated.

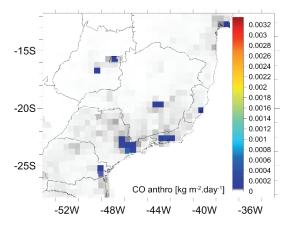


Fig. 3. Emissions of anthropogenic CO "default".

Fig.4 and Fig.5 show the results for  $PM_{10}$  and Fig.6 and Fig.7 the results for  $PM_{2.5}$ , and was observed the same behavior and differences between the inventories (Updated and default) as detected for CO.

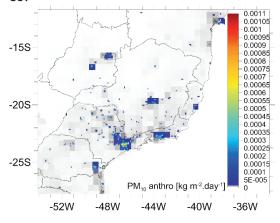


Fig. 4. Emissions of anthropogenic PM<sub>10</sub> updated.



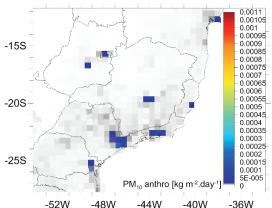


Fig. 5. Emissions of anthropogenic PM<sub>10</sub> "default".

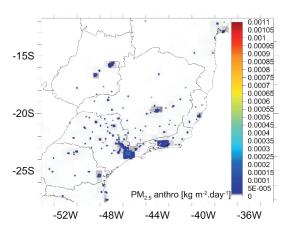


Fig. 6. Emissions of anthropogenic PM<sub>2.5</sub> updated.

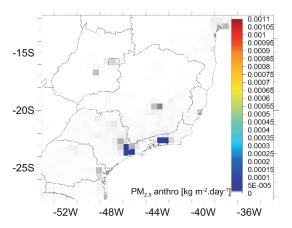


Fig. 7. Emissions of anthropogenic PM<sub>2.5</sub> "default".

## **EXPECTED RESULTS AND CONCLUSIONS**

Obtaining a high-resolution emissions inventory is complex and requires many input data to achieve high quality results, so it is important to note that the PREP-CHEM-SRC is a great tool for developing these inventories, especially for regions that do not have this information. For Brazilian Southeast the scenarios with updated emissions have a high

resolution and indicates more areas with pollutant emissions, characteristic that have to be validated with air quality simulations.

The validation of these emission inventories will be done with its application in photochemical models and the comparison of the results with measured data from monitoring stations. This will provide a depth analysis on the emissions and dispersion behavior of the pollutants and it is expected that the inventory with the updates achieve better results.

It is also expected that with this increase of pollutant emissions of the updated inventory, the urban centers will have a greater impact on each other.

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# Case Study on Espírito Santo's Carbon Dioxide Emissions and Geological Storage

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Abstract: According to the Kyoto Protocol, planning an ecologically sustainable future is the greatest challenge of the 21st Century. Current patterns of energy resources and energy use are shown detrimental to the welfare of mankind in the long run. The integrity of essential natural systems is already at risk because of the climate change caused by the intense emission of greenhouse gases into the atmosphere. In this context, the Carbon Capture and Storage (CCS) technology is a promising activity that aims to reduce the emission of gases responsible by the greenhouse effect and climate change mitigation through  $CO_2$  capture, transport and storage in suitable geological formations (saline aquifers, coal reservoirs, oil and gas reservoirs). However, the lack of maturity of the private and public sectors, with respect to the management of projects of this nature and their widespread use, prevents the advancement of such technologies in the state of Espírito Santo and therefore in Brazil. Inserted in this context, in this case study and brief literature review, we address the  $CO_2$  amissions at Espirito Santo and the geological environments conducive to the application of CCS projects at Espírito Santo state, Brazil. Therefore, it is concluded that CCS projects are possible deployment in the state of Espírito Santo, this is because in addition to the geological structure of oil and gas reservoirs in the Espírito Santo basin contribute to good results (as, in most cases, are sandstone reservoirs with presence of seal rock), the potential of the potential of hydrocarbon fields studied in this paper (Gas Filds Canapu, Cangoá, Peroá and Camarupim) deserve national recognition.

Keywords: Carbon Capture and Storage. Carbon Dioxide Emissions. Climate Change. Global Warming.

## **INTRODUCTION**

Since the Industrial Revolution in the 18th century, fossil fuels have been used as an energy source, contributing to increase the concentration of  $\text{CO}_2$  (carbon dioxide) in the atmosphere. In Figure 1, an increasing global concentration of  $\text{CO}_2$  in the atmosphere (in parts per million - ppm) can be observed during the period of 1980-2016, this period is characterized by a significant increase in the use of fossil fuels as an energy source.

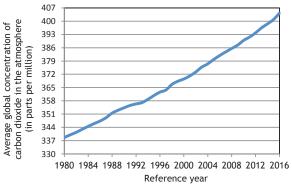


Figure 1. Concentration of carbon dioxide in the atmosphere over the period 1980-2016.

Due to this increase in  $CO_2$  emissions and its consequences, the traditional concept of global development incorporated environmental development. This incorporation resulted in the creation of a broader concept referred to as Sustainable Development, which is based on the inseparability of economic, social and

environmental development. The report "Our Common Future", released in 1987 (also known as the Brundtland Report), brought to attention the need of a new type of development that is able to sustain progress across the globe and to be achievable by developing countries in the long run (GAUSS, 2008). In this way, the concept of sustainable development, i.e., "meeting the needs of the present without compromising the ability of future generations to meet their own needs" (CMMAD, 1991) became established. According to Costa (2009), human actions, such as the burning of fossil fuels (coal, oil and natural gas), the use of aerosols, and biomass combustion, liberate Greenhouse Gases (GHG) into the atmosphere. Such gases are also released by other basic and intense economic activities, such cultivation and livestock production. The most abundantly released gases and therefore the most responsible for the greenhouse effect are nitrous oxide  $(N_2O)$ , methane  $(CH_4)$  and carbon dioxide  $(CO_2)$ .  $CO_2$  in particular has harmful effects on the environment, primarily due to the increasing speed with which it is being produced to meet the needs of today's consumerist lifestyle. The emission of GHG, especially CO<sub>2</sub>, causes global warming and consequently climate changes (IPCC, 2005). Carbon sequestration through the capture, transport and geological storage of CO<sub>2</sub> (CCS technology, Carbon Capture and Storage) is an important alternative for reducing emissions and stabilizing the atmospheric concentration of GHGs from a sustainable development perspective. It is known that the occurrence of natural  $CO_2$  accumulations (fields similar to natural gas fields) have great



potential as geological formations to store gases for thousands or even millions of years (KETZER, 2005; KETZER, 2008). With the inclusion of CCS as an activity of the Clean Development Mechanism (CDM) project, companies will invest more in projects of this nature due to the potential to generate Certified Emission Reductions (CERs), which are greatly advantageous for a company's image (DELGADO, 2007). According Frondizi (2009), the CDM is a mechanism based on the development of projects for which the private sector is responsible. Carbon credits are certificates that authorize greenhouse gas emissions to the atmosphere. Initially, the major industries in a country are selected and goals are set to reduce their emissions. Companies receive negotiable bonus in proportion to responsibilities, where each bonus, in dollars, is equivalent to a ton of pollutants (KHALILI, 2003). Companies that fail to comply with the progressive reduction established by law must buy certificates from successful companies. The system has the advantage of allowing each company to establish its own pace of compliance with environmental laws. These certificates can be traded on the Stock and Commodities Exchanges (KHALILI, 2003; RAVAGNANI, 2007; ÁVILA, 2009; REIS JR, 2012). the main obstacle for implementation in Brazil is the high cost of deployment and maintenance (RAVAGNANI, 2007). However, increased knowledge derived from research studies and practical experience contributes to the minimization of the involved costs. Also beneficial in this regard are the contributions of new technologies in the fields of capture, transport and geological storage of CO<sub>2</sub>. This study therefore consists of an exploratory and descriptive-analytical analysis of an important alternative for reducing emissions and stabilizing the atmospheric GHG concentration based on scenarios for the application of CCS projects. To achieve this objective, a literature review of the technology required for the geological storage of CO<sub>2</sub> was performed. Therefore, this research provides a discussion on the feasibility of CCS projects to reduce the emissions of polluting gases into the atmosphere.

## **METHODS**

This study consists of an exploratory and descriptive-analytical analysis of an important alternative for reducing emissions and stabilizing the atmospheric GHG concentration based on scenarios for the application of CCS projects. To achieve this objective, a literature review of the technology required for the geological storage of  ${\rm CO_2}$  was performed. Therefore, this research provides a discussion on the feasibility of CCS projects to reduce the emissions of polluting gases into the atmosphere. This paper studied the

potential storage in hydrocarbon fields - Canapu, Cangoá, Peroá and Camarupim.

### FINDINGS AND ARGUMENT

According to SEEG (2014), in the course of 10 years, Espírito Santo presented an approximate increase of 70.2% in greenhouse gases emissions to the atmosphere, when compared to what the state issued in 2003 and in 2013. Considering this rate (70.2% per decade) and the value of the total  $\rm CO_2eq$  emission reported in the ES inventory, a scenario with the following behavior of the GHG emission curve for the atmosphere in the ES (Figure 2).

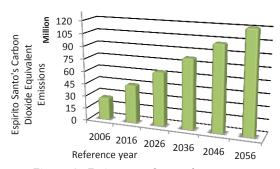


Figure 2. Estimates of greenhouse gases emissions to the atmosphere in Espírito Santo.

Hendriks (2004) shows that the compressibility of  $CO_2$  under typical reservoir studies is significantly larger than the compressibility of natural gas. This means that a void space within the reservoir can store a much larger volume of  $CO_2$  (measured at standard pressure and temperature conditions) than methane. Additionally, the mass of the stored  $CO_2$  is far greater than the mass of the natural gas because the weight of a mole of  $CO_2$  is much greater than that of methane. As a conservative measure, it was assumed that 75% of the void space created by exploiting natural gas fields could be replaced with  $CO_2$ . The equation 1 and equation 2 can help us calculates the  $CO_2$  storage potential.

$$M_3CO_2 = 0.75 * Vg_{tot} * R_{CO2/CH4} * \rho_{CO2}$$
 (1)

$$R_{CO2/CH4} = 2 * 10^{-7} * h^2 - 0.0015 * h + 4.1707$$
 (2)

 $M_3CO_2$  is the volume of  $CO_2$  that can potentially be stored (Mg);

0.75 is a conservative measure, such measure represents that 75% of the area can be filled by  $\text{CO}_2$ ;

 $V_{gtot}$  is the total gas volume (m<sup>3</sup>);

 $R_{CO2/CH4}$  is the volumetric ratio at reservoir depth (no unit): ration  $CO_2/CH_4$ ;

 $\rho_{CO2}$  is the density  $CO_2$  at surface conditions,  $1.98 \times 10^{-3} \; \text{Mg/m}^3;$ 

h is the reservoir depth.



With regard to geological storage, by means of the study, it can be seen that the Peroá Gas Field has the largest storage potential (more than 112.655 million tCO<sub>2</sub>), followed by the Camarupim Gas Field (38.231 million tCO<sub>2</sub>), the Canapu Gas Field  $(28.515 \text{ million } tCO_2)$  and, with the lowest potential, Cangoá Gas Field with approximately 11.617 million  $tCO_2$ . The four fields together have a potential of approximately 191.018 million tCO<sub>2</sub> (Figure 3). By means of the analysis, it is evident that, because it has the greatest  $CO_2$  storage potential (2.95 times greater than the Camarupim Gas Field, second place), the Peroá Gas Field will always have the highest gross income coming from carbon credits, unlike the Cangoá gas field, which has the lowest  $CO_2$  storage potential (9.70 times lower than the Peroá gas field) and, consequently, the lower gross income from carbon credits.

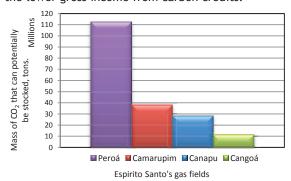


Figure 3. Estimates of mass of  $CO_2$  that can be stocked at gas fields in Espirito Santo.

Therefore, it is concluded that CCS projects are possible deployment in the state of Espírito Santo, this is because in addition to the geological structure of oil and gas reservoirs in the Espírito Santo basin contribute to good results (as, in most cases, are sandstone reservoirs with presence of seal rock), the potential of hydrocarbon fields studied in this paper (Canapu, Cangoá, Peroá and Camarupim) deserve national recognition.

### **CONCLUSIONS**

Carbon Capture and Storage (CCS) is a technology that can capture up to 90% of the carbon dioxide (CO<sub>2</sub>) emissions produced from the use of fossil fuels in electricity generation and industrial processes, preventing the carbon dioxide from entering the atmosphere. The increase in GHG emissions, primarily  $CO_2$ , to the atmosphere is due to the increase in world energy demand and is causing climate change and global warming. The need to mitigate climate change has led to the development of technologies to reduce the emission rate of these gases into the atmosphere. Carbon sequestration or CO<sub>2</sub> capture, transport and geological storage (CCS) is based on the principle of "returning carbon to the underground". CCS is an important alternative in reducing emissions and

stabilizing the atmospheric concentration of greenhouse gases from a sustainable development perspective.

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# Session 4 Model Evaluation and Analysis



# WRF MODEL VALIDATION FOR THE METROPOLITAN REGION OF BELO HORIZONTE, BRAZIL

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Abstract: 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. This paper presents the validation of the meteorological conditions using the Weather Research and Forecasting (WRF) model for the third most populated region in Brazil, the Metropolitan Region of Belo Horizonte (MRBH), composed by thirty four cities and located in the State of Minas Gerais. The simulation was permormed during 31 day (July 2015) to better represent the dry season of this area, the winter conditions of the MRBH. Simulations results were analyzed statistically against data from four meteorological stations of the National Institute of Meteorology (INMET).

Keywords: WRF, Validation, Metropolitan Region of Belo Horizonte, Meteorological stations.

#### **INTRODUCTION**

Urban regions with significant densities support the development of many and diverse activities that have the potential to modify, locally or regionally, the natural composition of the air as well as the balance of energy flow between the surface and the boundary layer by the land use changes (Offerle et al., 2005). The most affected layer, and also the most important one given its effect on the health and well-being of the population, is the troposphere. This compartment receives atmospheric emissions from anthropic activities, and also from natural sources, and disperses them according to its circulation dynamics.

According to the World Health Organization (WHO) (2016), approximately 3 million deaths a year are linked to exposure to outdoor air pollution. The strongest effects of air quality on health are attributable to fine particulate matter (PM2.5), followed by ozone (O3) and nitrogen dioxide (NO2). Thus, efforts within the research community to understand the local meteorology and air quality of urban areas have, considerably, increased over recent years. Meteorological data are key inputs in models such as CMAQ (Community Multi-scale Air Quality), in which is possible to simulate the distribution of emissions sources, long-range transport, and the ability of atmosphere to dilute pollutants.

The data required to understand the dynamics of the atmosphere involves the knowledge of processes and complex variables that also can be estimated by numerical models. Weather Research and Forecasting (WRF-ARW) is one of the most widely used meteorological models in mesoscale weather prediction. This computational resource can generate atmospheric simulations once the parametrizations related to several physical processes such as turbulence, convection of cumulus clouds and heat transfer using preprocessed predictions by a global meteorological model have been defined.

In the Metropolitan Region of Belo Horizonte (MRBH), located in the State of Minas Gerais, Brazil's southeast, very few studies have been developed in the area of meteorological modeling compared to other capitals in the country such as São Paulo/SP, Rio de Janeiro/RJ and Vitória/ES. With a territorial extension of 9,473 km<sup>2</sup>, the mentioned region currently formed by 34 cities, including the capital, Belo Horizonte, presented, in 2010, more than 4.8 million inhabitants which represented almost 25% of the state's total population. This region is responsible for producing 40% of gross domestic product of Minas Gerais (GDP)(Brazil Atlas, 2013; Minas Gerais, 2016). The typical climate of the Metropolitan Region of Belo Horizonte, according to the classification of Köppen-Geiger, is Cwa (humid subtropical climate) (ALVARES et al., 2013), in which the rainy season is concentrated in the months of November, December and January, and the dry season in June, July and August.



Thus, given the importance of air quality in the health of the population and representativeness of the mentioned region, this presents paper the validation of the meteorological condition in the RMBH, using the WRF model, for a month in the period of winter, in which conditions to dispersion are less favored due to the low intensity of rainfall and atmospheric stability. The purpose of this type of evaluation is to check the accuracy of the model applied in the representation of the real system, by comparing the output obtained experimentally with the model's prediction to the data observed in meteorological stations.

### **METHODS**

### Meterological modeling

The meteorological simulations were performed for the whole month of July of 2015, period of winter in the MRBH and low on precipitation intensity, by the non-hydrostatic, mesoscale Weather Research and Forecasting model, version 3.6.1. Four nested domains, centered at the coordinate19°48'57.60"S 43°58'08.40"W, have been set up: a larger domain on 27 km spatial resolution, the second domain on 9 km resolution. the third on 3 km resolution and finally, the innermost domain on 2 km resolution. The National Centers for Environmental Prediction (NCEP) Global Forecast System (GFS) data on a 0,5 x 0,5° horizontal resolution have been used to provide the initial and boundary conditions required by the WRF model while 32 sigma layers have been used for the vertical resolution of the model. A spin-up of 48h was applied in the simulations so the impacts of trading conditions were minimized.

The parameterizations chosen to simulate the meteorological conditions of the MRBH were based on the best result obtained by Reboredo et al. (2015) for the city of Bogota in Colombia, modifying only the microphysics option, as the following: WSM3 (microphysics), RRTM (longwave radiation), Dudhia (shortwave radiation), Revised MM5 Monin-Obukhov (surface layer), Noah land-surface model (land surface), BouLac (planetary bound layer) and Betts-Miller-Janjic (cumulus).

### Model validation

Simulation results were analyzed according to the statistical indexes and benchmarks (Column 3-Table 2) suggested by Emery et al. (2001). The statistical indexes are: Mean Bias (MB), Mean Absolute Gross Error (MAGE), Root Mean Square Error (RMSE) and Index of Agreement (IOA).

### Meterological modeling

For the model validation were used data from meteorological automatic surface stations of the National Institute of Meteorology (INMET), located at MRBH. The evaluated variables were: air temperature, specific humidity and vector wind. The description of the four stations used with their respective location, geographic coordinates and altitude as shown at Table 1. In addition to the mentioned stations, validation was also carried out using data from an altitude weather station, located at the Belo Horizonte International Airport/ Tancredo Neves, in the city of Confins/MG.

Table 1. Meteorological stations in the MRBH

Location - City/	Geographica	Alt.	
State	Latitude	Latitude Longitude	
Pampulha - Belo	19°53'02.20"	43°58'09.83"	854
Horizonte/ MG	S	W	
Cercadinho- Belo	19°58'48.12"	43°57'31.14"	1,200
Horizonte/ MG	S	W	
Florestal/MG	19°53'07.43" S	44°25'00.78" W	754
Rola Moça -	20°01'54.24"	44°00'40.49"	1,199
Ibirité/ MG	S	W	

#### FINDINGS AND ARGUMENT

Data obtained from the simulation as well as the data observed in the four meteorological stations were used to calculate the statistical indexes which are summarized in Table 2. Values that did not meet the benchmarking intervals are marked in red.

Table 2. WRF simulation performance evaluation using statistical indexes for the MRBH

evaluation using statistical indexes for the Milbir						
Variable	Indexes	Bench.	Flor.	R.M.	Pam.	Cerc.
	MB (K)	≤± 0.50	0,15	-2,26	0,90	-1,34
Temp.	MAGE (K)	≤ 2.00	2,43	2,41	1,36	1,66
	IOA	≥ 0.80	0,82	0,73	0,91	0,85
Wind	MB (m.s <sup>-1</sup> )	≤± 0.50	0,55	0,60	1,05	-1,94
speed	RMSE (m.s <sup>-1</sup> )	≤ 2.00	1,04	2,06	1,65	2,78
Wind	MB (°)	≤± 10.00	-5,90	9,65	-9,06	- 18,34
direction	MAGE (°)	≤ 30.00	27,56	29,66	22,24	30,35
	MB (g.kg <sup>-1</sup> )	≤± 1.00	0,08	-0,02	-0,05	-0,06
Specific humidity	MAGE (g.kg <sup>-1</sup> )	≤ 2.00	0,001	0,001	0,001	0,001
	IOA	≥ 0.60	0,53	0,49	0,58	0,56

For the variable temperature, the mean bias indicates that the parameterization is



underestimating data for the Cercadinho (Cerc.) and Rola Moça (R.M.) stations and overestimating it for the Pampulha (Pam.) station, not meeting, in the three cases, the proposed benchmarking range. The first two stations and in which the distance from the recommendation was more significant, are related to greater altitudes (1,200 m approximately). Other studies such as the one developed by Kriza et al. (2012) have also noted such fact imputing it to the limitations of WRF model related to its insufficient vertical resolution and the predominant land use class approach to calculate air temperature. The worse results, however, were obtained for the Florestal (Flor.) station in which the associated error between the simulated and observed value were substantially higher with a low index of agreement.

Wind speed also presented under overestimation beyond limits of the recommended interval being more significant for the Cercadinho station when RMSE is analyzed. In regarding to the parameterization proposed wind direction, underestimated data for the Cercadinho station as well. Mean absolute gross error also indicates the uncertainty related to the simulated data. The mentioned station sits next to a higher hill (~1,500m at northeast) which can act as an obstacle and impact on wind measures. It is also known that WRF has limitations in predicting wind direction when terrain is complex (Reboredo et al., 2015) like in this case where station is located in a green region surrounded by urbanized areas.

Lastly, the modeled data for specific humidity presented low absolute gross errors for all of the stations not meeting, however, benchmarks suggested for IOA indicating there is little agreement between results. Given the various limits of benchmarking not met, it is recommended the realization of new rounds of simulation using different parameterizations in order to improve WRF performance for the Metropolitan Region of Belo Horizonte, being this paper only a preliminary study.

## **ACKNOWLEDGMENTS**

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# Analysis of the CAM-Chem Ozone and Carbon Monoxide Global Distribution Using Derived Satellite Data

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Abstract: We present a global data set of surface tropospheric ozone (O3) and carbon monoxide (CO) with 1.0°×1.0° spatial resolution from the Atmospheric Infrared Sounder (AIRS) and Measurements of Pollution in Troposphere (MOPITT) satellite instruments for the period 2010-2014. Additionally, we compared the concentration of these pollutants with two versions of the National Center for Atmospheric Research (NCAR) Community Atmosphere Model with Chemistry (CAM-Chem) based on Model for Ozone and Related Chemical Tracers (MOZART), a component of the Community Earth System Model (CESM). In this work, we used the CAM-Chem model that considers only tropospheric chemistry and a model with the same configurations which also includes mechanisms of reactions in the stratosphere. Ozone observations (satellite from AIRS) and CO (MOPITT) were combined with CAM-Chem models results for the analysis. The comparison between the model simulations and the O3 and CO concentration satellite observations shows that both models can reproduce observed temporal and spatial distributions.

Keywords: Carbon monoxide, ozone, AIRS, MOPITT, CAM-CHEM

### **INTRODUCTION**

Both atmospheric gases and aerosols have been increasingly recognized as key components of the dynamic and complex Earth system. Earth's atmosphere and its evolution have regulated its chemistry. The impact of chemistry on the atmosphere or vice versa is a strongly coupled process that has remained one of the most challenging tasks for the modeling community. The two-way feedbacks between meteorology and chemistry are important in applications like Numerical Weather Prediction (NWP), Air Quality (AQ) forecasting, climate modeling and Earth System modeling with the details of processes represented being markedly different among the applications.

Tropospheric ozone (O3) is produced by the photochemical oxidation of carbon monoxide (CO), methane (CH4), and nonmethane volatile organic compounds (NMVOCs) in the presence of nitrogen oxides (NOx = NO + NO2). O3 is a potent greenhouse gas and harmful surface air pollutant, with implications for climate, human health, and agricultural productivity. Current global models

can capture the observed large-scale spatial and seasonal patterns of ozone concentrations but there is a large uncertainty in its driving forces, as reflected by the large differences between models in ozone production and loss rates (IPCC, 2007). The Brazilian Earth System Model (BESM) simulations have a great potential to contribute not only to the Brazilian climate modeling community, but also to the international efforts on global climate and climate change research. Currently, the Center for Weather Forecasting and Climate Studies of the National Institute for Space Research (CPTEC/INPE) in Brazil is working towards the implementation and tests of the aerosol and chemistry components in BESM. The Brazilian . Global Model (BAM) Atmospheric atmospheric component in BESM. CAM-Chem is the aerosol and chemistry component of the Community Earth System Model (CESM), from the National Center for Atmospheric Research (NCAR), based on Model for OZone and Related Chemical Tracers (MOZART) with modal representation of aerosols (MAM3), which is being implemented in BAM. This study compares the global data of CO from the MOPITT satellite with the CAM-Chem



simulations considering tropospheric chemistry. Other experiment was carried out with the same configuration and also considering stratospheric chemistry. The O3 simulations are compared to AIRS satellite in order to determine the skill of the model to represent O3 behavior.

## DATA AND METHODOLODY

In this study, we used satellite data of both pollutants. CO, from Measurements of Pollution in Troposphere (MOPITT) satellite instruments, and O3, from Atmospheric Infrared Sounder (AIRS) both with 1.0°x1.0° spatial resolution for the period January 2010-December 2014.

The simulations were designed using the CAM-Chem model with tropospheric chemistry including 103 species (experiment F\_2000\_MOZMAM\_CN), and a version including stratosphere chemistry, adding up to 122 species, including heterogeneous reactions (experiment STRATMAM3\_CN), for the same period of satellite data. The experimental design included 1.9°x2.5° lat/lon model spatial resolution (96x144 grid points) and 30 vertical levels, from surface level up to 10 hPa.

The spatial and temporal distribution of CO and O3 concentrations simulated over the globe during 2010-2014 were compared to MOPITT and AIRS satellite data, respectively.

To conduct the comparison between model and satellite data, the simulations were interpolated to MOPITT and AIRS resolution (Deeter et al., 2003, Lamarque et al., 2012, Aumann et al., 2003).

#### FINDINGS AND ARGUMENT

According to Figure 1 (upper panel), characteristic feature observed in Asia is that the highest CO concentrations occur over eastern China, around 550 ppbv, due to urban air pollution. High CO concentrations, probably associated to biomass burning, are observed over southeast Asia, in countries such as Bangladesh, Myanmar, Thailand, Laos, Cambodia, Malaysia and western Indonesia regions (around 350 ppbv) and over the Indian subcontinent (around 250 ppbv), mainly during springtime (Streets et al., 2003). In Europe, CO concentrations are in general spatially homogeneous (Figure 1, upper panel), reflecting the greater urbanization of the continent. The highest concentrations (around 250 ppbv) occur in densely industrialized areas such as the central portion of the continent, including Germany, the Netherlands and Poland, through east of Ukraine, west portion of Russia, as well as industrialized regions of Italy, France, and the British Isles. In the African Continent, high CO concentrations, around 250 ppby, occur in central and western regions due to biomass burning in the Congo's equatorial forest and in the forest-savvana transition in central Africa.

In North America, the highest concentrations, around 300 ppbv, are observed over the eastern portion. In this region, the Commission for Environmental Cooperation in Montreal identified two "pollution rivers" along which the pollution flows. One of them originates in the Ohio River Valley and flows eastward across southern Ontario and Quebec, and the, enters Northeastern United States. The other pathway begins on the East Coast of the United States and streams up into Canada. Higher concentrations around 250 ppbv are observed in California state, near Mexico.

In South America, the highest concentrations, around 250 ppbv, are observed in Brazil, over the Amazon Forest arc of deforestation, in the states of Mato Grosso, Pará, Rondônia, Acre and Amazonas, and on the Brazilian border with Bolivia due to the biomass burning, associated to the agriculture in these regions close to the Amazon Forest and the expansion of the agricultural frontier in this region.

In general, both CAM-Chem simulations efficiently represent the spatial distribution of CO, except for some areas with overestimation, like central Africa and Central South America.

The spatial distribution of satellite derived O3 is showed in Figure 2 (upper panel). The highest concentration of O3 over the Northern Hemisphere is probably associated to anthropogenic emissions. Specially over North America, Asia, Europe and North Africa, the observed concentrations are around 55 ppbv. Both CAM-Chem experiments overestimate O3 over the Northern Hemisphere and underestimate the concentration over South America.

#### CONCLUSIONS

The O3 satellite derived observations from AIRS and CO (MOPITT) were used to subjectively compare the CAM-Chem model results with two different configurations, one using tropospheric chemistry and the other also considering stratospheric chemistry. The comparison between the simulations and satellite observations show that the two models can reproduce the temporal spatial distributions of both pollutants.

Contrarywise, the inclusion of stratospheric chemistry (figures 2 and 3, bottom panels) did not improve the results, in spite of increasing computational time. Compared to the simulations including only tropospheric chemistry (figures 2 and, middle panels), it produced a generally negative bias for CO, and for O3, results are unclear and still subject to analysis. Further research and improvements are required in order to understand the complex relations between tropospheric and stratospheric chemistry to and increase model precision and performance.



#### Monoxide Carbon - 2010-2014

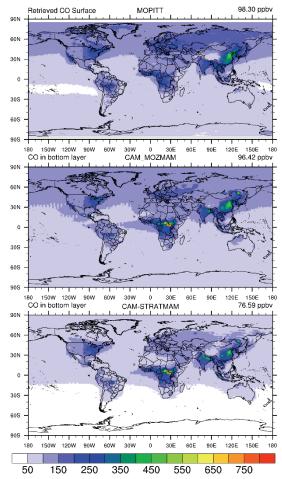


Figure 1. Comparison of CO mean annual CAM-Chem models simulations with tropospheric and stratospheric chemistry (middle and bottom panels, respectively) with the MOPITT sensor (upper panel) for the period 2010-2014.

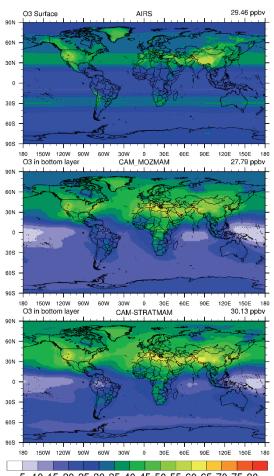
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#### Ozone - 2010-2014



5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 Figure 2. Comparison of O3 mean annual CAM\_Chem models simulations with tropospheric and stratospheric chemistry (middle and bottom panels, respectively) with the AIRS sensor (upper panel) for the period of 2010-2014.

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# SOLUTION OF THE DIFFUSION-ADVECTION EQUATION WITH DIFFUSION COEFFICIENT DEPENDING ON DISTANCE OF SOURCE

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#### Abstract.

The phenomenon of dispersion of pollutants in the atmosphere is modeled through the diffusion-advection equation. In the present work, a solution of the diffusion-advection equation was obtained, with diffusion coefficient dependent on the distance of the source using the new He-Laplace method. To validate the model, results were compared with data from the Copenhagen experiment. Results of the model with a diffusion coefficient dependent on the source have shown to be better than those with average vertical diffusion coefficient.

Keywords: He-Laplace, diffusion equation, homotopy

### INTRODUCTION

The dispersion of pollutants in the atmosphere is a phenomenon that occurs in a daily basis, which directly affects the quality of life of humans, as well as our planet. Such phenomenon is mathematically modeled via the diffusion-advection equation. However, in the literature, an analytical solution for such equation covering a real-life problem has not yet been found. Analytical and numerical methods were used while aiming to solve this problem - finite differences method (Debnath, 2012), Adomian decomposition method 1994), variational iterative (Adomian, (Golbabai, 2007), integral transform (Biazar, 2009), Laplace decomposition method (Khan, 2009), among others - but all these have their limitations. In such sense, the present work aims to evaluate the new He-Laplace method (which is the combination of the Laplace transform with the homotopy perturbation method), using a diffusion coefficient dependent on distance of the source, on the solution of the twodimensional advection-diffusion equation. The great advantage of this methodology is its simplicity in obtaining an analytical solution.

#### **METHODS**

The modeling of dispersion of pollutants in the atmosphere can be represented by the two-dimensional advection-diffusion equation:

$$U(z)\frac{\partial c(x,z)}{\partial x} = \frac{\partial}{\partial z} \left( K_Z(x) \frac{\partial^2 c(x,z)}{\partial z^2} \right) \tag{1}$$

Where U(z) is a function that represents the vertical profile of the average wind velocity in the longitudinal direction and  $K_z$  is the vertical diffusion coefficient. In this study, the vertical diffusion coefficient is only dependent on the longitudinal distance of the source, so that it can be written as:

$$K_Z(x) = \propto f(x)$$
 (2)

Thus, to obtain the solution of Eq. (1) it is possible to make a change of variable as follows:

$$x^* = \int_0^{x'} f(x') dx'$$
 (3)

Where  $x^*$  holds its original dimension [L] and  $\alpha$  is the dimensional part of the diffusion coefficient [L<sup>2</sup>/T]. Therefore, equation (1) can be rewritten as:

$$U \frac{\partial c(x,z)}{\partial x^*} = \propto \frac{\partial^2 c(x,z)}{\partial z^2}$$
 (4)

For simplicity, without loss of generality, we consider U and a constants. For the solution of equation (4) it is necessary to determine its boundary conditions. Thus, we have the condition of zero flow of contaminants on the surface (ground) and at the top of the vertical domain:

$$K_Z \frac{\partial c}{\partial z} = 0$$
 at  $z = 0$  and  $z = h$  (5)

Where h is the height of the planetary boundary layer (PBL). In addition, we have a source with emission rate Q at the height of source,  $H_S$ :

$$c(0,z) = \frac{Q}{II} \delta(z - H_s)$$
 (6)

Where the Dirac Delta function,  $\delta$  (.), is approximated by the following expression:

$$\delta(z - H_S) = \frac{1}{h} \left[ 1 + 2 \sum_{n=1}^{\infty} [\cos(\lambda_n z) \cos(\lambda H_S)] \right]$$
(7)

Being the eigenvalues given by:

$$\lambda_n = \frac{n\pi}{h}$$
  $n = 1, 2, 3, ...$  (8)

Thus, the source condition can be rewritten as:

$$c(0,z) = \frac{Q}{Uh} \left[ 1 + 2 \sum_{n=1}^{\infty} [cos(\lambda_n z) cos(\lambda H_S)] \right]$$
 (9)

Here is the novelty of the present work, using the He-Laplace method (He, 2008). The Laplace Transform is applied in Eq. (4), for the x variable. Together with its inverse, one obtains:



$$c(x,z) = c_0 + L^{-1} \left[ \frac{\alpha}{sU} L \left[ \frac{\partial^2 c(x,z)}{\partial z^2} \right] \right]$$
 (10)

Where  $c_0$  is given by Eq. (9). Therefore, to obtain the other terms of the series solution, we have the following equation:

$$c_n = L^{-1} \left[ \frac{\alpha}{sU} L \left[ \frac{\partial^2 c_{(n-1)}}{\partial z^2} \right] \right] \qquad n = 1, 2, 3.. \quad (11)$$

With the general solution of Eq. (10) given by:

$$c(x,z) = c_0 + c_1 + c_2 + \dots + c_n$$
 (12)

Thus, one obtains for the first term,  $c_1$ :

$$c_1 = -\frac{\alpha x^*}{U} \frac{2Q}{Uh} \sum_{n=1}^{\infty} \lambda_n^2 \cos(\lambda_n z) \cos(\lambda_n H_S) \quad (13)$$

By grouping the other terms according to equation (12), the resulting expression is given by:

$$c(x,z) = \frac{Q}{Uh} + \frac{2Q}{Uh} \sum_{n=1}^{\infty} \cos(\lambda_n z) \cos(\lambda_n H_S).$$

$$\cdot \left\{ 1 - \frac{1}{1!} \frac{\alpha x^*}{U} \lambda_n^2 + \frac{1}{2!} \left( \frac{\alpha x^*}{U} \right)^2 \lambda_n^4 + \cdots \right\}$$
(14)

Finally, by replacing the variable  $x^*$  in equation (14), one obtains the final solution:

$$c(x,z) = \frac{Q}{Uh} + \frac{2Q}{Uh} \sum_{n=1}^{\infty} cos(\lambda_n z) .$$

$$.cos(\lambda_n H_S) e^{\left(-\frac{\lambda_n^2}{U} \int_0^{x'} f(x') dx'\right)}$$
(15)

It is readily observed that Eq. (15) is a Gaussian solution. The diffusion coefficient depends only on z variable (average) given by (Degrazia, 1997):

$$K_{z}(z) = 0.22w_{*}h(z/h)^{1/3}.$$

$$\left(1 - \frac{z}{h}\right)^{1/3} \left[1 - \exp\left(-4\frac{z}{h}\right) - 0.0003\exp\left(8\frac{z}{h}\right)\right]$$
 (16)

Where w is the convective velocity. The coefficient dependent on the longitudinal distance of the source is given by:

$$K_z(x) = \gamma U x \tag{17}$$

where

$$\gamma = (\sigma_w/U)^2 \tag{18}$$

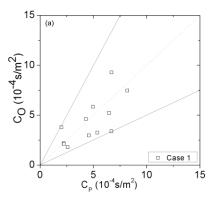
Where  $\sigma_w$  is the variance of the vertical velocity.

## FINDINGS AND ARGUMENT

The simulations performed with Eq. (15) were confronted with the traditional Copenhagen

experiments (Gryning, 1984). For such purpose, a constant diffusion coefficient (average in z variable) was used and another, dependent only on source distance.

Figure 1 shows the scatter plots considering Eq. (16) in the model, for average wind velocity measured at 10 m height (Case 1) and 115 m (Case 2).



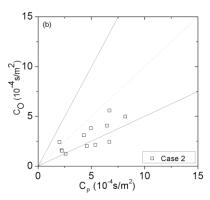
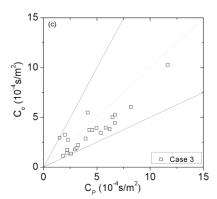


Figure 1. Scatter plot of Observed ( $C_{\rm o}$ ) and Predicted ( $C_{\rm p}$ ) concentrations by the model, normalized with the emission rate (C/Q), using the average vertical diffusion coefficient: (a) velocity measured at 10 m and (b) velocity measured at 115 m at the height of source. Dots between lines have a two-factor.

Figure 2 shows the scatter plots considering Eq. (17) in the model, for average wind velocity measured at 10 m (Case 3) and 115 m (Case 4).





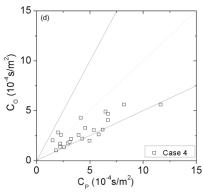


Figure 2. Scatter plot of the Observed ( $C_o$ ) and Predicted concentrations by the model ( $C_p$ ), normalized with the emission rate (C/Q), using the diffusion coefficient dependent on the distance from the source: (a) velocity measured at 10 m and (b) velocity measured at 115 m at the source. The dots between the lines have a two-factor.

Table 1 (below) shows the statistical results of the comparison of models. The best results are for normalized mean square error (NMSE), Fractional bias (FB) and standard deviation (FS) close to zero and correlation factor (COR) and two-factor (FAT2) equal to 1.

Table 1: Statistical index of model results.

Case	NMSE	FAT2	COR	FB	FS
Case 1	0.09	0.96	0.85	0.04	-
Case 2	0.32	0.78	0.87	0.43	0.43
Case 3	0.12	1.00	0.90	0.22	0.20
Case 4	0.36	0.83	0.84	0.43	0.57

It is readily observed from Figure 2 (a) and Table 1 that results are slightly better for Case 3, dependent on distance from the source, with wind at 10 m height.

## **CONCLUSIONS**

In this work, the He-Laplace method was used to solve a linear problem of the two-dimensional advectiondiffusion equation using a constant vertical diffusion coefficient and another dependent on the longitudinal distance of the source. Best results have shown to be from the model combined with the diffusion coefficient dependent on the distance from the source.

Although it is necessary to use a numerical method to deal with real situations, it is useful to first examine possible analytical solutions to obtain a known framework and test solutions. In this sense, analytical solutions are useful for a variety of applications, such as: providing approximate analyses of alternative pollution scenarios, conducting sensitivity analyses to investigate the effects of various parameters or processes involved in contaminant transport, extrapolation over large times and distances where numerical solutions may be impractical, serving as screening models or benchmark solutions for more complex transport processes that cannot be solved exactly, and finally validating more comprehensive numerical solutions of the governing transport equations. Finally, it is important to emphasize that the great advantage of this methodology is its simplicity in obtaining an analytical solution.

### **ACKNOWLEDGEMENTS**

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<sup>8</sup>GRYNING, S.; LYCK, E. Atmospheric dispersion from elevated sources in an urban area: comparison between tracer experiments and model



### EVALUATION OF THE WRF MODEL FOR THE STUDY OF THE METEOROLOGICAL ENVIRONMENT OVER THE TROPICAL ANDES DURING EL NIÑO

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Abstract: Meteorology in the tropical Andes is strongly influenced by the ENSO phases and complex terrain. Here we evaluate the capability of the ERA Interim reanalysis data to represent the meteorology in the mountainous central portion of the Colombian Andes, and show that this representation is improved via dynamical downscaling using the WRF regional climate model. We use precipitation for our evaluation because of three main reasons: it is a key descriptor of the atmospheric environment; it is highly sensitive to both ENSO and orographic effects; and there are available observations to compare with simulation results. We focused on the dry season of the El Niño years (the driest condition) in the 1998-2012 period. We hypothesize that ERA Interim limitations relate to its poor representation of the complex topography in the region, which is improved by WRF. This suggests that using the meteorology provided by ERA Interim by itself may be more informative. The potential to improve reanalysis meteorological data via WRF dynamical downscaling is fundamental for improving environmental management and decision-making in mountainous areas of the tropics.

Keywords: Dynamical downscaling, tropical Andes, model evaluation, WRF, ERA-Interim.

#### **INTRODUCTION**

Two of the main challenges of meteorological modeling lie in the adequate representation of climate variability (e.g. ENSO) and orographic effects. This is particularly relevant in the tropical Andes where meteorology is highly sensitive to both ENSO and orographic effects (Poveda et al. 2011). Regional climate models (e.g. the Weather Research & Forecasting System, WRF, Skamarock et al. 2008) are perhaps the most indicated to represent these regions, as their resolution and fine representation of processes allows an improved representation of, for example, topography-climate interactions (Heikkilä et al. 2011). However, modeling studies need to consider the model's performance and its capacity to represent the spatiotemporal behavior of the variables of interest and the processes that impose variability on these (Curry & Webster 2011). Here we evaluate the capability of the GCM-derived ERA-Interim reanalysis to represent meteorological features (particularly precipitation) in the Tropical Andes of Northwest South America under the influence of ENSO phases for the 1998-2012 period. Further, we evaluate the potential of WRF to perform dynamical downscaling of ERA-Interim during the dry season of El Niño years for the same period, in a strategic sub-region that represents an Andean tropical valley in Colombia.

#### **METHODS**

To assess ERA-Interim representation of precipitation features in the tropical Andes, and further if WRF downscaling improves such representation, we develop three specific steps:

(a) assessment of the performance of ERA-Interim compared to observations; (b) evaluation of the capability of multiple WRF configurations for reproducing observations; and (c) assessment of whether WRF dynamical downscaling provides added value to ERA-Interim information. To do this, we analyze two spatial domains that include (i) a regional scale that covers most of Northwestern South America (NWSA domain; Fig. 1A), and (ii) a local scale domain that centers in the central Andes of Colombia (Antioquia Reservoir Region - ARR; Fig 1B). This region is generally characterized by a complex topography with slopes that reach values of up to 87%.

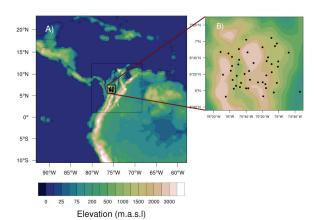


Figure 1. A) Nested domains with the North Western South America (NWSA - thinner box), and B) the Antioquia Reservoir Region (ARR - Thicker box) and detail ground precipitation observation stations. Elevation from WRF.



Observations of precipitation in both spatial domains were obtained from TRMM (Tropical Rainfall Measuring Mission, 3B43 product), GPCC V7 (Global Precipitation Climatology Center) and CRU TS3.21 (Climate Research Unit). In addition we used ground-based observations from the National Institute of Hydrology, Meteorology and Environmental studies of Colombia (IDEAM) for 45 rain gauges distributed across the ARR (Fig 1B).

We implemented WRF model version 3.7.1 (Skamarock et al. 2008) over two spatial domains with resolutions of 10 and 30 km, and 35 vertical levels. Initial and boundary conditions are from ERA-Interim using two-way nesting (Debreu et al. 2012). Sea surface temperatures from ERA-Interim were updated every six hours. To restrict largescale circulation, we used spectral nudging without forcing the boundary layer. We selected WRF single moment six class (WSM6) microphysics scheme, NCAR Community Atmosphere Model (CAM) radiation scheme, Noah multiprocess (Noah-MP) land surface model and Mellor-Yamada-Janjic (MYJ) planetary boundary layer scheme. Cumulus convection is a critical process in the tropics, so we tested three cumulus convection schemes: Betts-Miller-Janjic (BMJ), Kain-Fritsch (KF) and Grell 3D (G3D). The September-February semester of 2009-2010 was used for this sensitivity analysis. Best results were obtained with the KF scheme (we will highlight this by saying WRF-KF). All WRF simulations were run for the September-February semester. The period between September and November was used as spin-up, and the results from December to February were used for the analysis in all El Niño years between 1998-2012.

#### **RESULTS AND DISCUSSION**

During El Niño, ERA-Interim adequately represents the seasonality of precipitation but generally overestimates its magnitude (Fig. 2). The largest bias (greater than 100%) occurs during the dry season (DJF). WRF-KF improves the representation of both magnitude and spatial distribution of precipitation for the DJF trimester during El Niño years in the NWSA domain, when compared to ERA-Interim data (Fig. 3).

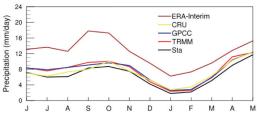


Fig 2. Annual cycle of precipitation in the ARR for El Niño years as represented by ERA-Interim, other gridded sources, and ground observations.

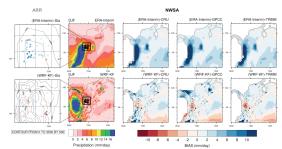


Fig 3. ERA Interim (top) vs. WRF-KF (bottom) biases for mean precipitation during DJF of El Niño years. Contours in the left column represent topography used by either ERA Interim or WRF-KF.

For the ARR domain, WRF-KF downscaling improves all aspects of the representation of precipitation. For instance, the representation of magnitude is much improved as the spatial correlation switches its sign from negative for ERA-Interim (R=-0.13) to positive for WRF-KF (R= 0.10). The representation of spatial variability is also improved by WRF-KF when compared to surface observations (SD/SD<sub>o</sub>=1.73 to ERA-Interim and SD/SD<sub>o</sub>=1.11 to results from WRF-KF), and WRF-KF estimations of precipitation approach very closely the values from other gridded information sources (Taylor diagram in Fig. 4A). WRF-KF not only improves the representation of spatial distribution, but also the representation of the temporal evolution when compared to ground observations of precipitation (Fig 4B).

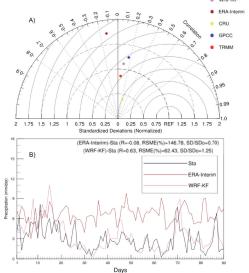


Figure 4. A) Taylor normalized diagram comparing ERA-Interim and WRF-KF representation of spatial distribution of precipitation. B) Daily evolution of the precipitation (averaged over ARR) from ERA-Interim, WRF-KF and surface observations (Sta).

Both during DJF of El Niño years.



An accurate representation of the topographical features is critical for adequately reproducing meteorological patterns in the tropical Andes. The ERA-Interim representation of the topography for the Tropical Andes is highly simplified, with an imprecise representation of the altitude variability of the western and central mountains range, that merges both branches of the Andes, and ignores the central river valley at -75.80 degrees of longitude (Fig. 5A).

This failure to correctly represent the topography may have effects in the observed bias in the representation of precipitation for the ARR domain. Local circulation systems occurring in valleys produce ascending winds that contribute to the formation of precipitation in the western flank of the central Andes (López and Howell, 1967; Fig. 5B). WRF uses a more detailed resolution that is able to better capture the spatial variability of topography (Fig 5A). When WRF-KF dynamical downscaling is performed, the inaccuracies associated with the representation of precipitation ERA-Interim are significantly improved, particularly for magnitude and spatial variability. Additionally, we analyzed the ERA-Interim and WRF representations of surface winds; the finer topography used by WRF captures better the influence of topography on surface winds and the variability generated on surface temperature. This is particularly important in air quality modeling of cities located in complex terrains (Fig 6).

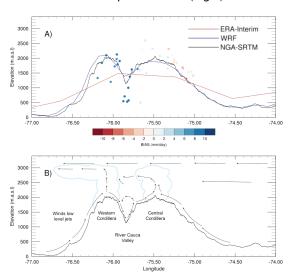


Figure 5. A) Representation of ARR's mean latitudinal elevation profile in ERA-Interim and WRF as compared to NGA-STRM. Dots indicate bias in ERA-Interim estimations of mean daily precipitation for 1998-2012 compared to ground observations of precipitation. B) Adapted from López and Howell (1967), schematic representation of regional wind circulation leading to observed patterns of precipitation.

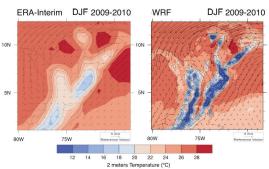


Figure 6. ERA-Interim vs. WRF, spatial distribution of 2 meters temperature and 10 meters wind vectors (DJF 2009-2010).

#### **CONCLUSION**

The ERA Interim reanalysis fails to represent important features of the meteorology in the tropical Andes, likely as a consequence of its coarse representation of topography. ERA Interim generally overestimates precipitation during the dry season of El Niño years. This representation of precipitation is improved via WRF downscaling, likely as a result of a better representation of meteorological phenomena over complex terrain. Collectively, these results highlight the importance of regional climate models to inform decisions related to meteorology in the tropical Andes. In synthesis, in regions with complex topography, global models data needs to be refined to represent meteorological processes and their influences on pollutants and moisture transport.

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#### Evaluating BRAMS Carbon Monoxide Operational Forecasts over the Metropolitan Area of São Paulo

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#### Abstract:

BRAMS model carbon monoxide (CO) operational forecasting for 24h, 48h and 72h forecast lengths were evaluated using measurements from Osasco and Congonhas monitoring stations of the State Environmental Company (CETESB). The studied period ranges from May 2012 to December 2015. Annual averages, diurnal and monthly annual mean cycles were analysed, and results show that CO concentrations have been decreasing over time, which was not reproduced by the BRAMS model forecasting. For the monthly annual cycle, the model is able to capture the monthly variability, indicating peak monthly concentration in June, similar to observations. All forecasting lengths represent the diurnal cycle properly, showing the two concentration peaks of the rush hours as in observed data. Even though the model tends to underestimate CO values for both sites (approximately 0.7 ppm in Osasco and 0.5 ppm in Congonhas), correlation coefficients are higher than 0.7 for the monthly annual and diurnal cycles. Based on these first results, it is possible to conclude that CO forecasting by the BRAMS model is reliable enough to be potentially used as a tool to aid population and policymakers on air quality public policies. More research including other localities and pollutants are still necessary for a better evaluation of the BRAMS model.

Keywords: Carbon Monoxide, urban pollution, BRAMS, environmental modeling, air quality forecast

#### **INTRODUCTION**

Carbon monoxide (CO) is among the gases that deteriorate air quality in industrialized locations or places with a major vehicle fleet such as the Metropolitan Area of São Paulo (MASP) and Campinas. CO is considered highly dangerous due to its toxicity and because it is a chemical asphyxiant. Therefore it is important to monitor and forecast CO concentrations, and then define promote public policies which better environmental management and public health of cities in general, especially where urbanization rates are present.

In the last 10 years, due to advances in computational resources, several numerical weather and climate prediction models integrate atmospheric chemistry transport models, such as the Brazilian Developments on the Atmospheric Modelling System (BRAMS, Freitas et al., 2017).

In the Center for Weather Forecasting and Climate Studies of the National Institute for Space Research (CPTEC/INPE), the BRAMS model has been used for operational forecasts and also for research in weather and air quality modelling since 2003, in a limited area domain to South America

(Freitas et al., 2009, Longo et al., 2010, Freitas et al., 2017). This model simulates the transport, removal and chemical transformations of gases and aerosols, as well as the atmospheric physics, dynamics and surface feedbacks in an integrated way (Freitas et al., 2017).

Performing objective evaluation of the chemical variables provided by BRAMS model is vital to its improvement, aiming to make products of greater accuracy available for the population. Within this context, this work aims to evaluate the operational forecasting of CO by the BRAMS model for the MASP during 2012-2015.

#### **METHODS**

CO forecasting in the BRAMS operational model were evaluated during the period of May 2012 to December 2015. The model configuration of the version used in this period, named Chemistry Coupled Aerosol-Tracer Transport model to BRAMS (CCATT-BRAMS), was described in Freitas et al. (2009).

BRAMS emissions were generated using the PREP-CHEM-SRC tool, the preprocessor of trace gas and aerosol emission fields for regional and global



atmospheric chemistry models (Freitas et al., 2011). This tool considers emissions from industrial/urban, biogenic, biomass burning and volcanic sources. For the urban/industrial emissions, RETRO (REanalysis of the TROpospheric chemical composition over the past 40 years; http://retro.enes.org) and EDGAR (Emission Database for Global Atmospheric Research; Olivier et al., 1996; Olivier et al., 1999) were used. RETRO is a global emissions database with a temporal interval of 40 years (from 1960 to 2000), with monthly means evaluated on a  $0.5^{\circ} \times 0.5^{\circ}$  grid resolution. EDGAR provides annual global emissions of greenhouse gases and air pollutants for the year 2000 with 1° × 1° spatial resolution. Likewise, an urban vehicle emissions inventory for South America (Alonso et al., 2010) was used. Biomass burning emissions were estimated by the Brazilian Biomass Burning Emission Model (3BEM, Longo et al., 2010) within PREP-CHEM-SRC based on satellite remote sensing fire detections (Freitas et al., 2011) whereas the database for biogenic emissions was provided by the Model of Emissions of Gases and Aerosols from Nature (MEGAN, Guenther et al., 2006) with 0.5° x 0.5° spatial resolution.

During the studied period, the model was run with a 25 km spatial resolution and 40 vertical levels, over South America, for 24h, 48h and 72h of forecast length. The 24h forecast length (03Z to 00Z with 3-hour intervals) was called F24h, as well as F48h and F72h for the second and third integration days.

Model data were extracted from 2 grid points near the geographical location of Osasco and Congonhas, both surface monitoring stations from the São Paulo State Environmental Company (CETESB) which measure CO continuously. Their geographical locations are shown in Table 1. Observed CO concentrations in CETESB stations were collected with 3-hour frequency.

Besides their economic importance, these locations also present high concentrations of vehicular pollution.

Both model data and observations were used to compute mean diurnal, monthly annual cycles and also annual averages for 24h, 48h and 72h for the stations listed in Table 1, and compared through linear correlation in order to analyse their similarities.

Table 1: Municipality and geographical coordinates of the CO measuring stations.

Municipality	Geographical Coordinates
Congonhas	23°36'57"S/46°39'47"W
Osasco	23°31'33"S/46°47'31"W

#### FINDINGS AND ARGUMENT

Analysis of the observed annual mean for Osasco and Congonhas stations indicates a decrease in CO concentration in each year. This trend is linked to the public policies implemented in the state of Sao Paulo in order to decrease emissions, mainly from vehicular sources. Such results were showed in the study of Rozante et al. (2017) exploring CO variations in the MASP. BRAMS model forecasts present little yearly variation of CO concentrations in the studied period. This is associated with urban emissions in the model which did not change during the period of study. However, the increase observed from 2014 to 2015 could be associated to atmospheric transport from fire emissions in regions nearby MASP. During these years, there was an increase in the number of fires in Brazil according with INPE Fires Satellite Monitoring Program (<a href="http://www.inpe.br/queimadas">http://www.inpe.br/queimadas</a>). addition, local emission, especially vehicular sources, may impact the results of measurements at ground stations, in contrary to numerical simulations with 25 km x 25 km spatial resolution, since this grid pixel incorporates a wide area making it difficult to represent the emissions of some local sources.

In Fig. 1a, the observed monthly annual cycle of CO from Osasco station is shown along with the modelled data in the nearest grid point. The monthly annual cycle is well represented by the model, indicating a peak in June and a second peak between February and March. However, the model underestimates the concentrations, which is expected, since the spatial resolution is not fine enough to represent all small-scale processes which might be associated to the patterns observed in a single monitoring point. The correlation coefficients between observed and modelled cycles are approximately 0.84 for 24h, 0.74 for 48h and 0.76 for 72h forecast lengths. For Congonhas station (Fig. 1 b), the model also represents the monthly annual cycle well, but with a temporal lag. While the concentration peak occurs in August, the model forecasts the peak in June, also with a secondary maximum in March. Correlations between observed and modelled data in this station for the 24h, 48h and 72h periods were around 0.72, 0.75 and 0.54, respectively.

Concerning the mean diurnal cycle of CO concentrations, for the Osasco station (Fig. 2a), a peak is observed at 9h local time, and a secondary peak at 21h local time, and in Congonhas station (Fig. 2b), the peak occurs at 18h local time and the secondary peak at 9h local time. The model correctly represents the observed diurnal cycle, despite the underestimation. Correlations between the forecasted and observed data were higher than



 $0.75\,$  for Osasco, and higher than  $0.85\,$  for Congonhas.

The underestimation for the mean diurnal cycle for Osasco and Congonhas are 0.7 ppm and 0.5 ppm, respectively. There is no strong difference between the different forecast lengths, but 24h forecast most closely match the observations.

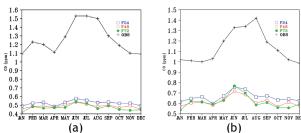


Figure 1: Mean seasonal cycle of CO in Osasco (a) and Congonhas (b)

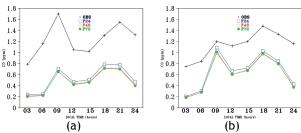


Figure 2: Mean diurnal cycle of CO in Osasco (a) and Congonhas (b)

#### **CONCLUSIONS**

The operational forecasting of CO concentrations for 24h, 48h and 72h from the BRAMS model was evaluated in the grid points nearest to the CETESB monitoring stations Osasco and Congonhas. The model underestimated concentration values for both stations. However, it was able to properly represent, with correlation coefficients higher than 0.70, the annual, seasonal and diurnal cycles of this pollutant in the study area.

#### **ACKNOWLEDGMENTS**

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# ACCURACY EVALUATION OF PHOTOCHEMICAL MODEL WRF-CHEM TO REPRESENT THE POLLUTANTS CONCENTRATION IN THE METROPOLITAN REGION OF SÃO PAULO

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Abstract: In this study we quantify the accuracy of the WRF-Chem model to predict the concentrations of pollutants in the Metropolitan Region of São Paulo (MRSP) using statistical tools. Environmental measurements were obtained in October 2015 in the CETESB Air Quality Station installed at the Institute of Energy and Nuclear Research (IPEN USP) of atmospheric concentrations of nitrogen oxides (NO, NO2 and NOx), carbon monoxide (CO), ozone (O3) and Fine Particulate Matter (PM2.5). Ozone precursors toluene and xylene were included in the study as well. They were quantified with the Gas Chromatograph Clarus 500 installed at Lapat (Analysis laboratory of Atmospheric Processes). The samples were collected on the roof top of IAG-USP and were compared with the simulated concentrations.

The numerical model Weather Research and Forecasting with Chemistry (WRF-CHEM), operates in the Lapat's (Laboratório de Análise dos Processos Atmosféricos) computational infrastructure and MASTER (Laboratório de Modelagem de Sistemas de Tempo e Estudos Numéricos) IAG-USP, using as the chemical mechanisms RADM2 (Regional Acid Deposition Model version 2) and MADE / SORGAM (Modal aerosol Dynamics model for Europe - Secondary Organic aerosol Model) was used for chemical treatment of the gas phase and for the description of aerosols.

Statistical Indices showed good agreement of WRF-chem model in predicting the pollutants ozone and carbon monoxide, with low positive bias and FAC2 (Fraction of the predictions that are within a factor or two) and a, satisfactory correlation, close to 0.65.

For the hydrocarbons xylene and toluene, precursors of ozone and secondary organic aerosols, the indices obtained by the model were suitable, with FAC2 of 0.5 and a slight negative bias. But low correlations were observed between the model and the environmental data for these compounds due to the uncertainty in the description of the emission of these compounds. For nitrogen oxides in turn (emitted mainly by heavy vehicles using diesel) we found the opposite: good representation of daily behavior with the identification of maximum and minimum concentrations, returning good correlation coefficients (near 0.6) but their mean values were overestimated, with bias of 66% and 60% for nitrogen monoxide and dioxide respectively.

Finally, the fine particulate matter (PM2.5) has not been well described by numerical modeling with all statistical indices unsatisfactory, showing that further refinement is needed. The model tends not to represent the daily cycle correctly (correlation near 0.3) nor their average concentrations (average bias of + 56%). In the MASP the issuing of the PM2.5 results from various sources, among them anthropogenic (incomplete biomass burning, metal derived from brake discs abrasion, resuspension, etc.) and biogenic (soil particles, sea salt, etc.); and secondary processes such as nucleation and coagulation, making this modeling complex function of the number of variables involved.

Keywords: Ozone, Ozone precursors, WRF-Chem, Statistical avaluation methods

#### **INTRODUCTION**

Among the largest agglomerations in the world, the Metropolitan Region of São Paulo (MRSP) has more than 19.7 million inhabitants and a complex relationship between land use, energy needs, urban mobility and possible environmental and human health impacts, of which air pollution is of particular concern.

The vehicle emission is the main responsible for the pollutants contribution to MRSP, due to its expressive fleet of more than 8 million vehicles, according to the Company of Technology and Environmental Sanitation of the State of São Paulo (CETESB).

NUANCE (Narrowing the The Uncertainties in aerosol and climate change) project consists of a series of subprojects focused on the study of the formation, evolution and deposition of primary particles and (Andrade et al., 2016). In this work, we present the results of the modeling of air quality in the atmosphere. In this study we intend to analyze the accuracy of the WRF-Chem model in predicting atmospheric pollutant concentrations using statistical tools, such as ozone (O3), nitrogen oxides (NO, NO2 and NOx), carbon monoxide (MP2.5) and the precursor hydrocarbons of ozone, toluene and xylene in the MRSP



The LAPAt (Laboratory of Analysis of Atmospheric Processes) provides on its page data of the numerical forecasts generated by the WRF-Chem model and they can be accessed at: http://www.lapat.iag.usp.br/aerossol/wrf9/). We have in figures 1A ~ 1D images of these predictions for ozone obtained in the mentioned page

#### **METHODS**

Environmental data were obtained for 48 hours (from 20:00 on 10/27/2015 until the same time as 10/29/2015 with hourly resolution) of the atmospheric concentrations of ozone (O3), nitrogen oxides (NO, NO2 and NOx), carbon monoxide (CO) and fine particulate material (MP2.5) at the CETESB Air Quality Station installed at the Institute of Energy and Nuclear Research - IPEN USP.

For the ozone precursors hydrocarbons, toluene and xylene were quantified by Chromatograph (LB), LAPAt in their laboratory installed on the IAG-USP terrace, and then compared them by means of statistical indices: (Mean bias (MB), Mean normalized error root (NMSE), correlation index (R) and Fraction of predictions that are within a factor or two (FAC2)) with the concentrations obtained by the numerical simulation of the WRF-Chem model.

#### FINDINGS AND ARGUMENT

The statistical indices shown in Table 2 indicate that the WRF-CHEm model performed well in predicting concentrations of ozone pollutant (Figure 2A) and carbon monoxide pollutants. Correlations with measurements were close to 0.6, low ozone positive bias, being slightly more pronounced for carbon monoxide, finally FAC2 values are above 0.75. The hydrocarbons xylene and toluene obtained FAC2 0.5 and slight negative bias. In Table 2 we noticed low correlations between model and environmental data, which is visible if we analyze Figure 2B.

For nitrogen oxides we find the inverse of hydrocarbons: good representation of the daily behavior with schedules of maximum and minimum concentrations identified (Figure 2C), returning good correlation indexes (close to 0.6); But their mean values are highly overestimated, where the bias obtained was 66% and 60% for the Monoxide and Nitrogen dioxide in that order.

Finally, the fine particulate material (PM2.5) shown in figure 2D was not well described by the model which obtained unsatisfactory statistical indices and; As well as nitrogen oxides, need further refinement. The model did not correctly reproduce mean concentrations (mean bias of + 56%) or the daily cycle (correlation <0.3).

Mean values and standard deviations of the simulated and measured data are presented in the table 1

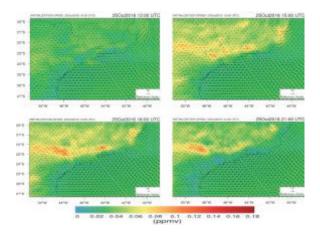


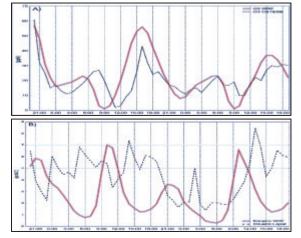
Figure 1: WRF-CHEM model prediction for ozone concentration and wind on a 9km grid surface

Table 1: Mean values and standard deviations from modeled (model) and observed (obs) concentrations

PoButaert	Means (model - obs)	Standard Deviation (model - obs)
NO2 (ppb)	28.6 - 11.4	11.9 - 4.2
NO (ppb)	10.9 - 3.7	12.2 - 3.5
NOx (ppb)	40 - 15	19 - 6.5
O3 (ppb)	23.1 - 20	14.8 - 10.2
CO (ppb)	511 - 382	272 - 84
Xilene (ppbC)	3.0 - 4.1	2.1 - 0.2
Toluene (ppbC)	2.7 - 4.4	1.8 - 0.3
PM 2.5 (µg/m <sup>3</sup> )	12.2 - 5.5	2.4 - 4.7

Table 2: WRF-CHEm Statistical evaluation indices

Pollutant	FAC2	MB	$\mathbf{R}$	NMSE
NO2 (ppb)	0.26	17.17	0.67	1,17
NO (ppb)	0.47	7.21	0.51	4,00
NOx (ppb)	0.28	24.3	0.63	1,39
O3 (ppb)	0.77	2.74	0.64	0,30
CO (ppb)	0.85	129	0.58	0,36
Xilene (ppbC)	0.5	-1.1	0.28	0,47
Toluene (ppbC)	0.44	-1.7	-0.03	0,81
PM 2.5 $(\mu g/m^3)$	0.40	6.85	0.28	1.02





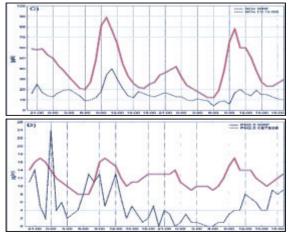


Figure 2: Variation of measured concentrations (dashed black line) and simulated by WRF-Chem (solid red line) for the period from 10/27/2015 to 10/29/2015 of the compounds ozone (a), toluene (b) nitrogen oxides (c) and fine particulate matter(d)

#### CONCLUSIONS

According to the indices obtained, we can infer that the WRF-CHEm model provides very assertive concentrations of pollutants with well-described formation / origin, such as ozone and carbon monoxide; In the first case associated with daytime cycle and incident solar radiation or primary emission of light gasoline vehicles, in the case of carbon monoxide

However, pollutants with higher reactivity and / or with primary sources of complicated spatial distribution are not well described by photochemical modeling. This is a direct result of deficiencies in the description of sources in the emissions inventory. This was evidenced by the median indices of nitrogen oxides and unsatisfactory fine particulate matter.

The model was generally adequate in describing the environmental concentrations of hydrocarbons xylene and toluene precursors of secondary organic aerosols and ozone. The low correlations observed are a reflection of the high reactivity of the compounds and the difficulty of adjusting a measure at grid points (of the simulation) with a measure at an experimental site.

As possible alternatives to improve the model, we can suggest that new experiments such as those promoted in the Jânio Quadros and Rodoanel Leste Tunnel are carried out. In this way, it would be possible to improve the methodologies for describing the emission factors of the mobile sources and the dispersion of pollutants within the MRSP

Another factor that needs to be better evaluated involves the emission of stationary and evaporative sources; Of these sources originate important atmospheric contaminants hydrocarbons such as benzene (gasoline) and acetaldehyde (ethanol),

precursors of ozone among other secondary pollutants.

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# Session 5 Policy and Decision Support



#### RESULTS FROM THE BRAZILIAN AUTO OIL PROGRAM

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Abstract: The environmental impact due to the use of an especific type of fuel can bring serious implications to the productive sector. The estabilishment of emission standards for atmospheric polutants must be based on scientific knowledge aiming to guaranty a better air quality, in particular over urban areas. This work presents some model results obtained during the numerical experiments from the Brazilian Auto Oil Program, which has as one of its goals to verify the impact that different emission scenarios, based on laboratory derived emission factors, may have on air quality over the main urban areas in part of south and southeast Brazil. Simulations were made based on the reference year of 2011, with emission scenarios for different years and situations. The main focus was on the sensitivity of ozone concentrations to the emissions. Main results include the very accurate values for ozone concentrations over large periods of time and the strong effect that traffic modal (use of a larger number of buses in substitution to particular vehicles for example).

Keywords: Air quality improvment, WRF/Chem, emission inventories, air pollution, ozone.

### INTRODUCTION (Heading Trebuchet MS, 11 font size, bold)

Governmental actions seeking the improvment of air quality have been introduced in many countries. In particular in Brazil, programs like PROCONVE and PROMOT, were very important to guarantee a low level of pollutant concentrations, not only over urban areas, but also in remote regions from the main sources. However, these procedures not always are suficient to avoid air quality violations for all regulated pollutants. For example, Pérez-Martínez et al. (2015) and Carvalho et al. (2015), based on air quality data provided by the Environmental Agency of Sao Paulo State (CETESB), showed that, although the concentrations of most of pollutants are decreasing with time, ozone concentrations still being a reason for concern, with an increasing tendency along the period studied by them. Therefore, experimental and numerical studies must be conducted in order to provide better informations about appropriated regulations in terms of fuel composition and engine technology. With that in mind, the Brazilian Auto Oil Program was conducted with the aim of to provide accurate information about vehicular emissions, considering actual fuels in use and fuels that still in development, and the impact that such emissions can have on pollutant concentrations, especially ozone.

#### **METHODS**

In order to analyze the impact that vehicular emissions can have on ozone concentrations, we used the WRF/Chem model (Grell et al., 2005). For the emissions we used information from different sources, including tunnel measurements performed in the Metropolitan Area of Sao Paulo (MASP, (Martins et al., 2006; Pérez-Martínez et al., 2013), the official emission inventory provided by CETESB (e.g CETESB, 2010; 2012), and the emission factors obtained during Brazilian Auto Oil Program laboratory experiments. Figure 1 shows an example of the emissions used and the domain used during the simulations.

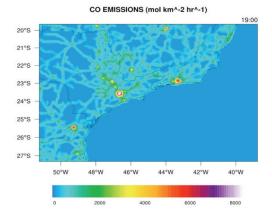


Figure 1. Example of pollutant emissions used in the WRF-Chem model and the domain of simulations



Table 1	<ul> <li>Emission</li> </ul>	factors	used in	the	WRF-CI	HFM (a	km-1)

	-					(5	,·	
	Category		CO NOx	PM10	COVs			SO2
	category		NOX	17/10	exaust	carter	evaporative	302
	Gasoline	6.50 <sup>(1)</sup>	0.50 <sup>(1)</sup>	0.15 <sup>(1)</sup>	1.17 <sup>(4)</sup>	2.00 <sup>(4)</sup>	0.170	0.03 <sup>(1)</sup>
Light	Ethanol	6.50 <sup>(1)</sup>	0.50 <sup>(1)</sup>	0.15 <sup>(1)</sup>	2.17 <sup>(4)</sup>	1.50 <sup>(4)</sup>	0.035	0.03 <sup>(1)</sup>
Lig	Flex-Fuel	6.50 <sup>(1)</sup>	0.50 <sup>(1)</sup>	0.15 <sup>(1)</sup>	0.10 <sup>(4)</sup>			0.03 <sup>(1)</sup>
	GNV	6.50 <sup>(1)</sup>	0.50 <sup>(1)</sup>	0.15 <sup>(1)</sup>	0.44 <sup>(4)</sup>			0.03 <sup>(1)</sup>
>	Trucks	4.95 <sup>(2)</sup>	19.12 <sup>(2)</sup>	0.44 <sup>(2)</sup>	2.05 <sup>(4)</sup>			0.61 <sup>(2)</sup>
Неаvу	Urban buses	1.84 <sup>(3)</sup>	10.23 <sup>(3)</sup>	0.35 <sup>(3)</sup>	2.05 <sup>(4)</sup>			
エ	Road buses	1.36 <sup>(3)</sup>	7.75 <sup>(3)</sup>	0.26 <sup>(3)</sup>	2.05 <sup>(4)</sup>			
	Motorcycles	4.2 <sup>(3)</sup>	0.15 <sup>(3)</sup>	0.05 <sup>(4)</sup>	1.41 <sup>(4)</sup>	1.20(4)		

- (1): Emission factors estimated by Jânio Quadros tunnel experiment in 2011
- (2): Emission factors estimated by Rodoanel tunnel experiment in 2011
- (3): Based on 2010 CETESB's Air Quality Report (CETESB, 2011)
- (4): Based on 2009 CETESB's Air Quality Report (CETESB, 2010)

#### FINDINGS AND ARGUMENT

Figure 2 shows the results obtained during two simulations with the WRF-Chem model in the point correspondent to Parque D. Pedro II CETESB station. The red line in the figure represent the concentrations provided by the model when using the emission factors calculated during the Brazilian Auto Oil Program and emission distribution correspondent to Figure 1. As we can see, the results represent very well the measured ozone concentrations at that station, including the diurnal cycle of the pollutant and periods of larger concentrations and its decreasing by the end of the period. This result show was that with the new emissions the model can be used with a certain level of security, both for air quality forecast and for public policies stabilishment.



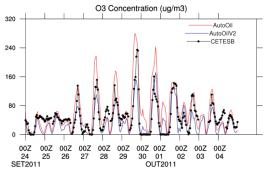


Figure 2. Time series of simulated and observed Ozone concentrations based on Parque D. Pedro II station. Red lines indicate the results obtained with the emission factors from Auto Oil while blue lines represent an increase of 2.9 % on the urban buses.

Blue lines in Figure 2 correspond to the emission scenario were the urban buses fleet was increased by 2,9 % in substitution to private light duty vehicles. As we can see, ozone concentrations can be as lower as 50 % during peak hours in most of the days simulated. This show us how powerfull this action can be in improving the air quality in the region and also the importance of the use of this numerical tool in providing information for public policies stabilishment. Although we showed the results for only one station, the same staments can be applied to other locations in the MASP.

#### **CONCLUSIONS**

Aiming to provide more accurate information on procedures to improve the air quality in urban regions, a Program including field experiments and numerical simulations were performed. Laboratory experiments provided better emission factors which were used to build an more accurate emission scheme for the WRF-Chem model. With these new emissions, the model was able to provide high quality results, representing very well the ozone concentrations in the Metropolitan Area of São Emission scenarios considering substitution of private light duty vehicles by public transportation confirmed the effectiveness of this procedure, contributing for decreasing ozone concentrations around 50 % in some hours of the simulated period.

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# ESTIMATING THE EFFICIENCY OF EMISSION CONTROL POLICIES ON IMPROVING LOCAL AIR QUALITY USING NUMERICAL MODELS: A CASE STUDY IN AN INDUSTRIAL MUNICIPALITY IN SÃO PAULO, BRAZIL

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Abstract: Growing levels of urbanization in developing countries have generally resulted in increasing air pollution, due to higher activity in the transportation, energy, and industrial sectors. The identification and understanding of the multiple pollutant sources' contribution to air quality in such sectors, locally and regionally, is essential to designing an effective emission control policy. Air quality modelling associated with emission scenarios is an important tool that can provide guidance on the most efficient and effective air quality management strategy. This work focuses on Piracicaba, an industrial municipality with a total area of 1378 km<sup>2</sup> and a population of 365 thousand inhabitants, located in the state of São Paulo. After updating its air quality standards in 2013 to levels suggested by the World Health Organization, the state of São Paulo has proposed a state-wide stationary and mobile sources emission reduction program, singling out locations in which air quality levels do not comply with the updated standards. Control strategies proposed so far focus on local stationary sources, (mainly sugar-alcohol, automotive and steel industries) largely underestimating vehicle emissions and regional contributions from the neighbouring Metropolitan Area of São Paulo to the local air quality. This work aims to model this scenario by preparing spatially and temporally averaged emissions from local industrial sources, using mandatory monitoring data and process-based estimations, along with vehicle emissions obtained through locally adapted emission factors and the road network provided by the OpenStreetMaps platform. This data will be processed using SMOKE which, along with a local and regional WRF meteorological model, will serve as an input for modelling emission reduction scenarios and estimating their effectiveness in achieving the expected air quality levels. It is anticipated that preliminary results will show that the afore mentioned pollutant emissions can be compared with levels initially considered by local authorities when designing the emission control program, as well as estimating the influence of regional emissions in local air quality.

Keywords: Air quality management, emission control policies, air pollution, numerical models, air quality modelling

#### **INTRODUCTION**

Clean air is a basic and essential requirement to human health and wellbeing. For this reason, atmospheric pollution represents a significant risk to population. The first studies to report on this correlation date from the mid-twentieth century, but recent studies continually report evidences of adverse effects on health of air pollution following both acute and chronic exposure (MANNUCCI et al., 2015).

Prevention of the negative effects of air pollution starts by correctly identifying the most active pollutants in a certain region and determining maximum concentration levels acceptable in order to guarantee the wellbeing of general population wellbeing. These levels are established as Air Quality Levels (AQS) that serve as a fundamental guideline for air quality management programs from national and regional environmental agencies. For this reason, AQS definition process must also consider monitoring criteria and data access and disclosure to governing bodies and general public (SANTANA et al., 2012).

Based on AQS, air quality management programs must employ instruments that provide a holistic perspective of the multiple factors that influence air quality degradation in an area, in order to adopt the most effective and efficient emission control strategy. Among these are air quality monitoring networks, emissions inventories, sources monitoring and dispersion modelling, environmental licensing, as well as post-control instruments.

The nationally adopted AQS in Brazil are established by Resolution 03/1990 of the Brazilian Conselho Nacional de Meio Ambiente (CONAMA, National Environmental Council). These can be considered outdated if compared to the Air Quality Guidelines Global Update 2005 (WHO, 2006), because of its permissive levelsan and for disregarding relevant pollutants, such as fine particulate matter (diameter <2.5 $\mu$ m, PM<sub>2.5</sub>).

Ahead of the update of national AQS, the states of São Paulo and Espírito Santo have, in 2013, updated their state-wide AQS to WHO levels. As recommended by the Guidelines, both states have established intermediary progressive levels, that



should be targeted leading up to a full state-wide adoption of final standards. Both states have since released emission control programs for its main pollutant sources, in order to achieve the progressive target levels.

The goal of this work is to critically analyse the emission control strategy being proposed for the state of São Paulo, and evaluate its potential efficiency and effectiveness in improving air quality locally and regionally.

São Paulo's control actions are stated in two major programs: Programa de Controle de Emissões de Fontes Estacionárias (PREFE, Fixed Sources Emissions Control Program) and Plano de Controle da Poluição Veicular (PCPV, Vehicular Pollution Control Plan) (CETESB, 2014). Both programs aim to achieve targeted levels in critical control areas within the state by prioritizing emission control actions. But these present conceptual problems: PREFE and PCPV are not well integrated with other state policies and with each other, e.g., both programs adopt distinct methodologies when defining control areas, disregarding potential synergic or conflicting interactions that may undermine its effectiveness (LIU et al., 2014).

The first edition of PREFE defines control actions guidelines for the 2014-2016 period based on 2010-2012 air quality monitoring results. The two year gap in-between can be a source of misinformation when suggesting control actions, in which a pollutant can be already under control when a emission reduction plan is being put into practice (Table 1).

Table 1. PM<sub>10</sub> averaged annual mean 1<sup>st</sup> intermediary AQS exceedance in Piracicaba in 2010-2012 and 2013-2015 periods

Monitoring	SP 1 <sup>st</sup> Intermed.	Averaged Annual Mean		
Monitoring Stations	AQS	2010-2012	2013-2015	
	MI1	$(\mu g/m^3)$	(µg/m³)	
Piracicaba - Algodoal (M)	40	49	38	
Piracicaba (A)	40	-	37	

Reference: adapted from (CETESB, 2016)

PREFE defines seven control areas (*Regiões de Controle*, RCs) in which occurrences of exceedances of the new proposed AQS have been registered in air quality monitoring results. Piracicaba, an industrial municipality with a total area of 1378 km² and a population of 365 thousand inhabitants, is one of those RCs (figure 1), in which coarse particulate matter (diameter <10 $\mu$ m, PM<sub>10</sub>) was considered the main pollutant of concern.



Figure 1. RC7 Piracicaba Reference: (CETESB, 2014)

The proposed control strategy focuses on local industries, mainly steelmaking, sugar-alcohol and automotive as the most significant in the region. This potentially underestimates long range transport pollutant contributions from the neighboring Metropolitan Area of São Paulo (MASP), a megacity of 21 million inhabitants that face many air quality challenges and where concentrations of regulated pollutants frequently exceed AQS (ANDRADE et al., 2017).

For these reasons, great uncertainties can be distilled from the proposed emission control program, regarding its effectiveness. Numerical air quality modelling, a tool extensively used to evaluate air quality management programs, will be used to evaluate the Piracicaba case. Different emission reduction scenarios are considered in order to investigate which actions could prove more efficient in achieving the desired ambient air quality levels.

#### **METHODS**

In order to appropriately represent the Piracicaba case, considering long, medium and local range emissions, as well as secondary pollutant formation mechanisms, the Community Multiscale Air Quality Modelling System (CMAQ) will be used. It is Eulerian tridimensional multipollutant and multiscale model recommended by USEPA for an integrated medium to long range assessment of air quality management strategies.

In order to be used as input data for CMAQ, an updated spatially and temporally averaged emissions inventory from local industrial sources will be prepared, considering mandatory emissions monitoring data as well as process-based estimations using emission factors. Vehicular emissions will be prepared through the model REMI (R-Emissions-Inventory) that uses locally adapted emission factors, and the road network provided by the OpenStreetMaps platform. In order to define boundary conditions for the Piracicaba region, the nested domains technique will be used, adopting



two regional larger scale domains centered around the area of interest (Piracicaba): a regional domain considering the state inventory, and larger domain employing the global 3D GEOS-Chem model (PEDRUZZI, 2016). A spin-up 48h period will be used to account for initial conditions. In order to establish meteorological conditions, numerical regional model WRF will be used considering 3 nested domains centered in the Piracicaba Region.

The emissions inventories, pre-processed using SMOKE, and meteorological model will serve as input for modelling a base scenario and seven other emission reduction scenarios using CMAQ. These scenarios will consider percentage emissions reductions in alternating fixed and vehicular sources. For validation, the base scenario modelled results will be compared to the air quality monitoring network results using statistical tests.

#### FINDINGS AND ARGUMENT

Preliminary evaluation of local industries mandatory emission monitoring results from 2013 have shown many discrepancies to the database used in the first edition of PREFE, based on a voluntary reporting initiative from 2008, not published (table 2).

Table 2. Annual PM emissions from Piracicaba local industries from 2 databases

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		Annual PM emission (t)			
Industrial		2008	2013		
Industrial	Type	voluntary	mandatory		
Source		reporting	monitoring		
		inventory	results		
ArcelorMittal	Steel	2,54	139		
Hyundai	Auto	=	90		
Raízen	Energy	702	320		

Recent air quality monitoring results have shown that, much like MASP, the pollutant that is currently exceeding the intermediary AQS is ozone, averaging 151  $\mu g/m^3$  during the 2013-2015, compared to the 140  $\mu g/m^3$  1st intermediary AQS. Considering that ozone formation is a complex mechanism, involving different pollutant precursors and environmental factors, an accurate local and regional emission inventory becomes essential for the design of an appropriate emission control strategy.

#### **EXPECTED RESULTS AND CONCLUSIONS**

This study aims to provide an updated detailed temporally and spatially averaged emission inventory for the region of Piracicaba. It also aims to provide an estimative of local vehicular emissions and regional emissions sources that affect the Piracicaba region, through medium and long range transport.

A detailed revision of current local industrial process and emission control technologies will be prepared in order to adjust assumptions regarding their influence in local air quality. The quantification of MASP area emissions also proves essential for this discussion, considering its volume and regional significance (ANDRADE et al., 2017).

These inventories will provide insight into the scale of contribution to local air quality degradation from these sources that can be used to provide guidance to police makers. Subsequently, these will be used as input for a more detailed air quality modelling platform that will be able to quantitatively evaluate the effectiveness and efficiency of the proposed emission control strategy by PREFE and PCPV in São Paulo, and allow for the testing of alternative strategies.

Beyond the expected academic motivation, the expected result of this work is highly applicable to current national air quality management scenario, and it can be reproduced to other regions in order to help design appropriate policies that will help communities improve air quality and general wellbeing.

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### AIR QUALITY SIMULATIONS DURING DRY SEASON OVER SAO PAULO METROPOLITAN AREA UNDER RCP 8.5 SCENARIO WITH WRF-CHEM

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Abstract: Coupled meteorology and chemistry models have become an important tool to assess future scenarios that consider the feedbacks between these two components (e.g., aerosol-cloud interactions). In line with this, the main goal of this study is to evaluate the capability of the on-line coupled Weather Research and Forecasting model with Chemistry (WRF-Chem) to simulate air quality and weather interactions over southeast Brazil, with especial focus over Sao Paulo Metropolitan Area (SPMA) under a changing climate.

In this study, air quality simulations are being conducted for dry-season (June, July and August) during a 5-year period between 2006 and 2010. The simulations are carried out using WRF-Chem v.3.7.1 under the Representative Concentration Pathways 8.5 (RCP 8.5) climate scenario. The simulation domain is based on that for air quality forecast performed by IAG-USP. The CB05 gas-phase chemical mechanism coupled with the MADE/VBS aerosol module is used to account for organic aerosol formation and evolution. Meteorological initial and boundary conditions are taken from NCEP Final Operational Global Analysis data. Chemical initial and boundary conditions are generated from the decadal simulation outputs of a modified version of the Community Earth System Model (CESM)/the Community Atmosphere Model version 5.3 (CAM 5.3) with advanced chemistry and aerosol representations. The meteorological and chemical predictions are compared against observations from the Sao Paulo State Environmental Protection Agency (CETESB) air quality network and satellite retrievals. Results are being analyzed and the major findings and the policy implications will be presented and discussed.

Keywords: WRF-Chem, RCP 8.5, air quality, Southeast Brazil, Sao Paulo Metropolitan Area.

#### INTRODUCTION

Because air quality is also affected by weather condition and vice versa, in the context of climate change, the use of coupled meteorology and chemistry models has become an important tool to assess future scenarios in considering the feedbacks between these two components. Examples of these feedbacks are aerosol-cloud interactions, changes in dry and wet deposition, variation on chemical production, loss rates and natural emissions production (Jacob & Winner, 2009). For that reason, theses models can be used to forecast impacts on future air quality because of change in emissions and climate scenarios (Coleman et al., 2013).

The main goal of this study is to evaluate the capability of on-line model Weather Research and Forecasting model with Chemistry (WRF-Chem) to simulate air quality and weather interactions over southeast Brazil, with special focus over Sao Paulo Metropolitan Area (SPMA). WRF-Chem could became an important instrument to assess the impacts of climate/emission scenarios on future air quality in Southeast Brazil and more specifically.

#### **METHODS**

We used WRF-Chem v3.7.1 to perform the simulation. WRF-Chem is being run with one domain based on Andrade et al. (2015). Model configuration is presented on Table 1, differences from previous studies are the use of the same radiation scheme for short and longwave radiation, a modern cumulus cloud parametrization scheme and a wind correction by topography.

Meteorological boundary conditions are taken from NCEP Final Operational Global Analysis data with and horizontal resolution of 1 °and 26 vertical levels every 6 hours. Chemical Boundary conditions are generated from the decadal simulation outputs of a modified version of the CESM /CAM5 which also used CB05 gas-phase mechanism.

Anthropogenic emission file is being created by using global emissions inventory from RCP 8.5 scenario for years 2000 and 2010 (Riahi et al., 2011). This information has a spatial resolution of  $0.5^{\circ} \times 0.5^{\circ}$  and a monthly average time resolution. Despite the inventory is well detailed, it doesn't have all the species of the gas-phase mechanism, the mapping for RCP to CB05 is based on Yahya et al. (2016), for the remaining species that RCP doesn't include, the emissions are estimated by



using local information from CETESB and field experiments performed over SPMA as showed in Vara-Vela et al. (2016). An example of the regridded emission of Carbon Monoxide (CO) for May on the simulation domain is showed on Figure 1.

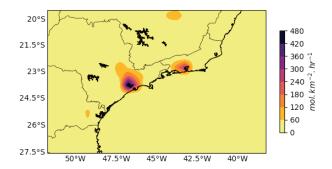


Figure 1. May emission of CO from RCP 8.5 emissions database adapted to the simulation domain.

Table 1. WRF-Chem configuration

Domain Attributes					
9 km x 9 km, 150 x 100	9 km x 9 km, 150 x 100 horizontal resolution,				
35 vertical levels					
Physics Configuration					
Longwave radiation	RRTM				
Shortwave radiation	RRTM				
PBL Scheme	YSU				
Surface Layer	Noah				
Cumulus cloud	Multi-scale Krain-				
	Fritsch				
Cloud Microphysics	Morrison double-				
	moment				
Topographic surface Activated					
wind correction					
Chemistry Configuration					
Photolysis scheme	Fast-J				
Gas-phase mechanism	CB05				
Aerosol mechanism MADE/VBS					

#### FINDINGS AND ARGUMENT

Simulation for the first two weeks of May of 2006 were carried out to evaluate the physics configuration. Figure 2 shows simulations of temperature at 2m (T2), relative humidity at 2m (RH2) and wind speed at 10m (WS) for Ibirapuera station. Performance statistics show that, with this configuration, T2 is slightly underestimates with a mean bias (MB) less than 0.5 °C for stations located

inside MASP, and the correlation coefficient (R) reach values above 0.9. RH2 is also underestimated, R values are above 0.7 while MB is than 10%. For WS, the topographic wind correction is efficient in reduce the overestimation of this parameter with MB less than 1.7 m/s and R higher than 0.5.

It is important to notice that RCP8.5 emissions can represent the emissions from the principal cities, for that reason, MASP and Metropolitan Area of Rio de Janeiro are well depicted, while Belo Horizonte and Curitiba present less spatial detail.

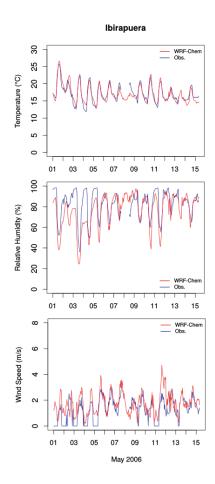


Figure 2. Simulation of temperature, relative humidity and wind speed at Ibirapuera station.

#### **CONCLUSIONS**

Sensibility tests proves that WRF-Chem represents well surface meteorological variables. Next steps are to run WRF-Chem using the new emission that includes RCP 8.5 scenario and local emissions, evaluate the results and start the dry-season multiyear simulations.



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## Projection of mortality and hospital admissions in public health attributable to air pollution in the state of espírito santo between 2017 and 2030

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Abstract: National air quality standards in Brazil were established in the 1990s and are now outdated in relation to international patterns. This creates a challenge for effective control of air pollution levels and contributes to increasing mortality and hospital admissions rates. In order to quantify the impact of adverse health outcomes due to the concentration of particulate matter in Espírito Santo, this paper aims to project the number of deaths, hospitalizations and amounts spent on public hospital admissions from 2017 to 2030. It considers a stationary scenario of air pollution by fine particulate matter (PM2.5), using the year 2014 as baseline. The results show that if air pollution continues at the current levels, it will cause an increase of 95% on the deaths from all causes between 2017 and 2030, as well as some 65 thousand hospital admissions and an estimated public health cost of \$ 36,2 million due to hospitalizations. The magnitude of these results demonstrates the need to implement more rigorous measures to control air pollution and to encourage clean energy transportation, among other public actions, in order to reduce damage to the health of the population and to diminish government spending.

Keywords: Air pollution, Public health, Hospital admissions, Mortality Particulate matter.

#### INTRODUCTION

According to World Health Organization, WHO (2005) clean air is considered a basic requirement of human health and well-being. However, air pollution continues to pose a significant threat to health throughout the world. More than 2 million premature deaths can be attributed to the effects of urban outdoor air pollution and indoor air pollution (caused by burning solid fuels. More than half of this burden of disease is borne by the populations of developing countries. In addition, by 2015, WHO has reported the early loss of about eight million lives worldwide from air pollution. Of these, about 3.7 million were due to external air pollution, which represents 46% of all sources of air-related pollutants. Recognizing it as an increasing threat to global public health, in an official report of the 68th World Health Assembly in May 2015, WHO determined that reducing atmospheric pollution could be a health indicator of post 2015 sustainable development policy (WHO, 2015).

Thus, air pollution has become an important risk factor for epidemiological health studies, since they have the most robust causal associations between long-term exposure to the pollutant and reduction of life expectancy (DOCKERY *et al.* LIPFERT, 1984; POPE *et al.*, 1995).

Air pollution has affected the health of the population, even when their levels are below what is determined by the legislation in force. The adverse effects of air pollutants on human health are a source of concern for environmental and public health regulatory agencies. Population

studies and epidemiological research have been used to identify these adverse health effects and to guide the development of practices and legislation to control emissions and air quality (BOTTONI et al 2013).

The population groups most susceptible to the toxic effects of air pollution are children under five years of age, elderly and individuals with chronic diseases (RITZ; WILHELM; ZHAO, 2006). This study has the objective of projecting mortality and hospital admissions attributable to air pollution in Espírito Santo State, Brazil.

#### **METHODS**

The methodology adopted was based on the work developed by Rodrigues et al. (2015), which includes projections of mortality, hospitalizations and projection of total expenditures with hospitalizations in the public health system, due to the pollution caused by the concentration of particulate matter  $(PM_{2,5})$  in the atmosphere. Concentration data were taken from state air quality monitoring stations. In order to calculate the projections, the following causes of mortality morbidity were considered: cardiovascular diseases, respiratory diseases in the elderly and respiratory diseases in children. Mortality is projected following the methodology established in Spiegel and Hyman (1998, apud Rodrigues et al., 2013) which uses a deterministic model for the projection as shown in equation 1:



$$O^{z,t} = \sum_{x} PO_{n,x}^{z,t} * O_{n,x}^{t}$$
 (1)

Where:

 $0^{z,t}$ = Number of deaths due to cause z in year t, corresponding to each year of the projection;

 $PO_{n,x}^{z,t}$ = Proportion of deaths due to cause z in year t for the age group x to x + n (five-year age groups);

 $O_{n,x}^t$  = Total deaths in year t for the age group x to x + n (five-year age groups).

The projected number of hospitalizations follows the fixed rate methodology proposed in STRUNK (2006, *apud* Rodrigues et al, 2015) therefore using the fixed hospitalization rate of 2014 and the population projected by IBGE (2013) by age group were considered for all the years of the projection which can be seen in equation 2:

$$I^{z,t} = \sum_{x} T I_{n,x}^{z,2014} * P_{n,x}^{t}$$
 (2)

Where:

 $I^{z,t}$ = Number of hospitalizations for cause z in year t, corresponding to each year of the projection;

 $TI_{n,x}^{z,2014}$  = Rate of hospitalization for cause z in 2014 for the age group x to x + n (quinquennial age groups);

 $P_{n,x}^{t}$ = Number of people in year t for the age group x a x + n (five-year age groups).

The projection of the total expenditure with public hospitalizations is calculated from the estimation of the number of hospitalizations resulting from the air pollution obtained in the previous projection. The average expenditure on hospitalizations for each of the causes was fixed at the same level as in 2014. Projected expenditures are at 2014 prices, as shown in equation 3:

$$G^{z,t} = \sum_{x} GMe_{n,x}^{z,2014} * I_{n,x}^{z,t}$$
(3)

#### FINDINGS AND ARGUMENT

Tables 1, 2 and 3 show the sum of deaths, hospitalizations and total expenditures with hospitalizations between 2017 and 2030 attributable to air pollution in a stationary scenario in which air pollution has remained the same since 2017.

The total number of deaths attributable to particulate matter (covering all age groups) increased by 95% in the analysis period, with 248 deaths in 2017 and a projection of 484 deaths by 2030 (Table 1).

Table 1. Projection of total deaths according to causes attributable to particulate matter  $(PM_{2,5})$  in the of State of Espírito Santo, 2017 and 2030

,,,,,,,,				
Deaths				
Causes	2017	2030		
Neoplasms	61	142		
Cardiovascular diseases	212	396		
Respiratory diseases in children	6	21		
Respiratório diseases in elderly	30	67		

In relation to public hospital admissions, different causes of morbidity were considered, so that they represented those with proven studies of the effect of the particulate material on health and respective concentration-response estimates.

These causes correspond to neoplasms, respiratory diseases and cardiovascular diseases, and in populations more susceptible to the effect of pollution, such as children and the elderly. As expected, cardiovascular diseases, considered the main cause in the country both in mortality and in morbidity, also appear as those with the greatest effect due to pollution.

Table 2. Projection of total hospitalizations of the public health system according to causes attributable to particulate matter  $(PM_{2,5})$  in the of State of Espírito Santo, 2017 and 2030

Hospital Admissions				
Causes	2017	2030		
Neoplasms	147	237		
Cardiovascular diseases	1415	2289		
Respiratory diseases in children	642	584		
Respiratório diseases in elderly	1455	2682		

Considering the stationary scenario of pollution, hospitalizations due to cardiovascular diseases would vary from 1,415 to 2,289 between 2017 and 2030 (Table 2), and spending went from about \$ 1,2 million to R\$ 2,1 million in the same period (Table 3).

Table 3. Projection of total hospitalization expenses according to causes attributable to particulate matter  $(PM_{2,5})$  in the of State of Espírito Santo, 2017 and 2030

Expenditure on hospital admissions (\$)					
Causes	2017	2030			
Neoplasms	55,197	88,810			
Cardiovascular diseases	1,298,302	2,099,808			
Respiratory diseases in					
children	165,054	147,423			
Respiratório diseases in					
elderly	494,587	911,764			



Cardiovascular diseases, although they do not represent the greater relative participation of hospitalizations among the four causes considered, are responsible for the higher percentage of hospitalization expenses, due to the high per capita cost of interventions for the treatment of this cause. Together with the expenditures of the other causes it was projected a public health cost of \$ 36,2 million due to hospitalizations from 2017 to 2030.

The hospitalizations attributable to air pollution by diseases of the respiratory tract in children have greater representativeness in hospitalizations as a whole when compared to projections of deaths, although their participation decreases over time. As the projections considered a scenario of hospitalization rate constant over time, this reduction reflects both the population decrease for the increase group and representativeness of respiratory diseases in the elderly. For this cause in the elderly group, there was an increase in hospitalizations attributable to the air pollution of 84% between 2017 and 2030. The relative participation of neoplasms remained practically unchanged.

In the study developed by Rodrigues *et al.*,(2013) in the state of São Paulo, the percentage variations in the projections were not very different when compared to the results in Espírito Santo. The greatest dissimilarity occurred in the projection of deaths due to respiratory diseases in children and the elderly, which may occur due to the difference in the concentration of particulate matter of each state and its health system.

As expected, the results of the projections were higher in the state of São Paulo, since it has larger area and population.

#### CONCLUSIONS

The goal of this study was to present estimates of the effect of pollution on health in the State of São Paulo, according to the WHO methodology for estimating deaths and diseases attributable to pollution (WHO, 2006). In addition, the study intends to contribute to the discussion of the harmful effects of pollutants caused mainly by motor vehicles, to draw the attention of society, public managers and entrepreneurs in search of alternatives of urban mobility, innovations in transport management and materials. As well as more stringent legislation and increase in the number of air pollution monitoring stations.

Such measures would serve as a guide for the implementation of local actions that result in improved air quality in the country. More specifically, studies such as this show that a crosscutting theme as important as air pollution should support intersectoral discussions between health and the environment in public policies and management plans to reduce the emission of air

pollutants, especially in large urban centers, as is the case of the Metropolitan Region of Espírito Santo.

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### Fine-Scale Modeling of Air Pollution Exposures during Commutes to School

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Traffic-related air pollutants can cause adverse health effects on human health in the near-field. Understanding how school location impacts children's air pollution exposure and the ability of children to walk and bike to school has been a policy issue of interest in recent years. This study analyzes children's air pollution exposure across an average school day—from the time they leave home in the morning to the time they return home from school. This research compares the daily average exposure for children walking to a local school in a heavy-diesel/heavy-traffic area compared to their exposure if they were required to be bussed or driven to a more remote school located in a low-diesel/low-traffic environment. The analysis also assesses how pollution exposure can be mitigated through policy interventions such as adoption of clean school bus fleets and improved school HVAC systems. We selected two neighborhoods in Detroit, Michigan with different air quality environments – heavy-diesel/heavytraffic and low-diesel/low-traffic – with a synthetic sample of students. Students were analyzed for commutes to their high traffic neighborhood school and for commutes to the re-located school in the low traffic neighborhood. Home-toschool commuting routes were created for three modes: walk, automobile, and school bus. Air pollution exposure along each route was estimated using R-LINE - a near-road dispersion model, and an application initially developed for the Near-Road Exposures and Effects of Urban Air Pollutants (NEXUS) study, to capture conditions in 2010 during typical school travel periods for the Detroit metropolitan area. Daily average exposures for six pollutants (Benzene, CO, NOx, PM2.5, EC, OC) were estimated across 5 phases of an average school day (AM Commute, Unload, School Day, Load, PM Commute). We will present results from this study focusing on evaluating cumulative daily exposures for school children for different commute modes in each of the two school populations, as well as when bussing children from a high-diesel/high-traffic neighborhood to a remote school in a low-diesel/low-traffic environment, and for assessing potential benefits when infiltration factors were adjusted to model effects of clean bus technology and improved school HVAC.



### Projecting Changes in Fuel Loads, Fire Activity and Wildfire Emissions into the Future: Case Study Over the Southeastern US

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Wildfires have posed a significant challenge for 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 wildfire areas burned and wildfire emissions will trend in the future are important for developing sound policies on the management of air quality and natural resources. The increasing frequency of catastrophic wildfires is being attributed to climate change, but other factors such as population and income growth, and the proximity of humans to wildland also play a role, particularly in the Southeastern US. Our methods take into account changes in both climate and socioeconomic factors that drive wildfires in this region. This case study over the Southeastern US applies these methods to examine the impacts of changes in fire weather and fuel load on wildfire emissions used to simulate future air quality. Results are presented for wildfire emissions trends in future under the RCP8.5 scenario of greenhouse gas emissions growth. The sensitivity of wildfire emissions to decadal changes in fuel load in response to climate change between now and mid-century is also examined.



### Impact of Projected Anthropogenic Emissions on Air Quality and Climate at Regional and Urban Scales

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To address the continuous lowering of the health-based air quality standards and identify efficient emissions control measures, there is a need to understand the relative contributions to air quality and health from individual source sectors. We used the Community Multiscale Air Quality (CMAQ) model instrumented with the Decoupled Direct Method (DDM), an advanced sensitivity analysis technique that allows us to estimate the influence of individual pollutants from individual sources or regions. We specifically focused on three individual source sectors – residential combustion, electric generating units and aircraft emissions. We considered direct residential combustion by state, leveraging Census and housing start data to determine spatial patterns of emissions within states, and modeled individual power plants in geographic groupings using a design of experiments that allow us to estimate the impacts for all major power plants on the grid. In addition, we also modeled each of the major airports in the U.S. We then estimated sensitivities of state-specific O3 and PM2.5 – key drivers of monetized health impacts - to individual precursor emissions. As CMAQ provides concentration estimates by grid cell, we were able to determine total public health benefits in terms of avoided mortality and morbidity (using BenMAP-CE) as well as the distribution of those benefits for directly modeled facilities and locations. A key outcome of this study was assessing the carbon reductions and health cobenefits from increased residential energy efficiency measures. We will present results from this study focusing on CMAQ and BenMAP-CE results quantifying the air quality and health benefits associated with reduced residential heating and electricity generation from individual states and/or regions in the U.S. and further illustrate how the results from this approach can be used to develop damage functions across various emissions sectors for individual precursors for developing policy options.



### Chemical composition of Fine Particles and Incidence of Acute R espiratory Diseases in Children

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Abstract: The aim of this work is to investigate the association between fine particles concentration (PPM 2.5),, including its c omponents as chemical inorganic elements, black carbon and hospital admissions and outpatients attendances due to acute respiratory diseases in children up to 12 year s old living in urban and industrial areas , during winter (221//006//22013 to 21//009//22013)) and summer times in the South hemisphere (221//112//22013 to 19//003//22014)) periods.. Six portable MiniVol samplers were used to sample fine particles (PPM 2.5) at six sites in the region during a 24hour period in alternate days . They were weighted in a scale with 1 µm sensiti vity and the analysis of its components was carried out using the energy dispersion X - ray fluorescence technique and by the reflectance technique . Daily data of hospital admissions and outpatients attendances due to acute respiratory diseases in CID - 10 J00 - J99 groups were obtained in three hospitals (oone public and two private)) in children up to 12 - year old . To quantify the correlation between acute respiratory diseases to the pollutant concentrations and PM 2.5 concentration considering the effects of pred ictor covariables,, the Generalized Additive Model (GGAM)) with Poisson distribution was applied.. The results showed a higher risk of acute respiratory events in relation to the exposure to fine particles,, for six days of exposure, which the risk of 1,056 (IIC 95%%:: 1,003 - 1,110)) for each increment of 4.25 µg//mm<sup>33</sup> (iinterquartile interval)) in MP 2.5 concentration estimates a relative risk of 1.056 (((IIC 95%:: 1.003 - 1.111)) . The exposition occurring with a lag of six days of acute hospital attendance or adm ission.. With respect to c hemical components present in fine particulate showing a greater risk of causing acute respiratory diseases were Si - 1,, 22 RR (IIC 95%:: 1,15 - 1,29)),, S - 1,09 RR (IIC 95%:: 1,06 - 1,12)),, Ti - 1,09 RR (IIC 95%%:: 1,01 - 1,17)), the Black Carbon (BBC)) - 1,07 RR (IIC 95%%:: 1,03 - 1,11)) for a same day occurrence of exposure and outcome. For outcomes due to a two - day period after exposure,, the greatest risk of respiratory diseases in the short term is associated with the presence of Se - 1,1425 RR (IIC 95%%:: 1,0618 - 1,2293)) and Ni - 1,10 RR (IIC 95%%:: 1,0244 - 1,1937))..

Conclusion: Although WHO suggests a guideline for air quality associated with PM 2.5 (225 µg//mm³³ for short term exposure,, i..ee..,, 24h - mean concentration)),, WHO also states that it is not po ssible to identify a threshold that guarantees no health effects.. Similarly,, even though the 24h - mean concentration in MRGV did not exceed WHO´´ss guideline for PM2.5 during the period investigated in this work,, the results have clearly shown that there is a n association between PM 2.5 concentration and hospital

admissions and attendan ce of children up to 12 years old.. There are few studies in the literature associating the effects of chemical elements constituent of PM 2.5 in acute respiratory events.. More ef fective controls on pollutant emissions and strict enforcement are needed by public authorities to mitigate the deleterious effects of diseases in urban areas..

Keywords: Air pollution,, fine particles,, Inorganic particulate;; Black Carbon,, respiratory diseases, GAM.



### COMMUTER'S EXPOSURE TO FINE PARTICLES AND BLACK CARBON IN PUBLIC TRANSPORTATION BUSES

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Abstract: The objective of this study was to evaluate the concentration levels of  $PM_{2.5}$  and Black Carbon equivalent (BCe) during the main trips to the population that uses the public as a means of transportation in Londrina-PR. In this way, measurements and PM2.5 collections were performed at a human respiration rate (MIE pDR-1500 ™ monitor) in five bus lines and during periods of higher and lower user flow, totaling 240 hours of sampling. The purpose of this study was to characterize exposure levels at different times and their health potential in the population during the daily work and / or study routes. In terms of average concentration of  $PM_{2.5}$  and BCe were of 18.8 µg m³ and 7.8 µg m³, respectively. In addition, the exposure of commuters is not similar on the five lines and higher in times of greater flow of people. The moments of greatest exposure are those waiting at the urban terminals or near bus stops of a large vehicular stream. In this study, a major source of vehicle emissions, because the sampling was carried out directly inside the buses in urban routes, but the contribution of industrial sources and the burning of biomass and waste were identified. On average, 40.5% of  $PM_{2.5}$  mass is BCe, indicating a potential health effect during displacement, considering that it is known to be toxic.

Keywords: Fine particulate matter, Black Carbon, urban routes.

#### **INTRODUCTION**

The traffic displacement is considered to be one of the periods with the greatest exposure to atmospheric pollutants among the daily activities, especially in high-density urban areas (DUCI et al., 2003). According to the WHO report (2005) on the effects of air pollution on health, in many countries people spend an average of 1 to 1.5 hours in traffic. In addition, the levels of the main pollutants are particularly high on the busy roads and avenues, and in places where major urban transport runs, with the highest peaks during the morning (MORAWSKA et al., 2008; MORENO et al., 2009).

In this way, concentrations of air pollutants are higher in the microenvironment of urban traffic, resulting in a significant contribution to personal exposure, even if travel time does not represent more than 6 to 8% of the day (KAUR et al., 2007). Several studies saying that passengers who travel regularly can receive up to 30% of the total inhaled daily intake of Black Carbon and approximately 12% of the PM2.5 dose during that period (FONDELLI et al., 2008; DONS et al., 2011, 2012). Black Carbon (BC) is a primary pollutant composed of PM, associated mainly with fine and ultrafine fractions (BRIGGS and LONG, 2016). It is a byproduct of incomplete combustion of fossil fuels and biomass burning, considered a marker of components derived from combustion, widely associated with epidemiological studies (BRIGGS and LONG, 2016, HEAL et al., 2012, DONS et al., 2013).

In the last years, researchers investigated the health effects caused by PM from specific sources such as vehicular traffic. They found that BC rich are related to vehicle characteristics and result in effects on the cardiovascular and respiratory systems (US EPA, 2012; DONS et al., 2013, 2012). Thus, the BC has been widely used as a relevant marker of traffic related air pollution, characterizing mainly dieselpowered vehicles (LEE et al., 2014). Thus, the present study aims to evaluate the concentration levels of PM<sub>2.5</sub> and Black Carbon equivalent (BCe) during the main displacements carried out by the population that uses public buses as a means of transportation in the city of Londrina-PR.

#### **METHODS**

The public transport system of Londrina transports approximately 4.027.443 million passengers per month, and may suffer some variations according to the year, according to Londrina's transport and urban planning company.. The bus fleet has an average age of five years and use \$500 and \$10 diesel fuels, but in greater quantity the \$500. The times of greatest flow of users are in the and in the late afternoon, which was named of peak (P). Five bus lines were selected based on the greatest demands and covered all regions of the city. The lines were named according to the direction of their route, starting from the central region of the city to the directions East, West, South, North, and a fifth line North-South, according to Figure 1.



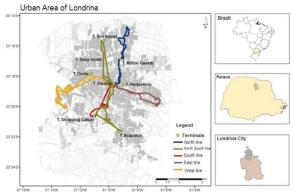


Figure 1. Localization of the study area and the selected commuter routes.

Each sampling was carried out for 8 hours, and therefore, several repetitions of the route were performed until adding up to 8 hours of measurement and collection of PM<sub>2.5</sub> in each line and period of peak (higher demand, 6 to 8 am. and 5 to 7 pm.) and non-peak (less demand, 8 am. to 5 pm.). In addition, in order to better characterize the exposure of the Londrina population during commuter in bus lines with higher demand of use, 240 hours of sampling were performed in the five lines in period between 6 am. to 7 pm in workdays without raining. A backpack containing a MIE pDR-1500™ personal monitor and collector (Thermo Fisher Scientific) was used, with the inlet out and positioned in the breathing zone. The equipment measured PM<sub>2.5</sub> concentrations every 1 minute, as well as collected particles up to 2.5 µm in PTFE filters (PALL Corporation). In addition to the monitor, the backpack contained a GPS DG-100 Data Logger (Global Sat).

#### FINDINGS AND ARGUMENT

In terms of mass concentration of the fine particulate matter, peak presented the highest mean concentration with 18.8  $\mu g$  m<sup>-3</sup>, while the non-peak mean concentration was 15.9  $\mu g$  m<sup>-3</sup>, suggesting higher exposure during peak activity, due to the greater activity of people and vehicles in this period.

The BCe was the one that presented a less variable behavior due to the characteristics of the sampling sites, that is urban and moving through the urban environment using buses as a means of transport, similar to the one performed daily by the population. The BCe in the urban environment has as main source of emission the burning of fuel. The line presented the highest concentrations during peak and non-peak, with mean  $PM_{2.5}$  concentrations of 20.7  $\mu g$  m<sup>-3</sup> and 23.2 μg m<sup>-3</sup>, respectively. The South line had mean concentrations of PM<sub>2.5</sub> of 17.8 µg m<sup>-3</sup> for the peak and 11.9 µg m<sup>-3</sup> for non-peak.

The west region line indicated a mean concentration for the peak of 18.0  $\mu g \ m^{-3}$  of PM<sub>2.5</sub> and for the non-peak 21.6  $\mu g \ m^{-3}$ . In the north line the mean concentration of PM <sub>2.5</sub> for the peak was 20.47  $\mu g \ m^{-3}$  and for the non-peak it was 11.1  $\mu g \ m^{-3}$ . The north line during peak obtained a mean PM<sub>2.5</sub> concentration of 18.4  $\mu g \ m^{-3}$ , during the non-peak the mean concentration was 11.4  $\mu g \ m^{-3}$ . According to Figure 2.

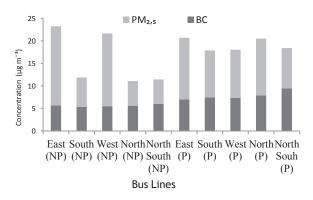


Figure 2. Average concentration of PM<sub>2.5</sub> and BCein each route, during time of peak (P) and non-peak (NP).

The variation of the time of arrival and exit of the buses, the different states of maintenance of the vehicles, the urban canyons present in the cities and the number of stops in the waiting points can contribute significantly to the variability of the concentrations of  $PM_{2.5}$  in the public transport. Being presented as peaks of temporal concentrations, that is, lasting only a few seconds. However, they contribute disproportionately to personal exposure to pollution (VELASCO e TAN, 2016).

On average, the concentration of BCe for the peak was 7.8  $\mu$ g m<sup>-3</sup> and 5.6  $\mu$ g m<sup>-3</sup> for the non-peak. The highest concentrations during peak may be related to the greater number of vehicles traveling the streets and avenues of the city, congestion and greater flow of buses in the urban terminals. The contribution of BCe in PM<sub>2.5</sub>, in average percentage terms, the peak lines contributed with 41.4% of the total PM<sub>2.5</sub> mass, while non-peak contributed with 39.3%, that is, was a more contribution from the BCe during peak. The lines that presented the highest concentrations of BCe during the peak were: the North-South line, with mean concentration of 9.4  $\mu$ g m<sup>-3</sup>, North with a concentration of 7.9  $\mu$ g m<sup>-3</sup>, South with 7.5  $\mu$ g m<sup>-3</sup>, followed by the West line 7.4  $\mu$ g m<sup>-3</sup> and East with 7.0  $\mu$ g m<sup>-3</sup>.

The North-South line presented the highest average concentrations of BCe, possibly because it is a line that runs most of the time on large avenues, not frequents areas with less flow of



vehicles, such as neighborhoods. In addition, it crosses part of its route by the highway BR 369, with the presence of heavy traffic and has passage through three urban terminals. That is, the waiting the passengers for the next trip is inside the urban terminal, with a large bus flow, and can influence the BCe concentrations of this line at peak, precisely because this pollutant is a marker of vehicular emissions.

For the non-peak the lines had the following average concentrations: North-South line 6.0 µg m , East with 5.6 μg m<sup>-3</sup>, North line 5,6 μg m<sup>-3</sup>, West 5,5  $\mu$ g m<sup>-3</sup> and South with 5.4  $\mu$ g m<sup>-3</sup>. The concentrations during the non-peak are smaller, which can be justified by the decrease of the vehicular flow, both in the routes traveled, as well as in the urban terminals. However, the North-South line continued to stand out in terms of higher mean concentrations of BCe, even for the non-peak. In the North sector of the city live the low income population, suggesting inequalities in the exposure even in the same mode of transportation, which are associated with higher time of trip. However, this issue should better addressed in future works.

#### **CONCLUSIONS**

In terms of mass concentration of  $PM_{2.5}$  and BCe, the period with higher demand presented the highest mean concentration. In the case of this study, the main source of emission is vehicular traffic, since the sampling was carried out directly within the buses on urban routes, but the contribution of industrial sources and the burning of biomass and waste was identified. On average, 40.5% of  $PM_{2.5}$  mass is BCe, indicating a potential health effect during displacement, considering that it is known to be toxic.

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# ESTIMATING THE EFFICIENCY OF EMISSION CONTROL POLICIES ON IMPROVING LOCAL AIR QUALITY USING NUMERICAL MODELS: A CASE STUDY IN AN INDUSTRIAL MUNICIPALITY IN SÃO PAULO, BRAZIL

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Abstract: Growing levels of urbanization in developing countries have generally resulted in increasing air pollution, due to higher activity in the transportation, energy, and industrial sectors. The identification and understanding of the multiple pollutant sources' contribution to air quality in such sectors, locally and regionally, is essential to designing an effective emission control policy. Air quality modelling associated with emission scenarios is an important tool that can provide guidance on the most efficient and effective air quality management strategy. This work focuses on Piracicaba, an industrial municipality with a total area of 1378 km<sup>2</sup> and a population of 365 thousand inhabitants, located in the state of São Paulo. After updating its air quality standards in 2013 to levels suggested by the World Health Organization, the state of São Paulo has proposed a state-wide stationary and mobile sources emission reduction program, singling out locations in which air quality levels do not comply with the updated standards. Control strategies proposed so far focus on local stationary sources, (mainly sugar-alcohol, automotive and steel industries) largely underestimating vehicle emissions and regional contributions from the neighbouring Metropolitan Area of São Paulo to the local air quality. This work aims to model this scenario by preparing spatially and temporally averaged emissions from local industrial sources, using mandatory monitoring data and process-based estimations, along with vehicle emissions obtained through locally adapted emission factors and the road network provided by the OpenStreetMaps platform. This data will be processed using SMOKE which, along with a local and regional WRF meteorological model, will serve as an input for modelling emission reduction scenarios and estimating their effectiveness in achieving the expected air quality levels. It is anticipated that preliminary results will show that the afore mentioned pollutant emissions can be compared with levels initially considered by local authorities when designing the emission control program, as well as estimating the influence of regional emissions in local air quality.

Keywords: Air quality management, emission control policies, air pollution, numerical models, air quality modelling

#### INTRODUCTION

Clean air is a basic and essential requirement to human health and wellbeing. For this reason, atmospheric pollution represents a significant risk to population. The first studies to report on this correlation date from the mid-twentieth century, but recent studies continually report evidences of adverse effects on health of air pollution following both acute and chronic exposure (MANNUCCI et al., 2015).

Prevention of the negative effects of air pollution starts by correctly identifying the most active pollutants in a certain region and determining maximum concentration levels acceptable in order to guarantee the wellbeing of general population wellbeing. These levels are established as Air Quality Levels (AQS) that serve as a fundamental guideline for air quality management programs from national and regional environmental agencies. For this reason, AQS definition process must also consider monitoring criteria and data access and disclosure to governing bodies and general public (SANTANA et al., 2012).

Based on AQS, air quality management programs must employ instruments that provide a holistic perspective of the multiple factors that influence air quality degradation in an area, in order to adopt the most effective and efficient emission control strategy. Among these are air quality monitoring networks, emissions inventories, sources monitoring and dispersion modelling, environmental licensing, as well as post-control instruments.

The nationally adopted AQS in Brazil are established by Resolution 03/1990 of the Brazilian Conselho Nacional de Meio Ambiente (CONAMA, National Environmental Council). These can be considered outdated if compared to the Air Quality Guidelines Global Update 2005 (WHO, 2006), because of its permissive levelsan and for disregarding relevant pollutants, such as fine particulate matter (diameter <2.5 $\mu$ m, PM<sub>2.5</sub>).

Ahead of the update of national AQS, the states of São Paulo and Espírito Santo have, in 2013, updated their state-wide AQS to WHO levels. As recommended by the Guidelines, both states have established intermediary progressive levels, that



should be targeted leading up to a full state-wide adoption of final standards. Both states have since released emission control programs for its main pollutant sources, in order to achieve the progressive target levels.

The goal of this work is to critically analyse the emission control strategy being proposed for the state of São Paulo, and evaluate its potential efficiency and effectiveness in improving air quality locally and regionally.

São Paulo's control actions are stated in two major programs: Programa de Controle de Emissões de Fontes Estacionárias (PREFE, Fixed Sources Emissions Control Program) and Plano de Controle da Poluição Veicular (PCPV, Vehicular Pollution Control Plan) (CETESB, 2014). Both programs aim to achieve targeted levels in critical control areas within the state by prioritizing emission control actions. But these present conceptual problems: PREFE and PCPV are not well integrated with other state policies and with each other, e.g., both programs adopt distinct methodologies when defining control areas, disregarding potential synergic or conflicting interactions that may undermine its effectiveness (LIU et al., 2014).

The first edition of PREFE defines control actions guidelines for the 2014-2016 period based on 2010-2012 air quality monitoring results. The two year gap in-between can be a source of misinformation when suggesting control actions, in which a pollutant can be already under control when a emission reduction plan is being put into practice (Table 1).

Table 1.  $PM_{10}$  averaged annual mean  $1^{st}$  intermediary AQS exceedance in Piracicaba in 2010-2012 and 2013-2015 periods

2010 2012 and 2013 2013 periods					
Manitanian	SP 1st Intermed.	Averaged Annual Mean			
Monitoring Stations	AQS	2010-2012	2013-2015		
	MI1	(µg/m³)	(µg/m³)		
Piracicaba - Algodoal (M)	40	49	38		
Piracicaba (A)	40	-	37		

Reference: adapted from (CETESB, 2016)

PREFE defines seven control areas (*Regiões de Controle*, RCs) in which occurrences of exceedances of the new proposed AQS have been registered in air quality monitoring results. Piracicaba, an industrial municipality with a total area of 1378 km² and a population of 365 thousand inhabitants, is one of those RCs (figure 1), in which coarse particulate matter (diameter <10 $\mu$ m, PM<sub>10</sub>) was considered the main pollutant of concern.



Figure 1. RC7 Piracicaba Reference: (CETESB, 2014)

The proposed control strategy focuses on local industries, mainly steelmaking, sugar-alcohol and automotive as the most significant in the region. This potentially underestimates long range transport pollutant contributions from the neighboring Metropolitan Area of São Paulo (MASP), a megacity of 21 million inhabitants that face many air quality challenges and where concentrations of regulated pollutants frequently exceed AQS (ANDRADE et al., 2017).

For these reasons, great uncertainties can be distilled from the proposed emission control program, regarding its effectiveness. Numerical air quality modelling, a tool extensively used to evaluate air quality management programs, will be used to evaluate the Piracicaba case. Different emission reduction scenarios are considered in order to investigate which actions could prove more efficient in achieving the desired ambient air quality levels.

#### **METHODS**

In order to appropriately represent the Piracicaba case, considering long, medium and local range emissions, as well as secondary pollutant formation mechanisms, the Community Multiscale Air Quality Modelling System (CMAQ) will be used. It is Eulerian tridimensional multipollutant and multiscale model recommended by USEPA for an integrated medium to long range assessment of air quality management strategies.

In order to be used as input data for CMAQ, an updated spatially and temporally averaged emissions inventory from local industrial sources will be prepared, considering mandatory emissions monitoring data as well as process-based estimations using emission factors. Vehicular emissions will be prepared through the model REMI (R-Emissions-Inventory) that uses locally adapted emission factors, and the road network provided by the OpenStreetMaps platform. In order to define boundary conditions for the Piracicaba region, the nested domains technique will be used, adopting



two regional larger scale domains centered around the area of interest (Piracicaba): a regional domain considering the state inventory, and larger domain employing the global 3D GEOS-Chem model (PEDRUZZI, 2016). A spin-up 48h period will be used to account for initial conditions. In order to establish meteorological conditions, numerical regional model WRF will be used considering 3 nested domains centered in the Piracicaba Region.

The emissions inventories, pre-processed using SMOKE, and meteorological model will serve as input for modelling a base scenario and seven other emission reduction scenarios using CMAQ. These scenarios will consider percentage emissions reductions in alternating fixed and vehicular sources. For validation, the base scenario modelled results will be compared to the air quality monitoring network results using statistical tests.

#### FINDINGS AND ARGUMENT

Preliminary evaluation of local industries mandatory emission monitoring results from 2013 have shown many discrepancies to the database used in the first edition of PREFE, based on a voluntary reporting initiative from 2008, not published (table 2).

Table 2. Annual PM emissions from Piracicaba local industries from 2 databases

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Industrial Source	Туре	Annual PM emission (t)				
		2008	2013			
		voluntary	mandatory			
		reporting	monitoring			
		inventory	results			
ArcelorMittal	Steel	2,54	139			
Hyundai	Auto	-	90			
Raízen	Energy	702	320			

Recent air quality monitoring results have shown that, much like MASP, the pollutant that is currently exceeding the intermediary AQS is ozone, averaging 151  $\mu g/m^3$  during the 2013-2015, compared to the 140  $\mu g/m^3$  1st intermediary AQS. Considering that ozone formation is a complex mechanism, involving different pollutant precursors and environmental factors, an accurate local and regional emission inventory becomes essential for the design of an appropriate emission control strategy.

#### **EXPECTED RESULTS AND CONCLUSIONS**

This study aims to provide an updated detailed temporally and spatially averaged emission inventory for the region of Piracicaba. It also aims to provide an estimative of local vehicular emissions and regional emissions sources that affect the Piracicaba region, through medium and long range transport.

A detailed revision of current local industrial process and emission control technologies will be prepared in order to adjust assumptions regarding their influence in local air quality. The quantification of MASP area emissions also proves essential for this discussion, considering its volume and regional significance (ANDRADE et al., 2017).

These inventories will provide insight into the scale of contribution to local air quality degradation from these sources that can be used to provide guidance to police makers. Subsequently, these will be used as input for a more detailed air quality modelling platform that will be able to quantitatively evaluate the effectiveness and efficiency of the proposed emission control strategy by PREFE and PCPV in São Paulo, and allow for the testing of alternative strategies.

Beyond the expected academic motivation, the expected result of this work is highly applicable to current national air quality management scenario, and it can be reproduced to other regions in order to help design appropriate policies that will help communities improve air quality and general wellbeing.

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### HEALTH AND ECONOMIC EFFECTS OF REDUCED PM<sub>2.5</sub> CONCENTRATIONS ON MORBIDITY IN THE GREAT VITORIA REGION

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Abstract: Association between PM<sub>2.5</sub> concentration and morbidity caused by respiratory diseases in children has been reported in the literature. The purpose of this study is estimate health and economic benefits from reduced PM<sub>2.5</sub> concentrations in the Great Vitoria Region (GVR). Monitoring data as well as emission inventory from 2010 was used into Community Multi-scale Air Quality Modeling System (CMAQ) in order to determine annual PM<sub>2.5</sub> concentration in each city. Population data for the age group (0-14) and economic variables were obtained from Brazilian Institute of Geography and Statistics (IBGE). Incidence rates and medical cost were attained from Computer Department of Unique System of Health (DATASUS). Besides, effect estimate (B) used is from an epidemiologic study derived for GVR. These data were placed as input files into BenMAP-CE in which health and economic effects were estimated considering three different thresholds established by State Decree 3463-R/2013. Cariacica already has its annual concentration below established levels considering only PM<sub>2.5</sub>, therefore, neither reduced cases nor savings were accounted. Vitoria presents the highest difference between modeled concentration and air quality thresholds. It implies the number of reduced cases will be 0.166% of the children studied in Vitoria. Vitoria would save \$20.6 million per year which represents 0.075% of the gross state product. These findings might be overestimated due to parameters used to calculate the relative risk and the simplistic economic analysis.

Keywords: Reduced PM<sub>2.5</sub>, respiratory morbidity, children, health effects, economic effects.

#### INTRODUCTION

 $PM_{2.5}$  (particulate matter with  $\leq 2.5 \mu m$ aerodynamic diameter) have been linked to mortality and morbidity in different age groups (Pope III et al., 1995; Cançado et al, 2006). This pollutant often result of fossil fuel combustion from vehicle exhaust and industrial production can not only penetrate deeply into the lungs but also enter the bloodstream, causing cardiovascular complications (UNICEF, 2016; Pražnikar Pražnikar, 2012). Children are highly vulnerable to this pollutant and develop diseases feasibly. Studies have shown strong association between PM<sub>2.5</sub> and respiratory morbidity in this age group (Tecer et al., 2008; Zhang et al., 2002; O'Connor et al., 2008; Nascimento, 2015). However, PM<sub>2.5</sub> concentrations in Great Vitoria Region are still of World Health Organization's recommendations which affect welfare. A State Decree 3463-R/2013 is an attempt to improve air quality but its implications are still uncertain. In this context, this study aims to evaluate benefits due to implementing the State Decree by analyzing the health and economic effects of the reduced fine particles concentrations on respiratory morbidity in children (0-14) in the Great Vitoria Region.

METHODS Study Area The study area (Figure 1) includes 4 cities of the Great Vitoria Region (GVR) where roughly 42.69% (1,500,392) of the state population reside and about 60% (\$16,518,382,727) of the gross state product is generated. In this region, many enterprises including steel and iron mining industry are located.

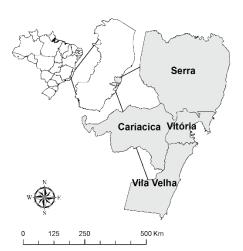


Figure 1. Study Area

#### Air Pollutant Data

Monitoring data from 8 stations of Automatic Air Quality Monitoring Network and emission inventory of Great Region developed by State Environmental



Institute in 2010 were used into Community Multiscale Air Quality Modeling System (CMAQ). Ground-level concentrations of  $PM_{2.5}$  were simulated for grid cells (1x1 km) for each hour in 2010. An annual concentration for each city was attained with VERDI 1.4 in which map created with data from Brazilian Institute of Geography and Statistics (IBGE) was also used.

#### **Health Data**

Morbidity data due to respiratory diseases (ICD 10: J00-J99) from Computer Department of Unique System of Health (DATASUS) and population data (Pop) from IBGE were obtained in order to calculate incidence rate (I). Health effects were estimated with the following equation:

$$C = I * Pop * (1 - e^{-\beta * \Delta P})$$
 Eq. 1

Where C represents either increase or decrease in number of cases based on baseline scenario,  $\Delta P$  is the change in pollutant concentration between baseline and control scenario and B is the effect estimate which is usually derived from epidemiologic studies.

In this analysis,  $\beta$  was acquired from Nascimento (2015). The author applied a Generalized Addition Model with Poisson regression to analyze the association between PM<sub>2.5</sub> concentrations in those 4 cities of the GRV and morbidity caused by respiratory diseases (ICD 10: J00-J99) in children in the 0-12 age group.

#### **Economic Data**

Medical expenses such as values of hospital services as well as medical services were acquired from DATASUS. Besides, mean length of stay (MLS) was also quantified from DATASUS data.

In addition, total income data (I) was attained from IBGE.

From these data, economic effects can be predicted as:

$$EV = H + MLS * \frac{I}{52 * 5}$$
 Eq. 2

Where EV indicates the total money saved or spent in those previous estimated cases (Eq. 1) and H is the mean hospital charge in 2010.

#### **Estimating effects**

In order to determine the health and economic effects from reduced  $PM_{2.5}$  concentrations, Environmental Benefits Mapping and Analysis Program - Community Edition (BenMAP-CE) was applied.

Three different control scenarios were defined take into consideration the three thresholds for annual concentrations of  $PM_{2.5}$  established by State Decree 3463-R/2013:  $20\mu g/m^3$  for second intermediate goal (Scenario 1 - S1);  $15\mu g/m^3$  for third intermediate goal (Scenario 2 - S2) e  $10\mu g/m^3$  for final standard (Scenario 3 - S3). For each control scenario, only city that has concentration above the air quality threshold had its  $PM_{2.5}$  concentrations reduced.

#### FINDINGS AND ARGUMENT

The following table presents annual  $PM_{2.5}$  concentrations for each city.

Table 1. Annual PM<sub>2.5</sub> Concentrations (in µg/m³) for baseline and control scenarios for each city in the study area.

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City	Baseline	S1	S2	S3		
Cariacica	8.01	8.01	8.01	8.01		
Serra	15.82	15.82	14.98	9.97		
Vila Velha	20.31	19.99	14.99	9.95		
Vitoria	29.34	19.95	14.96	9.98		

According to table,  $PM_{2.5}$  levels in Cariacica is already below the threshold for every scenario considered. While estimative of reduced cases was develop only for S2 e S3 for Serra, in case of Vila Velha and Vitoria all scenarios were analyzed. Especially Vitoria has the highest annual  $PM_{2.5}$  concentrations, which means the highest decrease that can reach 66% in the S3.

Those high differences between baseline and control scenarios are reflected in the estimative of the number of reduced cases (Figure 2).

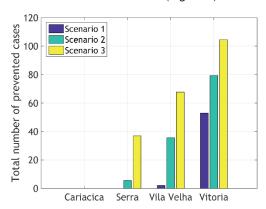


Figure 2. Estimate of Reduced Morbidity Cases in Children for each City

Since the annual  $PM_{2.5}$  concentrations in Cariacica do not differ among the scenarios, no case was predicted. In case of other cities, the estimate was directly proportional to the difference in  $PM_{2.5}$  concentrations between the scenarios. As expected, Vitoria exhibits more potential to reduce morbidity caused by respiratory diseases in children than other cities analyzed.

For the scenario 3, reduced cases represent 0.036%, 0.078% and 0.166% of the population in the 0-14 age group considered for Serra, Vila Velha and Vitoria, respectively. Nonetheless, the number of cases can be overestimated. It might occur due to B value (0.0089±0.0057) applied in this study. Its high standard deviation can contribute to overestimate the total number of cases. Besides, the use of annual concentration into BenMAP-CE may promote these high values owing to this model uses annual concentration as daily average. Also,



spatial distribution of the concentration and population was not considered which can bias the human's exposure.

Hence, the economic effects (Figure 3) are influenced by the previous result.

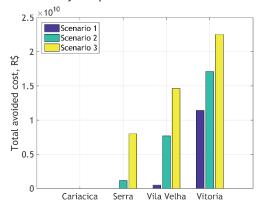


Figure 3. Expected Savings from Reduced Morbidity Cases in each City

The annual money saved with the more rigorous air quality standard established on the State Decree 3463-R/2013 is estimated in around R\$ 21.9 million (\$ 7.3 million); R\$ 40.0 million (\$ 13.3 million) and R\$ 61.8 million (\$ 20.6 million) for Serra, Vila Velha and Vitoria, respectively. It means 0.075% of the gross state product will be saved only in Vitoria. However, those values need to be analyzed carefully.

#### CONCLUSIONS

High PM<sub>2.5</sub> concentrations affect human health, especially children. Morbidity due to respiratory diseases is one of the possible effects caused by air pollution. This work presented estimate of the reduced cases as well as economic benefits. For the final standard determined by the Decree 3463-R, total reduced cases 0.166% of the population considered and savings may be 0.075% of the gross state product for Vitoria. Although these results are possibly overestimated due to B-value, annual spatial distribution concentration and no considered, it is an overall view of this issue. Therefore, further study is necessary in order to use daily average for each city; to develop new regression analysis to have more precise B with interference from confounding effects resulting from social and demographic aspects, to performer more meticulous economic analysis, to include presence simultaneous of intercorrelated pollutants and to contemplate spatial distribution of population and air pollutant concentration as well

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### Perceived risk, air pollution and annoyance: A compative study conducted by surveys

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Abstract: Interventions for reducing air pollution are important means for improving public health. However it is important to annalyse the regional context before to make definitive conclusions. This study aimed to analisy the effects of the intervention (closure the pallet making industry) with respect to perceived air pollution, risk perception and annoyance caused by dust. Surveys were performed before and after the intervention of a pelletizing plant. Individuals in the region of study aged 16-75 years were selected at random for participation in 2012 and in 2017. More than 200 respondents answered the questionnaire in both surveys. The two samples are representative of the population at the two points in time, and thus not identical. The main results shows that after the pelletizing plant were stopped theirs activities, the air quality was perceived as being less dusty, the residents were more sensitive to the industrial risk perception, and the respondents (sometimes and frequentely), related exposed to industrial risk and reported at fell annoyed by dust. Thus this results can helps the authorities to analyses the regional context before to determine an interventions and also to make definitive conclusions about this kind of impacts.

Keywords: Air pollution, annoyance, perception, risk, dust.

#### **INTRODUCTION**

Air pollution has brought a series of impacts to the environment due to damage in animals, and plant materials (Rotko et al., 2002, Klaeboe et al, 2008), affects quality life, health and well-being of humans (Egondi *et al.*, 2013), can cause disease (Llop et al., 2008; Blanes-Vidal, 2015) and also cause annoyance (Amundsen et al., 2008). In the Health Organization (WHO, constitution, health is defined as "a state of complete physical, mental and social well-being and not merely the absence of disease or infirmity". According to this definition, annoyance caused by air pollution qualifies as a public health problem as it can be an ambient stressor causing stress and diseases and affect the quality of life. In this context, a survey was conducted in January, 2012 among residents in the south of Espírito Santo state, on the east cost of Brazil. This region is a urban and industrialized area dominated by a pelletizing plants, treatment gas unit and also is a turistic region. The survey showed that air pollution, predominantly dust, was considered to be a major environmental problem, and about 80% of respondents reported fell annoyed by dust (Machado et al., 2014). However the main industry in this region stoped theirs activities since November, 2015 as a consequence of an environmental accident in tailings dam located in the state of Minas Gerais. As a consequence of the

accident the pelletizing plnat was stoped theirs activities, and as a result of this it was hypothesized that the residents in that region would: perceive the air quality as being less dusty(1), become more positive in their risk perception (2), report less annoyance due to air pollution (3). Thus, a second research was developed in January of 2017 to investigate these hypothesis. This study aim to analyze the effects of the intervention (stoped of the pelletizing industry) in relation to the perception of air pollution, perception of risk and annoyance caused by dust.

#### **METHODS**

This study is characterized as a qualitative research whose objective is to analyze the perception of a population about the annoyance caused by air pollution (Barnett, 1991). The sample size was calculated from the simple random sampling with proportional allocation described in Cochran (1977). Out of 200 respondents, aged 16-60 were selected randomly, by respecting the spatial distribution of the sample in sub-regions located around (1,5 km) the air quality monitoring stations. The surveys consisted of face to face interviews, ensuring direct contact between interviewer and respondent. The questionnaire considered different topics, such as: air pollution perception, perceived annoyance, consequences of



air pollution, perceived emission sources, risk perception and others. In this work we will present descriptive results and analysis on three selected of main hypotheses.

#### FINDINGS AND ARGUMENT

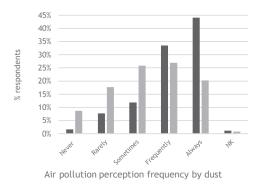
Table 1 presents the characteristics of the sample population according to gender for each survey. It was possible to observe the high participation of men in 2017 compared to 2012. This may be a consequence of the increase in the number of unemployed after the stoppage of the activities of the pelletizing plant.

Table 1. Opinons about risk perception

Surveys	Gender		
Jul veys	Men	Women	
2012 (n=242)	40,50%	59,50%	
2017 (n=555)	51,30%	48,70%	

An intersting and similar result in both surveys is about the importance of air quality, the most of respondents considering the air quality important. It means that independ of air pollutions emissions respondents are concerned about the importance of air quality in theirs lifes.

Analyzing the perception of air pollution, the dust is the form of more frequently answered in both survey. Howerer it is possible to see that the frequency of perception dust is significantly less in the 2017 survey compared with the 2012 survey (Figure 1). This result can be explained because in 2017 the pelletizing plants was not working.



■ 2012 Survey (n=242) ■ 2017 Survey (n=555)

Figure 1. Frequency of perception air pollution by dust

About risk perception (Table 2), in 2012 more than 90% of respondents said they felt at least somewhat exposed to industrial risks, and only 7% said they never felt exposed to risk. While in 2017, 35% of respondents said they did not feel more exposed to industrial risk. This result is consistent with the current situation of the region once the

industrial activities of the pelletizing plant are stopped. Moreover, in 2017 the population is aware of the environmental accident, which, although it happened in another state, caused human and animal deaths, pollution of flora and rivers, causing serious damage to farmers and ranchers.

Table 2. Opinons about risk perception

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	2012 Survey (n=242)	2017 Survey (n=555)		
	` ′	()		
Not exposed	7%	35%		
Little exposed	15%	23%		
Moderate exposed	27%	20%		
Very exposed	34%	14%		
Extremely exposed	17%	5%		
Not Know	0%	3%		

Compered booth survey, in figure 2, the percentage of annoyance caused by dust were reported to be less annoying and not annoying in the 2017. However, about 60% of respondents reported fell upset by the dust in 2017 while in 2012 more than 80% were annoyed. This result demonstrates that regardless of the contribution of the pelletizing plant the respondents relate to feeling annoyed by dust. This result is indicative of the importance to investigate other sources of air pollution that may contribute to reports of nuisance.

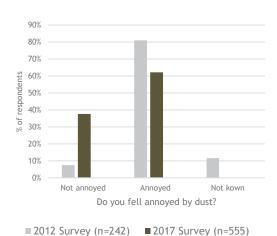


Figure 2. Related to fell annoyed by air pollution

This results can be comparable with the study conducted by Stenlund et al (2009) in Stockholm, where they found similar analysis in repect to this variables here investigated.

Although according to the environmental agency the data of dust monitoring afeter the accident (in november of 2015) shows that the flux of settled dust reduced but the contribution of vehicular and suspended soil dust are still significant in the region (see figure 3).



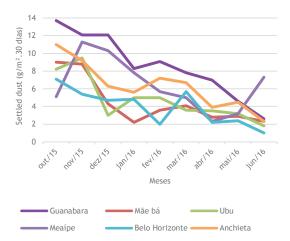


Figure 3. Time series of settled dust (source: IEMA, 2017)

#### **CONCLUSIONS**

The questionnaires surveys were conducted in south of Espírito Santo before and after an intervention that aimed to decrease air pollution (predominantly dust). This consisted of a stoppet pelletizing plant as a consequency of an environmental accident in Minas Gerais State in 2015.

As hypothesized, after the environmental accident in Minas Gerais, the activities in pelletizing plant in south of Espirito Santo stopped, thus the air quality was perceived as being less polluted by dust, the residents were more positive in their risk perception in 2017 compared to 2012, and they reported less annoyance due to dust. These results did not support that air pollution problemas are over now, because a significant percentage of respondents reported they still perceived air pollution by dust (at least), a high percentage of respondents aswered to fell exposed to risk, and a significant number of respondents reported to fell annoyed by dust. Considering that the pelletizing plants is a potential source of particulate matter, it can be concluded that reports of nuisance caused by dust do not come only from this source. In these respects, the intervention (stopped industries activities) can not be considered successful. We recommended to analyses the regional context/ variables in order to make a more complet conclusions.

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#### EXPOSURE TO AIR POLLUTANTS DURING COMMUTING IN SÃO PAULO

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**Abstract:** The aim of this study was to compare the exposure to particulate matter (PM<sub>2.5</sub>) and Black Carbon (BC) for typical commutes by bus and underground from 4 regions in São Paulo. The sampled regions were chosen due to the origin-destination availabe information. The highest BC concentrations were found in the bus and the highest PM concentrations in the underground. BC concentrations were lowest in the underground probably due to the relation of combustion sources and BC. The concentrations by bus were ruled mainly by the traffic conditions at the specific road of sampling.

Keywords: Personal exposure, Travel mode, Particulate matter, Black carbon.

#### INTRODUCTION

Among the several daily activities, commuting is considered one of the greatest periods of exposure to atmospheric pollutants, especially in the metropolitan areas with high vehicular density (DUCI et al., 2003). According to the World Health Organization (WHO) report (2005), which considers the effects of air pollution on health, the population spends on average 1 to 1.5 hours in traffic. Several studies have reported that frequent passengers can receive up to 30% of the total amount of Black Carbon (BC) and about 12% of the fine particulate matter during this period (DONS et al., 2011, FONDELLI et al. 2008).

São Paulo, one of the four megacities in South America and the most populous of them, has been extensively studied due to the effect of vehicle air pollution on health (LIMA et al., 2013, YOSHIZAKI et al., 2010, PERIN et al. Al., 2010) on urban scale. However, as the pollutants of vehicular emission circulate in an urban local scale and how much of this concentration effectively affects the population needs further research. There is a gap in the estimation of the exposure of pollutants due to different transport modes and exposure time.

The aim of this work was to determine which is the exposure and if there are differences between commuting modes and routes to  $PM_{2.5}$  and BC in São Paulo. For so, two different typical commuting routes in different transport modes were sampled in different daytime periods (morning and afternoon rush hour).

#### **METHODS**

#### Study Area

The Metropolitan Region of São Paulo (RMSP), located in southeastern Brazil, is considered a megacity with a population of 19 million people and

more than 8 million vehicles (BRITO et al., 2013). Only in the city of São Paulo, the state capital where the study was carried out, the population is more than 11 million inhabitants (IBGE, 2010). Consequently, the vehicular fleet of the municipality of São Paulo has been increasing alarmingly (DENATRAN, 2016), bringing problems not only in congestion and accidents, but also of health issues. Up to October 2016, approximately 8 million cars were accounted, which corresponds to 70% of the car fleet of the municipality of São Paulo.

#### Route selection and instrumentation

The routes were selected based on the Kernel maps made by the Geoprocessing Laboratory of the Polytechnic School of the University of São Paulo (LGP/EPUSP), which identified clusters of the places where the inhabitants more catch public transportation based on the data given by São Paulo Transport SA. (SPTrans). Figure 1 at *left* show us the origin and at *right* the destination. Predominantly, the origins with the largest number of ticketing are on the peripheral area of the city and the destination the center of the city.

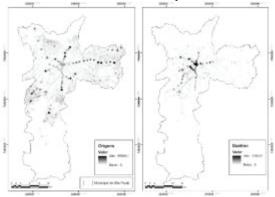


Figure 1. Kernel map of origin (left) and destination (right) made by the LGP/EPUSP for São Paulo municipality



The routes were selected covering the city in the East-West and North-South directions, which included the clusters identified with the largest number of ticketing and that had a reasonable travel time. We chose two routes each of which included two regions of the city (East/West and North/South) that intersected in the city center to simulate the movement that the population makes to go to work everyday.

The underground (UG) itineraries (Figure 2 at left) were called **Red** and **Blue** and the bus itineraries were called **E/W** and **N/S**.

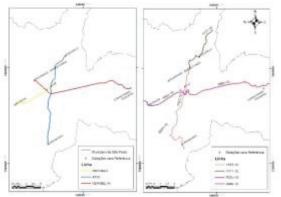


Figure 2. Subway routes (left) and bus routes (right) selected for sampling

#### Data Sampling and Management

We sampled  $PM_{2.5}$  and BC concentrations with a DustTrak II Aerosol Model 8530 (TSI) and MicroAeth Model AE51 (AethLabs), respectively, with a frequency of 10 seconds. The instruments were carried inside a bag, with the inlets positioned at approximately the breathing height of the carrier.

The sampling was performed over a total of 12 days between 19 September of 2016 and 23 February of 2017 at two different daytime periods (starting at 07:00 and 17:00 h local time). It was monitored a total of 24 samples equally distributed by route, transport modal and period.

The management of the data and the statistical analyses were made with the RStudio software (v 3.3.2, R Core Team, 2016) and ArcGIS 10.3 (Esri Inc.) was used for generating the concentration maps.

#### **RESULT AND DISCUSSIONS**

Table 1 and 2 shows the first quartil, median, mean, third quartil and maximum value of the sampled concentrations per route and per mode of BC and  $PM_{2.5}$ . The route corresponding to E/W showed the highest concentrations for BC (98,77  $\mu$ g/m³) and all

other statistical values. In the bus it was found the highest concentrations of BC.

For PM<sub>2.5</sub>, the maximum concentration levels were measured in the underground (200  $\mu$ g/m³). The mean values (46.17  $\mu$ g/m³ in the Blue line and 31.97  $\mu$ g/m³ in the Red line) are also much higher than in the buses (15.87  $\mu$ g/m³ in the E/W line and 20.62  $\mu$ g/m³ in the N/S line).

Table 1. Summary of statistics of BC concentration in µg/m³

	Lines	1st Qu.	Med.	Mean	3rd Qu.	Max.
Due	E/W	3.648	6.313	8.919	10.970	98.77
Bus -	N/S	2.425	4.592	6.643	8.152	86.68
110	Blue	3.022	4.691	5.974	7.212	73.67
UG -	Red	2.354	3.957	4.904	6.207	71.92

Table 2. Summary of statistics of  $PM_{2.5}$  concentration in  $\mu g/m^3$ 

	Lines	1st Qu.	Med.	Mean	3rd Qu.	Max.
Due	E/W	10	14	15.87	19	160
Bus	N/S	13	18	20.62	25	185
110	Blue	13	29	46.17	66	200
UG	Red	13	21	31.97	46	200

The statistical analysis was performed considering all the data avaiable for each line, that means that we didn't distinguish between periods of the day yet.

Figures 3 and 4 show the spatial variation of the concentrations of BC and  $PM_{2.5}$  for the bus in some routes sampled, as an example. The highest concentrations of air pollutants were expected to be found in the central area of the city of São Paulo, where there is a higher density of transport circulating, however, a well defined gradient can't be identified in the city center, what may suggest that concentrations sampled during the routes are mainly affected by the traffic conditions (Rivas et al., 2017). The concentrations of pollutants are much higher in the north and south areas of the city.





Figure 3. Spatial distribution of BC concentration in  $\mu g/m^3$ 



Figure 4. Spatial distribution of PM<sub>2.5</sub> concentration in µg/m<sup>3</sup>

#### **CONCLUSIONS**

The highest BC concentrations were found in the bus and the highest  $PM_{2.5}$  concentration in the underground. BC concentrations were lowest in the underground probably due to the relation of combustion sources and BC. The concentrations by bus were ruled mainly by the traffic conditions at the specific road of sampling.

As future work there will be: (1) Expand the analysis including period of the day influence and meteorological data; (2) Investigate better why the concentrations of all pollutants were higher on the north/south of the city of São Paulo; (3) include PM10 samples, (4) include car and bike measurements.

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## USING BENMAP-CE TO ESTIMATE THE HEALTH BENEFITS OF ALTERNATIVE AMBIENT AIR QUALITY STANDARDS

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Abstract: Urban populations around the world are increasing the pressure on the natural environment. As fossil fuel combustion increases, as land is cleared, as the number of consumers and their expectations rise, so cities are contributing to the degradation of the world's natural systems. With increasing urbanization, air pollution has become a public health problem, even when its levels fall short of current legislation. It is important to note that air pollution is not only a problem related to pollutant emission sources, but also topography and atmospheric conditions. Epidemiological studies relate air pollution to health, approaching issues such as epidemiological indicators in environmental health and assessment of exposure to air pollution. Among pollutants that can cause damage to human health and the loss of quality of life, particulate matter (especially fine particles) stands out as being more directly responsible for the health problems related to the respiratory system. In this context, the aim of this study is to estimate the health benefits of alternative ambient air quality standards of fine particles in Great Vitória using numerical results from the Community Multiscale Air Quality (CMAQ) and the Environmental Benefits Mapping and Analysis Program - Community Edition (BenMAP-CE) tool. The meteorological fields were modelled using the Weather Research and Forecasting model WRFv3.6.1 and for emissions was applied the SMOKEv3.5.1 using the current emissions inventory from local Environmental Protection Agency (IEMA). Some concentration-response functions proposed by cohort studies will be evaluated to calculate the number of attributable annual deaths corresponding to all causes, all non-accidental causes, ischemic heart disease, cardiovascular and lung cancer among persons aged over 25 years. To estimate exposure, it was used the CMAQ results for 2010 as reference scenario and the standard values of legislation and WHO as projected scenarios.

Keywords: BenMAP-CE, health benefits, fine particles, Great Vitória.

#### **INTRODUCTION**

Air pollution has become an important risk factor for epidemiological health studies since they have the most robust causal associations between long-term exposure to the pollutant and reduced life expectancy. Among the contemporary urban-environmental imbalances that affect human health are the air pollution (Chen et al., 2008; Carey et al., 2013).

An extensive body of epidemiological research has established a strong association between chronic exposures to fine particulate matter less than 2.5 µm (PM<sub>2.5</sub>) and ischemic heart disease, cardiovascular, lung cancer, all causes and all non-accidental causes mortality (Pope et al., 2002; Pope et al., 2004; Landen et al., 2006; Krewski et al., 2009; Crouse et al., 2012; Cesaroni et al., 2013).

The Region of Greater Vitória (RGV) (Figure 1) is located in the state of Espírito Santo which includes the cities of Cariacica, Serra, Viana, Vila Velha and Vitória. It is an urban region, of complex relief, highly industrialized and in process of expansion, being the air quality affected by the emission of pollutants from vehicular and industrial emissions, besides the logistics sector as port complexes and airport (IEMA, 2014).

The aim of this study is to estimate the health benefits of alternative ambient air quality standards of fine particles in Great Vitória using numerical results from the Community Multiscale Air Quality (CMAQ) and the Environmental Benefits Mapping and Analysis Program - Community Edition (BenMAP-CE) tool, with the year of 2010 as baseline scenario.

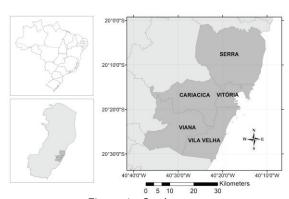


Figure 1 - Study area.

#### **METHODS**

#### Air pollution data

 $PM_{2.5}$  concentrations for baseline scenario were simulated with Community Multiscale Air Quality (CMAQ) model v. 5.0.2 applying a domain with horizontal resolution of 1 x 1 km², with 61 km by 79 km, centred in the Eurico Salles de Aguiar Airport (Vitória-ES). Three-dimensional meteorological



COMMUNITY MODELING AND ANALYSIS SYSTEM

fields were modelled using the Weather Research and Forecasting model (WRF) version 3.6.1 for 2010 and the SMOKE model v3.5.1 was applied to build an inventory of emissions, spatially and temporally resolved to RGV using the official state inventory emissions. The concentration fields were integrated over each city area with VERDI 1.4 program in order to obtain an annual concentration value that represents each city.

Two control scenarios were evaluated considering the Espírito Santo State Decree 3463-R/2013 which one stablishes a maximum annual concentration for PM<sub>2.5</sub> of 15  $\mu$ g/m³ (third intermediate goal) and 10  $\mu$ g/m³ (final/WHO standard), scenarios 1 and 2, respectively.

#### Population and mortality data

Population data was obtained from Instituto Brasileiro de Geografia e Estatística (IBGE - Censo Demográfico 2010) for each city by age group.

Mortality data due all causes (ICD-10: A00-Y98), all non-accidental causes (ICD-10: A00-R99), ischemic heart disease (ICD-10: I20-I25), cardiovascular (ICD-10: I20-I28, I30-I52, I60-I79) and lung cancer (ICD-10: C33-C34) was obtained from Departamento de Informática do Sistema Único de Saúde (DATASUS) which regulates mortality data in the Sistema de Informação sobre Mortalidade (SIM).

#### **Health Effects**

The health effects were estimated applying Equation 1:

$$\Delta Y = Y_0 * Pop * (1 - e^{-\beta * \Delta PM})$$
 Eq. 1

where  $\Delta Y$  is the change in health effects incidence (deaths cases);  $Y_0$  is the baseline incidence; Pop is the exposed population;  $\beta$  is the effect estimated which can be calculated from relative risks obtained from epidemiological studies; and  $\Delta PM$  is the air quality change.

The main characteristics of the epidemiological studies and concentration-response functions used for long-term mortality impact assessment of fine particles is presented in Table 1.

#### FINDINGS AND ARGUMENT

The annual concentration values ( $\mu g/m^3$ ) obtained for baseline scenario (2010) were:

Cariacica: 5.3 μg/m³;

• Sera: 8.2 μg/m<sup>3</sup>;

Viana: 6.3 μg/m<sup>3</sup>;

Vila Velha: 12.2 μg/m³;

Vitória: 15.8 μg/m³.

Table 1. Summary of the main features of selected concentration-response functions.

Health outcome	Reference	Age Range	Hazard ratio (95% CI)
	Pope et al. (2002)	30-99	1.06 (1.02-1.11)
All Causes	Krewski et al. (2009)	30-99	1.03 (1.01-1.05)
	Laden et al. (2006)	25-99	1.16 (1.07-1.26)
Non-	Crouse et al. (2012)	>25	1.15 (1.13-1.16)
Accidental	Cesaroni et al. (2013)	>30	1.04 (1.03-1.05)
	Pope et al. (2004)	30 -99	1.18 (1.14-1.23)
Ischemic	Krewski et al. (2009)	30-99	1.15 (1.11-1.20)
Heart Disease	Crouse et al. (2012)	>25	1.31 (1.27-1.35)
	Cesaroni et al. (2013)	>30	1.10 (1.06-1.13)
	Pope et al. (2002)	30-99	1.14 (1.04-1.23)
Lung Cancer	Krewski et al. (2009)	30-99	1.11 (1.04-1.18)
	Cesaroni et al. (2013)	>30	1.05 (1.01-1.10)
Cardiovascular	Crouse et al. (2012)	>25	1.16 (1.13-1.18)
	Cesaroni et al. (2013)	>30	1.06 (1.04-1.08)
	Laden et al. (2006)	25-99	1.28 (1.13-1.44)

Vitória obtained the highest annual  $PM_{2.5}$  concentration in RGV. According to the inventory of emissions, the main source of PM is vehicular (IEMA/Ecosoft, 2011). In addition, the region receives direct influence of emissions of particulate matter from two large companies, located in the same industrial complex and that both work with beneficiation of iron ore. 28 % of the particulate matter emitted by industrial sources in RGV are  $PM_{2.5}$  (IEMA/Ecosoft, 2011).

As Cariacica, Serra and Viana already obtained annual concentrations below the values established by the control scenarios (15 and 10  $\mu g/m^3$ ), the health benefits were estimated only for Vila Velha and Vitória. Therefore, the  $\Delta PM$  calculated for these two cities were:

- scenario 1: Vitória = 0.8 μg/m³;
- scenario 2: Vila Velha = 2.2 μg/m³;

Vitória =  $5.8 \mu g/m^3$ .

The estimate of reduced mortality cases is presented in Table 2 according to the health outcome and epidemiological studies.



Table 2. Estimate of reduced mortality cases.

Health	Reference	Vitória		Vila Velha
outcome	come		S2	S2
	Pope et al. (2002)	8.1	57.1	26.2
All Causes	Krewski et al. (2009)	4.1	29.2	13.3
	Laden et al. (2006)	21.4	146.5	68.6
Non-	Crouse et al. (2012)	17.7	121.6	56.9
Accidental	Cesaroni et al. (2013)	4.9	34.8	16.0
	Pope et al. (2004)	2.5	16.8	8.0
Ischemic	Krewski et al. (2009)	2.1	14.3	6.7
Heart Disease	Crouse et al. (2012)	4.0	26.8	12.9
	Cesaroni et al. (2013)	1.4	9.9	4.6
	Pope et al. (2002)	0.6	4.0	1.3
Lung Cancer	Krewski et al. (2009)	0.5	3.2	1.1
	Cesaroni et al. (2013)	0.2	1.5	0.5
Cardiovascular	Crouse et al. (2012)	2.4	16.5	8.3
	Cesaroni et al. (2013)	0.9	6.7	3.3
	Laden et al. (2006)	4.0	26.8	13.7

For each mortality indicator, the results varied depending on the selected cohort studies, which included different age range and provided different hazard ratios. The effect of using different estimates from the same cohort study, i.e. American Cancer Society cohort (Krewski et al., 2009; Pope et al., 2004; Pope et al., 2002) indicated a decrease by 49.4 % for all causes, 16 % for IHD and 16.7 % for lung cancer when using the Krewski's hazard ratio compared to those of Pope for scenario 1, for example.

The disparities among the cohort studies could be due to chemical composition of  $PM_{2.5}$  and its heterogeneous mix of particle sizes, thus encompassing the environmental characteristics of each area of study (geographic location, emission sources and pollutants mixtures), the variability among different populations, and the exposure assessment methodology.

The greatest health benefits resulting from a reduction in air pollution are observed in Vitória,

where the highest fine particle reduction concentration would be observed.

Since reductions in air pollution occur gradually after the implementation of environmental policies, the appearance of any concomitant health benefits could be expected to occur in a similar manner (Boldo et al., 2014).

#### **CONCLUSIONS**

Air pollution has become a growing concern in the past few years, with an increasing number of acute air pollution episodes in many cities worldwide. The actual impact of air pollution on health presented here shows the importance of adopting more restrictive air quality standards. Such information is essential to implementing, monitoring and evaluating policies that help to tackle air pollution while also protecting health. The importance of using local epidemiological studies to estimate health benefits is also recorded. Unfortunately, in Brazil, long-term cohort studies for PM<sub>2.5</sub> are non-existent.

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# Session 6 Regulatory Modeling and Applications



## EVALUATION OF SULFUR DIOXIDE AIR CONCENTRATIONS DURING CLAUS SYSTEM MAINTENANCE OF THE ARCELORMITTAL TUBARÃO COKE PLANT

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Abstract: Steel industry has a significant importance in the  $SO_2$  emissions at the Great Vitoria Region. Nonetheless,  $SO_2$  emission control system, as installed in the Arcelor Mittal Tubarão Coke Plant, denominated Claus system has a potential to recover this gas in the industrial plant, mitigating sulfur dioxide emissions and, consequently, impacts in air quality. In order to demonstrate the influence of this system on the air quality, the present study quantified the emissions for two different scenarios (normal operation and Claus maintenance). These scenarios were placed into AERMOD View and the results were analyzed following the CFR 40-51.166 Prevention of Significant Deterioration of Air Quality which presents a methodology of analysis of studies of atmospheric dispersion still unusual in Brazil. For the 24-hour average, baseline concentrations, which consist of monitoring data, for a single receptor point violated the air quality standard established by State Decree 3463-R/2013. In case of annual average, no infringement to those standards was observed. Thus,  $SO_2$  emissions from ArcelorMittal Tubarão neither contribute nor violate air quality standards in the Great Vitoria.

Keywords: Claus system, SO₂ emissions, air quality, Great Vitoria Region, ArcelorMittal Tubarão.

#### **INTRODUCTION**

Steel an mining industry are responsible for 75.5% of the total  $SO_2$  emissions emitted into the atmosphere in the Great Vitoria Region (IEMA, 2013). In this context, installation of  $SO_2$  emission control equipament is indispensable since some of them, as Claus, can reach efficiency higher than 90 (USEPA, 2015).

This system, installed at ArcelorMittal Tubarão Coke Plant, was paralyzed during 90 days which promoted additional  $SO_2$  emissions.

Hence, due to the importance of steel industry for these emissions, this study aims to demonstrate environmental benefits for the air quality in the Great Vitoria with the Claus system use.

In order that, the methodology of evaluation of violation or contribution to violation of Air Quality Standards, still unusual in Brazil, and follows what is proposed in the United States of America by the CFR 40-51.166 Prevention of Significant Deterioration of Air Quality was applied. This regulation is applicable to analyze impacts on air quality due to installation of new enterprises or modifications in industrial plants already existent.

#### METHODS Study area

An area 40x40 km  $(1,600 \text{ km}^2)$  was delimited. Cell grids  $(500 \times 500 \text{ m})$  covering the main cities in the Great Vitoria were defined. In addition, monitoring statios which belongs to Automatic Air Quality Monitoring Network (RAMQAr) were used as receptor points (Figure 1).

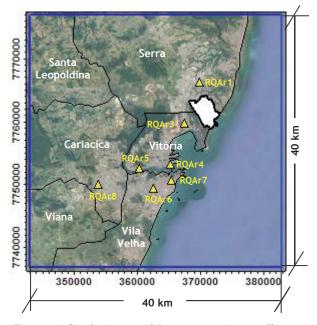


Figure 1. Study Area and Receptor points (yellow triangles).

#### **Emission Inventory**

The emissions were quantified for two different scenarios:

- Scenario #1: normal operation of the Claus;
- Scenario #2: Claus System shutdown for maintenance (from June 20th to September 17th).

 $\mathsf{SO}_2$  emission rates (Table 1) were provided by ArcelorMittal Tubarão.



Table 1. SO<sub>2</sub> Emission Rates

Source Name	Emission Rates [kg/h]			
Source Name	Scenario #1	Scenario #2		
Coke Plant	1,974.53	2,229.36		

Reference: Araújo et al (2016).

#### Air quality modeling

Emission rates as well as physical features of the sources were entered into an air quality model, AERMOD View® version 9.1.0. Two simulations were

- Annual three whole years modeled:
  - Scenario #1 (S1): Use of emission rate considering normal operation of the Claus in the 1,095 days ran (365 days x 3 years);
  - Scenario #2 (S2): Use of emission rate associated with Claus maintenance in 270 days out of 1,095 days ran (90 days x 3 years).
- Shutdown 270 days (90 days per year):
  - Scenario #1 (S1): Use of emission rate relates to normal operation during the simulated period;
  - Scenario #2 (S2): Use of emission rate corresponding to Claus maintenance during the simulated period.

Besides, surface meteorological data for three years of the analysis (2013, 2014 and 2015) were obtained from a surface station located in Vitoria Airport.

#### Modeled data processing

Results from model were compared with First Intermediate Goal established by State Decree No 3463-R/2013 (Air Quality Standards - AQS).

In order to verify whether Claus system use contributes or promotes violation of the AQS, simulated data were compiled by applying the CFR 40-51.166 Prevention of Significant Deterioration of Air Quality (USEPA, 2005) as follows:

- 1. <u>Determination of Reference Concentrations</u> (RC):
  - Second highest 24-hour average;
  - Highest average for the entire study period;
- 2. Determination of the Increment in the concentrations:
  - Increment in the concentrations due to Claus shutdown: RC<sub>S2</sub> - RC<sub>S1</sub>;
- 3. <u>Determination of Baseline Concentrations:</u>
  - SO<sub>2</sub> concentrations in the atmosphere resulting from measuring;

- Over each RAMQAr station: compilation of highest 24-hour and annual average;
- Sum: Baseline + Increment (item 2).

Afterwards, these concentrations are compared with AQS, following criteria below:

#### A. If Baseline > AQS:

SO<sub>2</sub> concentrations in the atmosphere violate the AQS.

#### B. If $RC_{S1} > AQS$ :

Emissions from steel industry violates the AQS during normal operation of the Claus;

#### C. If $RC_{S2} > AQS$ :

Emissions from steel industry altered during Claus System maintenance results in infringement of AQS.

#### D. If Baseline + Increment > AQS:

The increment in the concentrations does not promote violation of the AOS directly but it contributes.

The infringement analysis is divided in short-term (maximum 24-hour average) and long-term (annual average).

#### **RESULTS**

As example, Figure 2 illustrates SO<sub>2</sub> 24-hour reference concentrations, corresponding modeling which was denominated as Annual (Scenario #2). Highest sulphur concentrations occurred outside the more urbanized areas, which are surrounding the RAMQAr stations. In addition, no violation of AQS (60 µg/m<sup>3</sup>) was identified.

#### Application of CFR 40-51.666

Table 2 presents baseline concentrations. A single infringement of the AQS was noted in only one receptor point for 24-h average. For annual averages, violations of AQS were not observed.

Table 2. Baseline Concentrations [µg/m³]

RAMQAr	Station	24 hour <sup>a</sup>	Annual <sup>b</sup>
1	Laranjeiras	44,10	9,99
3	Jardim Camburi	26,30	10,94
4	Enseada do Suá	38,80	15,16
5	Vitória Downtown	69,80	14,81
6	Ibes	30,80	7,76
7	Vila Velha	35,00	10,97
8	Cariacica	14,50	6,15

- a. AQS 24 hour 60  $\mu g/m^3$ ; b. AQS Annual 40  $\mu g/m^3$ .



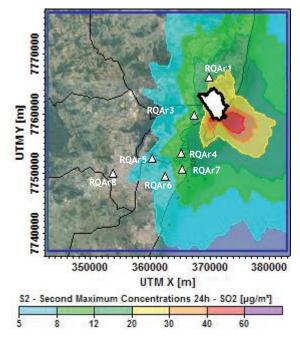


Figure 2. Second Highest 24-h Concentration for  $SO_2$  - Scenario 2

#### Short term

Table 3 exhibits increment in the  $SO_2$  concentrations caused by scenario 2 as well as the sum of this increment and baseline concentrations in each RAMQAr station. A single infringement of the AQS at the RQAr05 was a result from baseline concentrations (Table 2) and not really due to increments during Claus maintenance, which in both simulations (annual and shutdown) had low magnitude.

Table 3. Increment of the SO<sub>2</sub> Concentrations for Short Period

RQAr	Annual [µg/m³]		Shutdowr	n [µg/m³]
NQAI	Increment	Sum	Increment	Sum
1	0,25	44,35	1,60	45,70
3	1,48	27,78	0,74	27,04
4	0,47	39,27	0,99	39,79
5	0,82	70,62	0,82	70,62
6	0,61	31,41	0,76	31,56
7	0,11	35,11	1,13	36,13
8	0,37	14,87	0,37	14,87

#### Long term

In case of annual averages, no concentration violated or contributed to infringement of the AQS in the long period for both scenarios analyzed.

Table 4. Increment of the SO<sub>2</sub> Concentrations for Long Period

Eorig i eriod				
RQAr	Annual [µg/m³]		Shutdown [µg/m³]	
RQAI	Increment	Sum	Increment	Sum
1	0,07	10,06	0,30	10,29
3	0,07	11,01	0,25	11,19
4	0,08	15,24	0,33	15,49
5	0,05	14,86	0,18	14,99
6	0,05	7,81	0,20	7,96
7	0,08	11,05	0,30	11,27
8	0,02	6,17	0,09	6,24

#### **CONCLUSIONS**

By following the CFR 40-51.166 methodology, increments in the sulphur dioxide concentrations due to emission sources located in the ArcelorMittal Tubarão do not cause or contribute to violate the AQS in all scenarios and temporal references analyzed. The single violation of the AQS was a result from baseline concentration for short period (24- hour average) over the receptor point RAMQAr05 (Vitória Downtown). Therefore, Claus shutdown for maintenance does not promote or contribute to violate air quality standards in the Great Vitória Region.

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## Using Raw Materials Balance to Represent the Chemical Profile of a Group of Sources to Smooth the Collinearity Influence in CMB Applications

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Abstract: Chemical Mass Balance (CMB) was used to identify contributions to settled dust from industrial sources that process iron ore and iron ore pellets in Vitoria, Brazil. These processes take place mainly at a steel maker (seven million tons a year) and eight iron ore pelletizing plants (32 million tons a year). In a large port nearby the industrial installations 130 million tons of raw material and intermediate products are handled in a typical year, comprised of iron ore, coal, pellets and steel plain products. A chemical profile representing the sources of the steel maker was developed based on a mix of raw materials and intermediate products that reproduces the mean annual activity. This profile and other ones from known sources of the region were used in an apportioning study to explain the origin of ambient settled dust samples. This approach enables CMB to produce good separation of Iron and Carbon containing sources that otherwise would generate strong collinearities. The elemental analyses were performed by PIXE (Particle Induced X-ray Emissions) and TOT (Thermal Optical Transmittance) procedures. Mossbauer Spectroscopy was used to separate hematite from industrial origin and soil origin. Additional decision criteria were adopted based on body of evidence evaluation considering industrial inventories and a ranking of CMB solutions that took into account the importance of statistical indicators and main elements uncertainties archieved.

Keywords: Chemical Mass Balance, collinearity, settled dust, inventories, Mossbauer spectroscopy.

#### INTRODUCTION

This study refers to a single site used to collect settled dust in the region of Vitoria, Brazil, located five kilometres downwind from the major local industrial district. The receptor site is known as Ilha do Boi (IB). The objective to focus this study in only one site was to test the use of additional tools to improve the separation of sources when using CMB.

As the basic materials used in the production of steel and iron ore pellets are iron ore, coke, coal and sinter, strong collinearities can occur when CMB is used to apportion the elements found in samples among the potential sources of settled dust in the region under study. Iron is the dominant element in the samples, followed by Silicon, Aluminium, Elemental and Organic Carbon.

The basic hypothesis to be evaluated is if an overall profile representing the steel maker plant could smooth the Iron element predominance allowing the other industrial sources containing Iron to be identified.

The concurrent hypotheses are:

- 1. There is no evidence of high participation of particles with aerodynamic diameter less than 25  $\mu$ m in settled dust samples collected at receptor site IB;
- 2. The potential of chimneys emissions to be deposited at short distance is low considering their heights, the initial buoyancy and momentum components of plumes and the samples after the controls used (electrostatic preciptators and fabric filters) which indicate no more than 10% of particles emitted to be more than  $10\ \mu m$  in aerodynamic diameter;
- 3. The potential for generation of dust that can be deposited at short distances by wind action is in the interval 10 µm to 100 µm as inferred from granulometric distribution of each material evaluated and its density.



The main sources used for the study were ArcelorMittal steel maker plant (AMT), industrial source 2 (IS2), Iron ore in stock piles (IRON ORE), iron ore pellets in stock piles (PELLETS), coal (COAL), sea aerosols (SEA) and soils (SOILS).

#### **EXERIMENTAL PROCEDURES**

A composed sample collected during 2010 in IB by passive equipment was submitted to LASER difractometry and the results show the limits of 0.26% in mass below 25  $\mu$ m and 71.9% below 106  $\mu$ m. This is good evidence to be used now on what is to be searched but variations along at least 24 monthly samples must be studied before more defensible arguments can be established.

The main chimneys located at AMT site, responsible for thermochemical transformations that could represent new sources with chemical profiles different from raw materials and intermediate products are from 101 meters to 186 meters height after electrostatic precipitators and fabric filters controls. Although the local inventory addressed 8% to 49% of their mass emissions in the range greater than 10  $\mu$ m, a few tests with separation by inertial devices indicate less than 10% of mass emissions in that range.

The stacks located at the others industrial sites that could also promote thermochemical transformations are from 54 meters to 113 meters height. The local inventory used the classic PM10 = 0.63 TPM resulting in 37% of emissions in the greater than 10  $\mu$ m range, a very uncertain value.

The distance from nearest industrial sites to IB receptor is around 5000 m, the distance from AMT site to IB is 8000 m as shown in Figure 1. The particles emitted must travel above water surface under moderate mean wind speed (2 m/s to 4 m/s, representing 60.8% of total measured hourly wind data). Under these conditions low friction velocities are generated and it is expected that the deposition velocities of particles less than 10 µm in aerodynamic diameter can reach only 3 cm/s, as verified by Obatosin and Kenneth (2006).



Figure 1: Region of interest showing AMT site and IB receptor.

More recently Zhang and Shao (2014) discussed the influence of particle density, friction velocity, surface roughness and type of surface (stick wood, sand, plant and water) to test known schemes to calculate deposition velocities. In the experiments conducted, for water surface, under friction velocity 0.6 m/s and particles density 2200 Kg/m3 the authors found a 5 cm/s deposition velocity for 10 µm particles.

Even when the problem was studied taking into account all mineral dust in a region (Fukuoka, Japan), as described by Osada (2014), there was evidence that particles below 10  $\mu$ m are less than 20% of total dust deposited by dry processes.

During the 1670 seconds available for particle travel under 3 m/s wind speed, from the nearest industrial sites to IB receptor, a 50 meter downward displacement is expected. Based on these evidences it is possible that only emissions from chimneys around 50 m height could produce particles below 10  $\mu$ m that would deposit on surfaces at IB receptor.



Based on these evidences the sources IS2 is recognized as a possible group of contributors to settled dust at IB. This group is composed by similar chimneys and by fugitive dust from similar controlled metallurgical processes.

#### The built of AMT profile

The main raw materials and intermediate slab handled in AMT during 2013 were those shown in Table 1 with their size grain accumulated participation below 10  $\mu$ m and 100  $\mu$ m. When that information is combined with local inventories and with real data from material consumption and recirculation a quantitative parameter is created concerning the total potential emissions generated from handling raw material before being processed and from intermediate products.

An example of how this technique was used is shown in Table 2 that describes the composition of the transfer process at sinter plant.

Table 1: Materials handled at AMT during 2013 with the grain size accumulated participation under the limits studied.

timis statica.				
MATERIAL	ACCUMULATED PARTICIPATION BELOW 10 µm (%)	ACCUMULATED PARTICIPATION BELOW 100  µm (%)		
Slab type LD	24.1	89.5		
Slab type KR	13.2	92.3		
Coke	16.1	70.8		
COAL	16.6	83.8		
SINTER	34.0	91.4		
BLEND (ORE)	66.1	99.4		
PELLETS	35.0	100.0		

Table 2: The composition of the transfer process at sinter plant.

SINTER TRANSFER OPERATIONS				
material	Mass real consunmption (t/year 2013)	% Participation	Mass in sample* (au)	
sinter	4149404	0.4868	0.0998	
coke	136660	0.0160	0.0033	
Iron ore	2824593	0.3314	0.0679	
Fine material from sinter	1398338	0.1641	0.0336	
Material from gas cleaning	13932	0.0016	0.0003	
Total	8523355	1	0.205	

\*Mass values in sample are in arbitrary units (au).

After scanning all processes a global balance of materials can be built, coherent with raw materials purchased and reused and intermediate sub products generated. A physical sample of AMT profile was built where the final chemical composition will represent real independent variables since the potential for particle emissions that could be settled at IB receptor is completely described without intersections of chemical sets describing the sources.

In Table 3 the final AMT profile composition is shown and in Table 4 the final chemical composition of the sample is described after a statistical treatment on ten subsamples to keep the necessary homogeneous representativeness.



Table 3: AMT profile physical sample final composition. Mass values in sample are in arbitrary units (au).

AMT PROFILE COMPOSITION			
MATERIAL	MASS (au)		
sinter	1.0438		
coke	9.9590		
coal	7.5056		
pellets	4.8343		
iron ore	6.4736		
scrap KR	3.0387		
scrap LD	11.9963		
limestone	1.3083		
total mass	44.8512		

Table 4: AMT profile final chemical composition.

	Mean value	Experimental error
Element	(%)	(%)
Magnesium	0.8563	0.0216
Aluminium	1.3799	0.0166
Silicon	2.9636	0.0297
Phosphorus	0.1185	0.0056
Sulphur	0.6175	0.0076
Chlorine	0.0279	0.0030
Potassium	0.0316	0.0041
Calcium	9.7879	0.0977
Titanium	0.0868	0.0073
Chromium	0.0144	0.0024
Manganese	0.3916	0.0052
Iron	12.0911	0.1208
Copper	0.0016	0.0005
Zinc	0.0029	0.0005
Strontium	0.0262	0.0024
OC	13.1408	1.4675
EC	20.9967	1.7895

#### THE INDEPENDENCE OF AMT PROFILE

In Table 5 the sources used in this study are compared to AMT chemical profile and it is easily seen that its composition is quite different from the others. When using CMB procedures this difference will always prevent that some linear combination among others sources will reproduce, by chance, AMT real characteristics.

Table 5: Comparison among sources chemical profiles in (%).

Tuble 5, Comparison unlong sources enemical profiles in (70).										
Source	Na	Mg	Al	Si	Р	S	Cl	K	Ca	Ti
AMT		0.8563	1.3799	2.9636	0.1185	0.6175	0.0279	0.0316	9.7879	0.0868
Soils	0	1.045	7.52	23.885	0.241	0.065	0.089	1.1	2.49	0.589
Sea	40.0	0	0	0	0	3.3	40.0	1.4	1.4	0
Iron ore	0	0	0.047	0	0.041	0	0	0	0.018	0.03
IS2	0.106	0	0	0	0	2.209	0	0	0.285	0
Coal	0.117	0.132	0.031	1.8	0.038	0.102	0.028	0.162	0.319	0.13
Pellets	0	0.506	0.019	2.625	0.026	0.097	0	0.018	1.397	0.046



COMMUNITY MODELING AND ANALYSIS SYSTEM

Table 5: AMT profile final chemical composition in (%) - (continued)

				()
Source	Mn	Fe	OC	EC
AMT	0.3916	12.0911	13.1408	20.9967
Soils	0.071	5.532	0.15	0.07
Sea	0	0	0	0
Iron ore	0.077	60.0	0	0
IS2	0	76.12	2.424	0.633
Coal	0.002	0.77	23.594	68.3
Pellets	0.1	56.2	0.22	0

#### RESULTS OF CMB USE ON IB RECEPTOR SETTLED DUST SAMPLES

During 2012 and 2013 some monthly samples of settled dust were collected using passive devices at IB receptor site. The chemical compositions are shown in Figure 2. A general tendency was followed with predominance of Fe, followed by Si, OC, EC and Al. The most important difference occurs in sample 1012 with high values of Na and Cl concentrations.

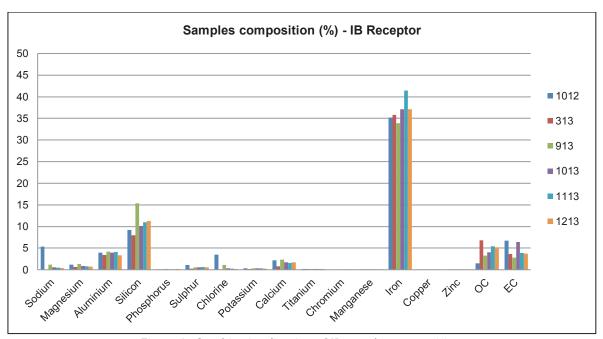


Figure 2: Graphic visualization of IB samples composition.

Table 6: CMB results.

SAMPLE	R2	Chi Square	% MASS	SOILS	SEA	IS2	COAL	PELLETS	OC (*)	AMT
1012	1.00	0.56	109.3	49	11	27	3	15	-	5
313	0.99	0.71	99.0	42	-	9	5	38	5	-
913	0.98	2.69	110.0	43	3	15	-	44	3	3
1013	1.00	0.48	105.6	55	1	20	-	19	3	7
1113	0.99	1.14	100.5	45	<1	21	6	25	-	3
1213	1.00	0.69	96.4	50	<1	21	4	18	-	1

<sup>(\*)</sup> Residual OC not explained.

The fitting achieved is good when considering the new AMT profile. All T statistics were higher than 4, and differently from previous applications of CMB in the same region it was possible to separate the IS2 source from pellets, both with high Fe contents. In table 06 is showing the high soils participation must be supported by



stronger evidence since it is a point of discordance among environmental authorities and technicians, nevertheless the values of statistics T for that source are beyond 12 and the obvious high participation of crustal elements in settled dust around the world as described by Zacco (2009).

#### ADDITIONAL ANALYSIS

As Fe is the most abundant element in the IB samples and is part of various sources profiles a well-established method was used to identify the characteristics under which this element is present in the sources and in the IB samples. The Mossbauer spectroscopy is a nuclear technique based on resonant absorption of gamma radiation emitted from radioactive source. The effects are restricted to low energy gamma radiation emissions (0 to 100 KeV). Mossbauer spectroscopy resolution is very good (one part in 1013) and it is possible to determine some parameters that characterize the Fe lattice in the material under evaluation. (Souza Jr et al., 2002).

To better describe the phases of Fe four parameters must be found after experiments at room temperature and at a very low temperature (25 K was used in this study). The parameters are: the second order Doppler parameter ( $\alpha$ ), the quadrupole splitting ( $\alpha$ /2 $\alpha$ ), the hyperfine field (BHF) and the area under each representation of phases. One important additional parameter is the Morin Transition, the change in the signal of  $\alpha$ /2 $\alpha$ 9 when the experiment is run under room temperature and under low temperature.

In Table 7 it is shown the characteristics of Pellets, Iron ore, AMT profile and soils at room temperature and at 25 K. All samples contain hematite but only in soils sample this phase doesn't undergo a Morin transition. So, the primary conclusion is that is possible to use the parcel of hematite in an ambient sample that doesn't exhibit Morin transition as a limit for soils participation.

Also, the other phases present in an ambient sample can be related to its participation in each source Fe contents.

Table 7: Mossbauer spectroscopy results.

Samples	Phases	& (mm/s) (± 0.05)	$\Delta/2\xi q \text{ (mm/s)}$ (± 0.05)	B <sub>HF</sub> (T) (± 0.2)	Area (%) (± 1)
Pellets		(= 3335)	(= 3335)	(= *;=)	(= -)
	-Fe <sub>2</sub> O <sub>3</sub>	0.36	-0.21	51.9	98
RT	SPM	0.36	0.62		2
25 K	-Fe <sub>2</sub> O <sub>3</sub>	0.48	0.43	54.3	100
Iron Ore		·			
RT	-Fe <sub>2</sub> O <sub>3</sub>	0.36	-0.21	51.8	98
25 K	-Fe <sub>2</sub> O <sub>3</sub>	0.49	0.42	54.3	100
AMT		•	•	•	·
RT	-Fe <sub>2</sub> O <sub>3</sub> -Fe <sub>2</sub> O <sub>3</sub> <sup>(*)</sup>	0.36	-0.22	51.7	98
	SPM	0.36	0.63		2
	-Fe <sub>2</sub> O <sub>3</sub>	0.48	0.39	54.3	85
25 W	-Fe <sub>2</sub> O <sub>3</sub> (*)	0.39	-0.10	53.1	6
25 K	-FeOOH	0.47	-0.24	50.2	8
	Fe/Si	0.59	2.44	-	1
Soils		·			
DT	Mix(-Fe <sub>2</sub> O <sub>3</sub> <sup>(*)</sup> / FeOOH	0,35	-0,24	50,2	32
RT	SPM	0.34	0.56		68
	-Fe <sub>2</sub> O <sub>3</sub> (*)	0,48	-0,17	53,4	9
	-FeOOH	0,46	-0,26	49,6	59
25 K	Fe <sub>5</sub> HO <sub>8</sub> .4H <sub>2</sub> O	0,49	-0,26	45,4	23
	FeOOH	0,41	0,50		4
	Fe-Si	0,58	2,38		5



#### **CONCLUSIONS**

The built of a material set representing all operations and processes that occurred in 2013 at Arcelor Mittal steel mill in Vitoria, Brazil, based on local inventory and real material movements, handling and use was successful in generating an independent chemical profile. The profile represents the potential for particle emissions in the range  $10 \mu m$  to  $100 \mu m$  (giant particles), supported by hypotheses applicable only to the studied conditions. Application of CMB produced good results and the limits of soils participation in the samples collected at the unique receptor could be proved using Mossbauer spectroscopy., Nevertheless there was strong evidence of crustal set of elements present in the samples.

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## Modeling the impacts of NO<sub>2</sub> vehicular emissions: A case study in Florianópolis, Brazil

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Abstract: Air pollution has been recognized as one of the worst environmental health risks at the present time. Recognizing potential impacts from road transport, the present study aimed to assess the impact of vehicular emissions of  $NO_2$  in Beira Mar Norte Avenue, in Florianopolis, Brazil. A bottom-up approach was applied in order to estimate emissions, and then AERMOD was used to simulate pollutant dispersion. The highest hourly concentration resulted in 932.7  $\mu g/m^3$ , and annual arithmetical average found was 120.9  $\mu g/m^3$ . Comparing simulations results with Brazilian air quality standards for  $NO_2$ , primary standards were exceeded 4,646 times, comprehending 68.6 hectares; and secondary standards, 12,186 times in 333.6 hectares. These concentrations were also considered high compared to literature, therefore the present study demonstrated that individuals in Beira Mar Norte Avenue surroundings were exposed to health effects from  $NO_2$  exposition.

Keywords: Vehicular emissions, air quality control, dispersion modeling, AERMOD.

#### INTRODUCTION

In urbanized cities, exhaust emissions from road transport represent one of the main sources of ambient air pollution. They arise from the combustion of fuels in internal combustion engines (EEA, 2013). In the Metropolitan Area of Sao Paulo, Brazil, of all atmospheric emissions in 2014, vehicles were responsible for 97.5% of all carbon monoxide (CO), 79% of hydrocarbons (HC), 67.5% of nitrogen oxides (NOx), 21.8% of sulfur oxides (SOx), 40% of MP10 and 37% of MP2.5 (CETESB, 2016). It demonstrates, thus, that vehicular emissions need to be assessed as a significant source of air pollution.

In Florianopolis, Brazil, there are no emissions inventories to account for mobile contribution. However, it is known this city has the highest number of vehicles per capita in Brazil: 0.79 vehicles/inhabitants (DENATRAN, 2016). Therefore, impacts from road transport in Florianopolis should be a major concern for ambient air quality control.

Recognizing risks associated to air pollution, countries all over the world have developed goals and limit values to control pollutant concentrations in ambient air (WHO, 2000). In Brazil, air quality standards have been defined by CONAMA N. 003/1990. This legislation defines as primary standards those concentrations of pollutants which should not be exceeded in order to prevent health effects; and as secondary standards, those concentrations which would result in minimum harm to individuals and the environment (BRAZIL, 1990).

Taking into consideration the Brazilian air quality standards, the present study aims to assess the impacts of vehicular emissions of  $NO_2$  in Florianopolis. The chosen study area is an important traffic route called Beira Mar Norte Avenue. In order

to estimate  $NO_2$  emissions, a bottom-up approach was applied. To simulate pollutant dispersion, the model AERMOD was used.

It was the first time a dispersion study for vehicular sources was conducted in the city, evidencing pollution from mobile sources is still an emerging issue in developing countries, even though emissions from vehicles have shown to be significant.

#### **METHODS**

#### Study area

Beira Mar Norte Avenue is located in Florianopolis, Brazil. The city has 421,240 inhabitants and total area of 675,409 km² (IBGE, 2010). The Avenue is considered the main route between Florianopolis' insular and continental portions. It also plays an important social role, considering its surroundings serve as an area for sports practice and recreation.

#### Estimating NO<sub>2</sub> emissions

Vehicular emissions were estimated for Beira Mar Norte Avenue following a bottom-up approach (Eq. 1). The method was applied in an extension (D) of 5,91 km along the Avenue, using Eq. 1:

$$E_{NO_2} = \sum N_{if} X F E_{if} X D \tag{1}$$

Emissions  $(E_{NO_2})$  were calculated using vehicular count for each category of vehicles (car, motorcycle, bus, etc.), with data collected from 14th to  $20^{\rm th}$  December 2010 provided by the Environmental Protection Agency of Santa Catarina state (FATMA). The Agency provided the number (N) of automobiles, light commercial vehicles, motorcycles, trucks and buses going through Beira Mar Norte Avenue. Categorization of vehicles occurred in terms of model year (i) and fuel type (f). For each category, emission was calculated according to its emission factor (FE). Total



emissions were used in AERMOD to simulate  $NO_{\rm 2}$  dispersion.

#### Meteorological and terrain preprocessing

Meteorological and upper air data from observations, combined with estimated surface characteristics were processed using AERMET, which provided the necessary boundary layer parameters to be used in AERMOD.

Meteorological data from observations were collected from a station located in Florianopolis and provided by Instituto Nacional de Meteorologia (INMET). From January 1st to December 31st of 2015, medium temperature was found to be 21.9 °C; dew point, 18.0 °C; relative humidity, 79.3 % and pressure readings reduced to mean sea level, 1015 mbar. Winds were predominant from North, with velocity up to 8 m/s and 7.5% of calms. Observed upper air data were obtained from National Oceanic and Atmospheric Administration (NOAA) website, collected from a station located in Florianopolis airport, with data from January 1st to December 31st of 2015.

Surface characteristics depend on surface uses and seasonal conditions. They were estimated according to AERMET User's Guide.

Terrain particularities were incorporated to simulations through AERMAP. In this case, the region's Digital Elevation Model from SRTM/NASA-SC was used as input, providing base elevation at each receptor and source, and terrain hill height scale.

#### **Modelling options**

In order to simulate receptors, a grid of 40.000 points was created. In relation to sources, they

were formed by 30 polygons along three ways in the Avenue, constituting line sources. Total area summed up  $147,657.43~\text{m}^2$ .

#### Compliance with ambient air quality standards

The compliance with ambient air quality standards was evaluated by comparing  $NO_2$  concentrations to the Brazilian legislation established by CONAMA N. 003/1990. Reference values are summarized in Table 1.

Table 1. Primary and secondary air quality standards stablished by CONAMA N. 003/1990.

	AAA. dillidat di ttillileticat average.							
Average	Primary	Secondary						
time	standard	standard						
1 hour	320 μg/m <sup>3</sup>	190 μg/m³						
AAA	100 μg/m³	100 μg/m³						

Reference: BRAZIL, 1990

#### FINDINGS AND ARGUMENT Emissions estimation

It was estimated, for the considered period, that vehicles emitted 5.45 g/s of  $NO_x$ . It is known that only a parcel of NO converts to  $NO_2$ , which is highly influenced by environmental conditions. As there has not been any previous studies in the region to evaluate  $NO_2/NO$  relationship, a conservative approach has been adopted based on US EPA recommendations for AERMOD use (EPA, 2014). It means full conversion of NO to  $NO_2$  was adopted for this case.

#### NO<sub>2</sub> dispersion

Short and long term areas of exposition to  $NO_2$  are shown in Figure 1 and 2 respectively.

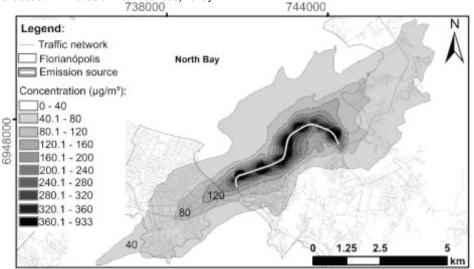


Figure 1. Maximum 1-hour concentrations of NO2 in Beira Mar Norte Avenue surroundings



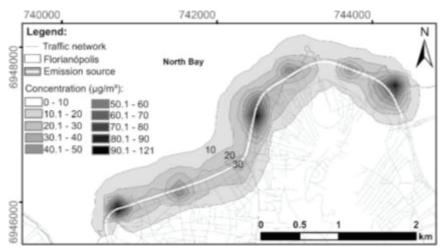


Figure 2. Annual arithmetic average of NO2 in Beira Mar Norte Avenue

Concerning both primary and secondary standards, critical 1-hour concentrations were found all along the Avenue. The highest concentration resulted in 932.7  $\mu$ g/m³. In relation to the annual arithmetical average (AAA), concentrations were critical in three locations along the Avenue and the highest value was 120.9  $\mu$ g/m³. In both cases concentrations were higher than those reported by the World Health organization. In the United Kingdom, NO<sub>2</sub> near road maximum concentrations were listed from 470 to 750  $\mu$ g/m³. AAA around the world ranged from 20 to 90  $\mu$ g/m³ (WHO, 2000).

As summarized in Table 2, It was found 4,646 occurrences of non-compliance with primary standards within 68.6 hectares. And also, 12,186 occurrences of non-compliance with secondary standards were found in 333.6 hectares.

Table 2. Results summary

Parameter	Result
Maximum 1-hour concentration	932.7 µg/m³
Maximum Annual arithmetic average concentration	120.9 μg/m³
Frequency of primary standards non-compliance occurrences	4,646
Primary standards non- compliance area	68.6 ha
Frequency of secundary standards non-compliance occurrences	12,186
Secondary standard non- compliance area	333.6 ha

#### **CONCLUSIONS**

Simulations demonstrated that both standards for  $NO_2$  were exceeded. Also, reference values were exceeded thousands of times, even though they should not be exceeded more than once a year. These results show that critical concentrations were not isolated cases.

Despite of important findings reached by this work, there are some concerns about the present evaluation, due to the lack of field measurements to validate the model results. Moreover, undefined  $NO_2/NO$  relationship in the study area was a limiting factor, which may have kept the present study from getting closer to reality.

Finally, the present study demonstrated that individuals in Beira Mar Norte Avenue surroundings could be exposed to health effects from NO<sub>2</sub> exposition, even considering only vehicular emissions of Beira Mar Norte Avenue. Therefore it evidences the importance of conducting a complete emission inventory in Florianopolis to assess all sources of air pollution. Also, it is recommended for future studies to monitor air quality in the area, to provide data for comparison with simulations.

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#### SOURCE APPORTIONMENT OF SETTLEABLE PARTICLES IN VITÓRIA, BRAZIL

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Abstract: Settleable particulate matter (SPM), especially coarser particles with diameters greater than 10 µm, have been found culprits for high deposition rates in cities affected by hinterland industrial activities. This is the case in cities, where industrial facilities are located within the urban sprawl and building constructions are still intense such as the case of Metropolitan Region of Vitoria (MRV), Espirito Santo, Brazil. Frequent population complaints to the environmental protection agency (IEMA) throughout the years triggered monitoring campaigns to determine SPM deposition rate and source apportionment. Eight different locations were monitored throughout the MRV and SPM was quantified and chemically characterized. Sources profiles were defined either by using US EPA SPECIATE data or by experimental analysis. Atmospheric fallout in the MRV ranged between 2 and 20 g/(m<sup>2</sup> 30 d), with only one monitoring station ranging from 6-10 g/(m<sup>2</sup> 30 d). EC, OC, Fe, Al and Si were found the main constituents of dry deposition in the region. Source apportionment by the Chemical Mass Balance (CMB) model determined that steel and iron ore pelletizing industries were the main contributor to one of the eight locations whereas resuspension, civil construction and vehicular sources were also very important contributors to the other stations. Quarries and soil were also considered expressive SPM sources, but at the city periphery. CMB model could differentiate contributions from six industrial source groups: Thermoelectric; iron ore, pellet and pellet furnaces; coal coke and coke oven; sintering, blast furnace and basic oxygen furnace; soil, resuspension and vehicles. However, CMB model was unable to differentiate between iron ore and pellets stockpiles which are present in both steel and iron ore pelletizing industries. Further characterization of source and SPM might be necessary to aid local authorities in decision-making regarding these two industrial sources.

Keywords: dry deposition, settleable particulate matter, dust fall, receptor model.

#### **INTRODUCTION**

Several works have shown that particles with diameters greater than 10  $\mu m, \ i.e. \ \dot{larger}$  particles, are responsible for the largest mass fraction of atmospheric fallout although they may account for only a small fraction of total airborne particles e.g. (Davidson et al. 1985). Lin et al. (Lin et al. 1994) showed that particles > 10 µm in diameter dominate atmospheric dry deposition. Although larger particles can be expected to have greater contributions to particles' dry deposition, they have not been characterized in many previous aerosol studies (Chen et al. 2015; Lue et al. 2010). Current accounts PM2.5 as the main sulphates and nitrates deposition contributors (Turpin et al. 2000), however Matsumoto et al. (2011) found a similar chemical composition for fine and larger particles.

Receptor models are normally used to determine source apportionment of ambient levels of fine and coarse particles in a specific location (de Moraes et al. 2016; Hu et al. 2014; Koulouri et al. 2008; Lee et al. 2008; Mazzei et al. 2008; Zhou et al. 2015). This approach is particularly useful for determining suspected air pollution culprits. Particularly, the Chemical Mass Balance (CMB) model has been widely used in source apportionment studies, focusing on trace elements (Bi et al. 2007; Kumar et al. 2001; Samara and Voutsa 2005). However only few focus on total SPM and larger size

particles (Crilley et al. 2017). When it comes to determine local environmental policy and management solutions, it is crucial to determine local air pollution culprits. Here, we will study the Metropolitan Region of Vitoria (MRV) in Espirito Santo, Brazil, where a grave problem of SPM nuisance affects local population for years now (de Souza et al. 2014; Melo et al. 2015). SPM is target frequent populace complaints to environmental agency in the MRV, with over 20% of the total complaints being related to air pollution during the years 2009-2013 (Melo et al. 2015). In the present work, spatial and temporal distribution of particles deposition rate and their chemical characterization in the urban and industrialized area of the MRV have been investigated and the contribution of natural and anthropogenic sources related to human and industrial activities were determined.

#### **METHODS**

SPM was collected in four containers at each receptor location M1-8 indicated in Figure 1. Containers were designed according to ASTM D1739 (ASTM 2004). Sampling was carried out with time periods of 30 days for 2 full years, from April 2009 to March 2011. Collected samples were analysed by a General lonex Corporation Particle-Induced X-ray emission (PIXE) to establish SPM chemical composition. For source apportionment, 22



industrial sources were considered (Figure 1). Source characterization was performed using a mixture of experimental sampling and chemical profile taken from SPECIATE 4.2. Using the CMB 8.2 model provided by the USEPA we ran source apportionment for the MRV.



Figure 1. Spatial distribution of the SPM collection sites and industrial sources in the MRGV.

#### FINDINGS AND ARGUMENT

The two-main ore-transforming industries are located next to each other: the steel industry (S13-S22) and the pellet aggregates industry (S8-S12) (Figure 1) and use the same ore as raw material.

5 Figure synthesizes elemental composition (mass percentage) monitoring station. Figure 5 shows EC, OC, Fe, Al and Si as the main constituents of dry deposition in the region. Si and Al are mainly related to crustal sources, and can be traced back to quarries, road resuspension and soil (Table 2). Fe contents seem to be the most irregular element monitoring across presenting its highest weight percentage at M3. M1, M4, M6 and M7 also show high Fe contents, but not to the same extent as in M3. M3 particulates show a relative Fe

percentage of about 35%, being 7 times larger than Si. Prevailing wet season winds are N-NE, indicating that possible sources are located Northeast of M3 - as suggested previously. Although Fe is a relative abundant element in natural sources around the MRV such as soil, quarries or resuspension (Table 2), Fe and EC are particularly abundant in iron ore (S10, S22) and other industrial related sources (Table 2). Therefore, Fe and EC can be associated with the emissions from steel and pellet industries (\$8-22 in Figure 1). Sources S8-S12 and S13-S22 are producers of iron ore, iron pellets, sinter, coal and coke, and have high Fe and EC present in their products (Table 2). In fact, the Fe concentrations in SPM is expressively larger in the region south of the industrial complex (Figure 5). Exceptions are M5 and M8, which seem to be located slightly off the prevailing wind direction during the wet season (Figure 2). EC and OC can be found in SPM at all monitoring stations. While OC is mainly linked to vehicle traffic emissions, EC is related to coal and coke emissions and can be traced back to steel and pellets industries (Table 2). OC concentrations are higher in the regions with the highest amount of traffic (M2, M8, M5, M4), but not substantially (Figure 5).

Ca levels are also considerably high (Figure 5), and may be linked to civil construction and steel and pellets industries (Table 2). It is possible to note that Ca levels are higher at M2 and M5. Although these monitoring stations are in the direction of main emissions from the industrial district (during wet season), the highest Ca concentrations are found where



the largest civil construction activities were occurring at the time of study (M2, M4 and M5). Although M3 is heavily influenced by steel and pellets industries (S8-S22), they do not show high Ca concentration levels. Since these locations do not have civil construction in their surroundings, Ca might be used as a tracer for this type of activity.

Although levels fine and coarse particles meet the Brazilian national standards, a prospective study about air quality annoyance in the MRGV demonstrated that 83.1% of respondents consider SPM deposition as nuisance (Alves et al., 2006). In average, M4 presents the highest deposition rates (Figure 4), and coincides with the highest level of annoyed population. In a previous study, M4 presented the highest percentage of extremely annoyed respondents (Melo et al. 2015). The effects of seasonality on population nuisance is explored elsewhere (Melo et al. 2015).

#### 4.3. Source Apportionment

Given the chemical composition at each monitoring station (M1-M8), source contributions were estimated using CMB. Figure 6 summarizes source contribution

percentages from April 2009 to November 2010. The period from April to November 2009 was grouped together due to the insufficient SPM mass for chemical characterization. The label *Siderurgy* embodies both industries of iron ore and steel manufacturing (S8-22), as referred to in section 3.

Siderurgy shows the main up as contributor to M3 (Figure 6c), previously hypothesized. M2, M4, M5, M6 mainly influenced and M7 are resuspension, civil construction and vehicular sources (Figure 6b, 6d-g). M5 is particularly influenced by vehicular traffic since it is located between several main highways (Figures 1, 5). Most of these monitoring stations are surrounded by streets of intense traffic and heavy construction works that could be driving the high contributions of sources as resuspension and civil construction. M7 and M8 stations show major source contributions of quarries and soil (Figure 6g and 6h). Since the outskirts of the MRV is characterized by unpaved roads and intense truck traffic, where M7 and M8 are located, soil and resuspension would then play a major role as SPM sources. Coal/Coke contribution can be seen at all



monitoring stations (Figure 6a-h), since OC and EC were widely spread across the MRV (Figure 5). However, *Coal/Coke* highest contributions are found at M2, M3 and M4. M3 and M4 are located opposite of steel and pellets industries (S8-S12 and S13-S22), on the direction of N-NE winds.

Α discretized analysis of source apportionment by subgroups was conducted for M3 aiming to better investigate and discriminate contribution from industrial Siderurgy is responsible for 57% of the total dry deposition at M3. Overall, all sources belonging to iron industries contributions, account for about 79% in this station (Figure S2), being ore and pellets stockpiles and pelletizing plant furnaces the main contributing sources (about 72%).

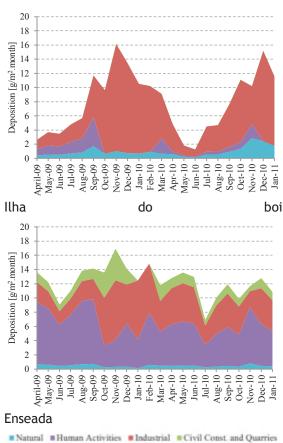


Figure 7. Temporal variation of SPM deposition rate [g/m².month] relative to sources contributions.

#### **CONCLUSIONS**

Conclusions should include (1) the principles and generalisations inferred from the results, (2) any exceptions to, or problems with these principles and generalisations, (3) theoretical and/or practical implications of the work, and (5) conclusions drawn and recommendations.

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## Session 7 Environmental Odours



### EXAMINATION OF INTER-ANNUAL VARIABILITY IN METEOROLOGY WITH IMPLICATIONS FOR ODOUR DISPERSION MODELLING

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Abstract: Inter-annual variability within meteorological input data required for odour dispersion modelling are investigated. In view of this need, we simulate a facility in the planning phase to assess the odour impacts from a single-point source using the AERMOD air dispersion model. To conduct the evaluations, the general odour criterion used by the jurisdiction of Germany was selected as reference. Equivalent maximum predicted concentrations and separation distances were determined for all weather years assessed individually or in combination. Accordingly, the low variability between the years reveals that a single year period was a sufficient length of the meteorological dataset to achieve consistent outcomes of potential odour impacts.

Keywords: air pollution, environmental odour, meteorology, dispersion modelling, AERMOD.

#### **INTRODUCTION**

Currently, different approaches are used throughout the world to regulate on environmental odour. Among the methods and tools that conceive such approaches, dispersion modelling stands out because it can be used both to evaluate the risk of odour impacts in planning stage assessments (future scenarios) and to enlighten assessment of odour impacts of existing facilities. This tool is categorized within regulatory frameworks as maximum impact standard (Brancher et al., 2017).

Once the odour concentration statistics in ambient air are calculated using suitable dispersion models, the outputs are compared against a jurisdictional immission standard or guideline, termed odour impact criteria (OIC). OIC are generally formed by a combination of three components: odour concentration threshold  $C_t$ (given in odour units per cubic meter or equivalent units, ou m<sup>-3</sup>); threshold percentile compliance value P (also specified as a threshold exceedance probability); the averaging time  $A_t$  used to calculate concentrations within the dispersion model (Brancher et al., 2017). For odour pollution, dispersion models are usually set to calculate concentrations over an integration time of 1 h or lower. If the OIC are specified with short time intervals to account for the ability of the human nose to perceive odour within a single breath, then a peak-to-mean factor F is normally required to adjust the odour concentration to the typically longer averaging times used in dispersion modelling (Schauberger et al., 2012; Piringer et al., 2016). Recently a new approach was suggested to determine the variance of the calculated ambient concentration to determine this F (Ferrero et al.,

2017). Therefore, short-time peak concentrations values derived habitually from 1-h averaging times can also be considered in the selection of OIC (Schauberger et al., 2012; Brancher et al., 2017). The OIC comprise regulatory limits or target values essentially used to outline compliance for potentially odour-generating facilities.

Odour regulation, worldwide, has proved delicate to establish a robust tool to assess and predict complaints. This is due to several reasons, as the strict connection with human appraisal. The processes leading from odour formation to annoyance and loss of amenity of the residents are complex. Both perception and appraisal of odour are factors that can interfere in this chain (EA, 2002). Among the challenging topics found presently in the field of environmental odour, Brancher et al. (2017) describes the difficulties in estimating odour emission rates, uncertainties in dispersion modelling, correlating exposure to annoyance and discusses on the net effect of these factors. Additional methodological procedures that still needs advances to make odour impact assessments more consistent are also reported in Brancher et al. (2017). To examine the consequences of variability in meteorology, for instance, and its implications to legislations is crucial for odour impact assessments based on predictions of dispersion models. This is mainly because distinguished impact patterns can be delivered if the assessments are conducted on a monthly, annual or multi-year basis over the meteorological file used to feed the dispersion model.

The investigation of inter-annual variability in meteorology used as input to perform an odour dispersion modelling study is the core issue of this



work. Consequently, we examined the variation that the length of the inputted meteorological file can provide on odour footprints. To this intent, a hypothetical scenario (proposed development) was developed to assess the odour impacts from a single-point source using the steady-state plume model AERMOD.

#### **METHODS**

#### Site description and odour source

A hypothetical scenario of odour emission was conceived in the city of Joinville, state of Santa Catarina (SC), located in southern Brazil. Joinville is representative of the industrial pole of SC with varied activities emitting odours into the environment (e.g., food, textile, foundry and metal industry). Odour emission from an idealised characteristic industrial facility were represented by a single-point source (vertical stack) located at -26.257876°, -48.866606°. The geometry of the source was assumed circular, with a height of 10 m from the terrain level and inner diameter of 1.2 m. The exit velocity and gas temperature were assumed at 7.0 m s<sup>-1</sup> and 313.15 K, respectively. Additionally, the odour emission rate (OER) was presumed continuous (i.e., 24 h day 1) and stationary in time, corresponding to 30,000 ou s<sup>-1</sup>. This OER corresponds to an odour concentration of approximately 3,790 ou m<sup>-3</sup> within the source.

#### Modelling set-up

The U.S. Environmental Protection Agency (USEPA) regulatory air quality model, AERMOD (version 16216r), through the graphic user interface AERMOD-View Version 9.3.0 developed by Lakes Environmental Software, was used to predict odour concentrations in ambient air. Default regulatory options were selected in accordance with the Guideline on Air Quality Models (USEPA, 2017). The modelling domain was inserted into a circular area of 1,5 km radius, with its center positioned in the odour source. Subsequently, the modelling domain was discretised using an uniform polar grid with 1296 receptor points along 18 concentric rings also centred in the stack. Moreover, the location of the receptors was distributed in 72 radial directions, with initial direction in 0° with increase of 5° clockwise. To assume average height of human nose, the receptors were positioned 1.5 m above the ground. SRTM1 contour map file from Shuttle Radar Topography Mission, with 30 m grid resolution, was used to address the topography of the site. Accordingly, the digital elevation model was built using the pre-processor AERMAP (version 11103). The modelling domain has elevations in the range from 3 m to approximately 73 m asl. Surface characteristics around the meteorological tower (i.e., albedo, Bowen ratio e surface roughness length) were determined in accordance with the procedures of AERSURFACE (USEPA, 2008) and

AERMET User's Guides (USEPA, 2016) using AERSURFACE utility (version 13016). With respect to the recommendations described in the Guideline on Air Quality Models (USEPA, 2017), the site was classified as urban and therefore urban dispersion option was selected. Background concentration was not assumed.

#### Meteorological data

Meteorological data were acquired from Joinville's Civil Defence for Cachoeira Area Central station CAC (-26.275094°, -48.849253°) at 1 h sample intervals for wind speed and direction, dry bulb temperature, net radiation and relative humidity. The weather years used to perform the modelling were the 3 most recent to this date (i.e. 2014, 2015 and 2016). CAC was considered the most representative station for the source location based on the proximity of the meteorological site to the source ( $\approx$  2.6 km), complexity of the terrain (topography between the surface station and the source location and is mostly flat), surface characteristics and the period of the data collection. However, CAC station does not have cloud cover and atmospheric pressure observations. Thus, these variables were collected at Joinville's airport SBJV (-26.224°, -48.797°) located about 7.8 km from the odour source. Gaps were consistently filled with established data substitution protocols (USEPA, 2000, 2016). Approximately 99% coverage of surface meteorological records was attained for all variables. It should be noted that substitution for missing data was not used to attain the 90% completeness requirement for regulatory modelling applications. Winds characterized as calm represented 6.35% of the observations; the dominant wind pattern for the site is blowing from north and the average wind speed is 1.18 m s<sup>-1</sup>. Since no upper air data is available for CAC or SBJV, the vertical profile of the atmosphere for 2014-2016 was obtained from Florianópolis airport's soundings SBFL (-27.67 $^{\circ}$ , -48.55 $^{\circ}$ ) situated nearly 160 km from the odour source. Both surface and upper air data were inspected using quality assurance procedures and validation, and processed using AERMET (version 16216). For the estimation of atmospheric stability, the Monin-Obukhov similarity theory is used by the model.

#### Selection of OIC components

The following components of OIC were selected as reference to perform the evaluations:

- $C_t = 0.25 \text{ ou m}^{-3}$ ;
- $P = 90^{th}$ ;
- A<sub>t</sub> = 1 h.

This criterion is currently used in German odour legislation. A constant F of 4 is applied to address hourly values from short-time concentrations of 1 s. As a  $C_t$  of 1 ou  $m^3$  is set, therefore, applying F, a  $C_t$  equals to 0.25 ou  $m^3$  for 1-h mean concentration is delivered.



#### FINDINGS AND ARGUMENT

The quantitative assessment of potential odour impacts showed that the 1<sup>st</sup> high odour concentration predicted for the entire period of evaluation was approximately 4.42 ou m<sup>-3</sup> located 40 m from the stack. On the other hand, the highest maximum odour concentration for the 90<sup>th</sup> percentile was about 0.92 ou m<sup>-3</sup> for a receptor placed 40 m from the source in 2014. Therefore, the locations of the maximum concentrations were found relatively close to the emission stack.

With respect to the examination of interannual variability, Figure 1 reports the contour plots using the OIC previously described for 2014 (red), 2015 (blue), 2016 (green) and 2013-2016 (black). The 0.25 ou m<sup>-3</sup> isoconcentration lobes follow primarily the prevailing wind direction (i.e. north) with similar separation distances for all years.

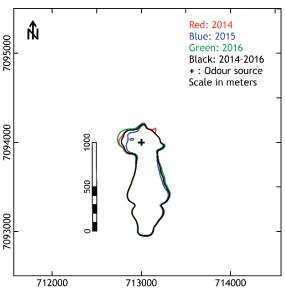


Figure 1. Contour plots for an odour concentration threshold of 0.25 ou m<sup>-3</sup>, 90<sup>th</sup> percentile and averaging time of 1 h for the meteorological years 2014 (red), 2015 (blue), 2016 (green) and 2013-2016 (black).

Table 1 shows the maximum predicted odour concentrations and largest separation distances from the source according to the impact assessment criterion established as reference. The results indicate that substantially different impact patterns were not observed for individual years or multi-year evaluations over the set of meteorological data used as input to AERMOD. The low variability between the 3 years demonstrate that a period of one year was a sufficient length of the meteorological dataset to achieve reliable results. Ordinarily, the wind statistic of a certain site will not change significantly for a measurement period of about 3 months. However, for a distinct seasonal pattern (e.g., Monsson) this could be a limiting factor for using a shorter period such as one year.

Table 1. Maximum predicted odour concentrations and largest separation distances from the source for the 0.25 ou m<sup>-3</sup> contour, 90<sup>th</sup> percentile and 1-h averages.

		Maximum odour	Largest
Period		concentration	separation
		(ou m <sup>-3</sup> )	distance (m)
	2014	0.92	1055
	2015	0.88	1054
	2016	0.80	1043
	2014-2016	0.85	1,051

#### **CONCLUSIONS**

The odour modelling assessment using AERMOD supplied a sufficient level of detail to detect a low degree of inter-annual variability in meteorology for the OIC selected to perform the evaluations. Therefore, these findings disclose that a single year of meteorological data was a sufficient length of meteorological data to adequately predict potential odour impacts.

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## Session 8 Air Pollution Meteorology



#### Extending Mesoscale and Global Meteorological Model Outputs to Assess Urban-Scale Impacts

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The WUDAPT (World Urban Database and Access Portal Tools, <a href="http://www.wudapt.org/">http://www.wudapt.org/</a>) is currently underway (Mills et al., 2015). WUDAPT collect, generate and provide gridded urban scale model-ready urban canopy parameters, including buildings, street canyon, impervious and vegetative surface fractions, surface roughness and reflectivity details, anthropogenic heating, and sky view factor (SVF) for all the world's major cities (with resolution of 120m). We present a conceptual design on the use of WUDAPT parameters, in a postprocessing mode of mesoscale meteorological models, to quantify urban scale metrics that reveal city characteristics on impacts associated with assessing heat stress risks to human health (e.g. Hanna et al., 2015), morbidity, energy, and human activity for selected cities, at high resolution grids. We present an interface to calculate appropriate indices using the model outputs such as dry bulb and wet bulb temperatures, surface radiation, and humidity, to develop appropriate urban indices using the WUDAPT parameters. For example WUDAPT -SVF values are expected to vary considerably throughout a city. With WUDAPT, the within grid heat stress index in operational mesoscale models could be spatially conditioned (weighted) with the spatial maps of SVF at the higher resolutions, enhancing its benefits for heat tress advisories, for assessing of impacts on mortality and morbidity, demand on energy, and to human activities. Overall, WUDAPT can be useful not only as input into a mesoscale and global weather/climate models to define urban canopy parameters, but it is also a useful dataset to independently consider with model output for an urban application of interest.



## INFLUENCE OF THE METEOROLOGICAL PARAMETERS ON AIR QUALITY OF THE ITABIRA CITY, MINAS GERAIS - BRAZIL

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Abstract: Air pollution in urban centers is a growing concern, as it has a significant impact on human health. However, some cities are affected by additional sources of pollution, such as particulate matter emitted by fires or due to mining activity. Itabira-MG is part of this context, as the main economic activity is based on the extraction of iron ore. In this work, the influence of meteorological parameters on monitored mass concentrations of coarse particulate matter ( $PM_{10}$ ) and total suspended particles (TSP) were investigated during 2014, 2015 and 2016 years for Itabira city. The results pointed out that high concentrations of  $PM_{10}$  and TSP are associated with dry days, low values of relative humidity, and intermediate values of temperature, solar radiation and wind speed. Multiple regression analysis has shown that, in fact, radiation and humidity are the most important parameters or that contribute most to the variability of  $PM_{10}$ . In the case of TSP, humidity and temperature are the most important parameters. However, in both cases, relative humidity was shown to be the most significant meteorological parameter and with a higher correlation with  $PM_{10}$  and TSP. The results also showed that there is a relationship between the concentration of particulates and the number of visits and hospitalizations due to respiratory problems.

Keywords: air pollution, meteorological conditions, human health.

#### INTRODUCTION

Mining has become very important for the economic and technological development of several countries and fundamental for the *dynamics* of the Brazilian economy. According to data presented by National Confederation of Industry (CNI, 2012), mining participates with 3% to 4% of national GDP and 20% of total exports in Brazil. Despite the economic benefits, mining has social and environmental impacts. Among these, we can mention the air pollution, with emission of particulates resulting from the mining activity and gases emitted by the equipment used for material extraction and processing (CPRM, 2002).

Among several fixed sources present in the Itabira city, mining activity is one of the most important. Productive ore mines operated by the Vale do Rio Doce company are located within the urban limits and therefore directly expose the inhabitants to emissions of particulate matter (BRAGA et al., 2007).

Meteorological conditions, such as local wind and rain patterns, are important because they determine a greater or lesser dilution of the pollutants that reach the receiver, that is, mainly the inhabitants of the city (VERMA and DESAI, 2008). For example, during winter, less rainfall and the higher number of thermal inversions worsen air quality, especially with respect to carbon monoxide (CO), particulate matter (PM) and sulphur dioxide

 $(SO_2)$ . Therefore, this study intends to analyze the influence of meteorological parameters on the dispersion of the total particles and particulate matter suspended (major pollutants due to mining) and the impact on human health.

#### **METHODS**

Itabira has an Automatic Air Quality Monitoring Network (AAQMN) composed of 5 stations arranged to optimize the coverage of the monitored area. The monitoring is continuous, with generation of hourly means of TSP and  $PM_{10}$  during 24 hours a day in 4 stations and a exclusively meteorological station, which measures the following parameters: wind speed and direction, temperature, relative humidity, pressure, solar radiation and rainfall.

The relationship between PM<sub>10</sub> and TSP concentration and meteorological parameters was investigated using descriptive, correlation and multiple regression analyses, as well as classification and cross-table techniques, as in Tecer et al. (2012), Akpinar et al. (2009), Lazzari et al. (2011) and Verma and Desai (2008).

Stepwise method was applied in the regression model, which is based on an algorithm that verifies the importance of the variables. Meteorological parameters are considered as independent variables and the response (or dependent variable) is the particulate matter.



The dispersion of the particulate will follow the predominant wind direction, which was also determined in this work, as shown by Figure 1 for the 2016 year.

Finally, in order to analyze the health impacts of pollutants, data on hospital admissions were collected directly from computerized databases (DATASUS), made available by the Ministry of Health to the hospitals that were contracted to the Unified Health System (SUS). In addition, data from the Municipal Health Department of Itabira was used, in order to determine the reference units or Family Health Centers (PSF's) of patients most affected by the respiratory problems.

#### FINDINGS AND ARGUMENT

The direction of the wind is extremely important when studying atmospheric pollution, since the pollutants move predominantly downwind; therefore, its direction determines the most affected areas. The prevailing wind direction varies by season and location.

In order to know the prevailing wind direction, a frequency analysis should be made. Figure 1 depicts the prevailing wind direction and its velocity, with the resulting vector (red line), in each season of the 2016 year.

In summer, the prevailing wind direction is generally southeasterly with speeds varying between 2.1 to 5.7 m/s. In autumn this direction holds, but now speeds range from 0.5 to 5.7 m/s. In winter and spring seasons, the direction is generally easterly and northeasterly.

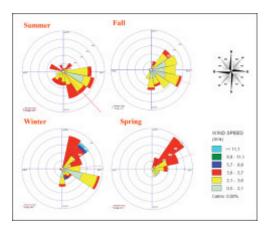


Figure 1. Seasonal Wind Rose (m/s) for 2016 year of Itabira AAQMN meteorological station.

Figure 2 shows the relationship between the meteorological parameters and the  $PM_{10}$  and TSP peak days. The classification categories for  $PM_{10}$ , TSP and meteorological parameters are defined by

the percentiles: <25th, >25th and <75th, and >75th for January of 2014 to September of 2016. High concentrations of PM<sub>10</sub> and TSP are associated with dry days, since a wet removal of particulate matter by rainfall takes place. High concentrations of PM<sub>10</sub> and TSP are also associated with a temperature range of 19.2-23.6°C. The increase of relative humidity is associated with higher concentrations of particulate matter and total particles. High concentrations of PM<sub>10</sub> and TSP are associated with intermediate values of radiation and wind velocity. Typically, the increase of wind speed is associated with greater pollutants transport and dispersion. However, the wind is greatly influenced by the topography and obstacles to its passage, as well as the roughness of the surface.

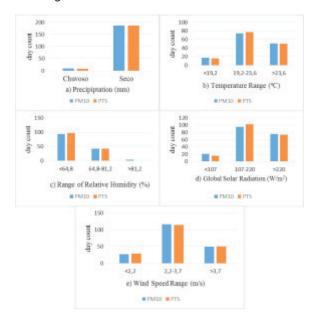


Figure 2. Relationship between the meteorological parameters and peak days in concentration of PM<sub>10</sub> and TSP: a) precipitation (mm), b) temperature (°C), c) relativity humidity (%), d) global solar radiation (W/m<sup>2</sup>), e) wind speed (m/s).

Multiple regression analysis was performed to investigate the behavior of particulate matter and total particles in relation to meteorological parameters, and to evaluate which parameters are more important or contribute most to the concentration of the pollutants. The period analyzed is from August 2015 to September 2016.

The meteorological variables explain 60% of the variability in  $PM_{10}$  and 69% in TSP. Radiation and, especially, relative humidity are the most important and significant variables for  $PM_{10}$ .

Regarding to TSP, regression by the Stepwise method, points to relative humidity, radiation and



temperature as the most important and significant variables. However, the relative humidity and temperature presents the higher coefficients. The relative humidity has correlation of with  $PM_{10}$  and TSP.

Figure 3 shows the relationship between the number of hospital admissions for patients with respiratory problems and concentration of particulates. There is a link between the concentrations of PM10 and TSP with the hospital admissions of the elderly and people aged from 15 to 49 years. In the autumn of 2014 and in the spring of 2015, the admissions of children between 0 and 4 years old was higher as well as the concentrations of particulate matter and total particles. In the spring of 2015, there was an increase in the hospital admissions in all age groups, accompanied by a significant increase in PM10 and TSP concentrations in the same period.

The correlation between the concentrations of  $PM_{10}$  and hospital admissions for the age group of 5 to 14 years is 0.97 (significant at 95% level) for the 2015 year and equal to 0.91 (significant to 90%) for the age group of 15 to 49 years. The correlation with TSP is also significant at 90% and equal to 0.92 for the age group of 5 to 14 years old in the year 2015.

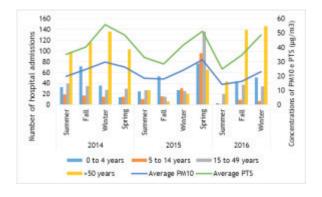


Figure 3. Number of hospital admissions for patients with respiratory problems and concentrations of PM<sub>10</sub> and TSP (μg/m³).

#### CONCLUSIONS

The results pointed out that high concentrations of  $PM_{10}$  and TSP are associated with dry days, low values of relative humidity, and intermediate values of temperature, solar radiation and wind speed. Multiple regression analysis has shown that, in fact, radiation and humidity are the most important parameters or that contribute most to the variability of  $PM_{10}$ . In the case of TSP, humidity and temperature are the most important parameters. However, in both cases, relative humidity was shown to be the most significant meteorological parameter and with a higher correlation with  $PM_{10}$  and TSP. The results also showed that there is a

relationship between the concentration of particulates and the number of hospitalizations due to respiratory problems.

It was not possible to analyze the daytime cycle of the particulate matter in order to know if a higher concentration is directly associated to a period of the day, since the monitored data presents only the daily averages.

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#### MECHANISMS OF AIR POLLUTION TRANSPORT IN URBAN VALLEYS

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#### Abstract:

The transport of air pollutants emitted from urban areas located in valleys can be strongly restricted by local meteorological phenomena such as low-level temperature inversions and different mechanisms of recirculation or stagnation of air pollution. By means of idealized numerical simulations, here we study the mechanisms of air pollution transport resulting from the interplay between a low-level temperature inversion and an urban heat island in urban valleys having different widths. We identified two mechanisms of air pollution transport. The first mechanism describes closed slope-flow circulations that lead to an accumulation of pollutants near the base of the sidewalls. The second mechanism is driven by an urban heat island-induced circulation below the inversion layer, which tends to concentrate the air pollutants in the valley center and can form an elevated polluted layer. The persistence of these types of mechanisms could cause severe air pollution episodes in urban valleys.

Keywords: urban valleys, pollutants transport, temperature inversion, UHI, modeling.

#### INTRODUCTION

Topography plays a major role in controlling the atmospheric boundary layer over complex terrains, thereby affecting the mechanisms of air pollution transport in urban valleys. The transport of air pollutants emitted from urban areas located in valleys results from the interaction between several phenomena which can include low-level temperature inversions, urban heat island (UHI) effects, the development of slope and valley winds (Gohm et al. 2009), and different mechanisms of recirculation or stagnation of air pollutants (Gohm et al. 2009). Different combinations of these factors can strongly influence the air pollution transport in valleys (Gohm et al. 2009; Lehner and Gohm. 2010; Rendón et al. 2014) and, therefore, may lead to severe air pollution events with important implications for public health.

In present work we investigate the effect of valley width on the daytime evolution of the flow field and the mechanisms of air pollution transport resulting from the interplay between the temperature inversion and the urban heat island in urban valleys. We do this through idealized simulations performed with the numerical model EULAG (Prusa et al. 2008).

#### **METHODS**

The model EULAG adopted in this study has been throughly documented in the literature (Prusa et al. 2008) and has already been applied to study the daytime evolution of the thermal wind circulation in valleys (Schimidli et al. 2011; Rendón et al. 2014, 2015). The basic idea was to simulate and compare the daytime evolution of the inversion

layer and the air pollution transport in two urban valleys with different widths, which will be referred to as narrow and wide valleys. Both simulations were performed during the daytime between 0600 LST (Local Standard Time) and 1800 LST, starting with a condition of temperature inversion, and are identical but for the width of the valley floor that was set to 4 km and 12 km for the narrow and wide valleys, respectively. The surface of both valleys is divided into homogeneous areas of urban and rural land cover, which differ in their heating and roughness.

To obtain insights on air pollution transport, we assume that a passive tracer is continuously emitted from the urban area. The surface flux of passive tracer is given by 17 kg hour<sup>-1</sup> km<sup>-2</sup>, based on measurements of annual carbon emissions from an urban area of about 360 km<sup>2</sup> in the Aburrá river valley in Colombia.

#### **RESULTS AND DISCUSSION**

The breakup of temperature inversion (BTI) progresses faster in the narrow valley, mainly because its atmosphere is more heated during the daytime than the atmosphere in the wide valley (Fig. 1). At 0600 LST, the  $\theta$  (potential temperature) profiles in the center and along the sidewalls are identical in both valleys; afterwards, the narrow valley atmosphere is heated faster. In both valleys the BTI follows a pattern characterized by a small displacement of the top of the inversion layer and a continuous rise of its bottom.

The flow field within the CBL (convective boundary layer) is characterized by the development of



updrafts and downdrafts (Fig. 2), the expected structure that arises when turbulence generated by buoyancy due to upward heat flux from the surface dominates relative to turbulence generated by mean shear.

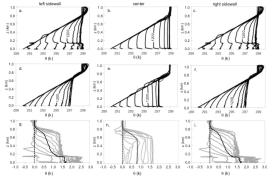


Figure 1: Vertical  $\theta$  profiles from 0600 to 1800 LST in the narrow (top) and wide (middle) valleys, at the left sidewall (left), the midvalley (center) and the right sidewall (right). The bottom shows the hourly differences between the profiles in the narrow and wide valleys.

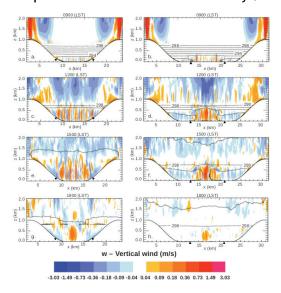


Figure 2: Longitudinal mean fields of the cross-valley w in the narrow (left) and wide (center) valleys. Isentropes are shown every 1 K. The black triangles mark the edges of the urban area.

The spatial distribution of these updrafts and downdrafts differs between the two valleys. While in the narrow valley randomly spaced updrafts and downdrafts develop over the whole valley floor (Fig. 2c,e), in the wide valley floor updrafts prevail in the center over the urban area whereas downdrafts prevail over the rural areas (Fig. 2d,f). In the wide valley the inversion layer becomes shallower in the center due to the larger depth of

the CBL over the urban area as compared to that over the rural areas.

Although the emission rates of tracer from the urban areas are exactly the same in both valleys, the time-spatial distribution of the tracer differs between them (Fig. 3).

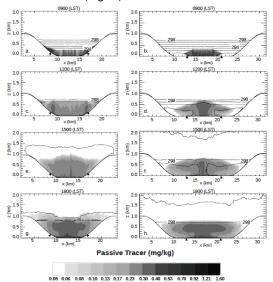


Figure 3: Passive tracer mixing ratio (mg kg<sup>-1</sup>) in the narrow (left) and wide (center) valleys. Isentropes are shown every 1 K. The black triangles mark the edges of the urban area.

In both valleys the tracer remains substantially trapped within the valley atmosphere owing to the capping effect of the persistent inversion layer. However, the more polluted regions are not the same in the valleys because of differences in the flow field and the associated air pollution transport mechanisms. The first mechanism of air pollution transport is a "smog trap" formed by a closed slope-flow circulation that traps pollutants over the lower parts of the sidewalls in the narrow valley, but not in the wide valley (Fig. 3, panels a and c). In the wide valley, the interaction between the slope flow and the UHI is weakened due to the separation between the urban area and the sidewalls. In the narrow valley, there is a strong interaction between the slope flow and the UHI, and the smog traps result from the interplay between the slope flow, the UHI and the temperature inversion. The second mechanism is driven by the UHI-induced circulation below the inversion layer, which tends to concentrate the tracer in the valley center and can form elevated polluted layers (Fig. 3d,f,g,h). This circulation persists in the wide valley during the afternoon and leads to an accumulation of pollutants in the center of the valley. The prevailing upward flow in the center which feeds the divergent flow below the inversion leads to the formation of an elevated



polluted layer that extends beyond the limits of the urban area (Fig. 3d,f,h). This same mechanism drives the distribution of the tracer in the narrow valley in the afternoon (Fig. 3e,g). In the narrow valley there is a transition between the two mechanisms of transport of pollutants during the day.

Figure 4 summarizes the main features of the temporal evolution of the flow field, the inversion layer, and the tracer distribution observed in this study. Our results suggest that a major implication of the UHI on the BTI is that the thermal contrast between the urban area on a valley floor and the rural surface of the sidewalls strongly restricts the mass transport by the upslope winds and, consequently, largely prevents the descent of the inversion layer that has been observed in previous studies of the BTI in valleys. Three of these circulations where identified. First, a circulation near the base of the sidewalls that develops when the upslope winds are detrained toward the center due to the inversion layer (Fig. 4a). A second type of circulation near the base of the sidewalls develops when the UHI forces downslope winds linked to ascending flows that are restricted by the inversion layer (Fig. 4c). The third type of circulation describes the low-level UHI-induced circulation that concentrates pollutants in the valley center and causes the development of an elevated polluted layer below the inversion layer.

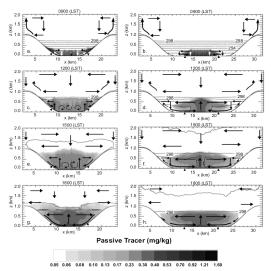


Figure 4: Schematic of the evolution of the flow field associated with the tracer distribution. Arrows indicate mean flow and turbulent eddies. The shadowing indicates the tracer mixing ratio.

#### **CONCLUSIONS**

The width of an urban valley affects the lifetime and evolution of low-level temperature inversions

mainly because of its influence on the heating of the atmosphere confined within the valley, as well as its effects on the structure of the flow field that develops below the inversion layer.

The breakup of inversion layers in valleys where an urban area is concentrated on the valley floor is likely to be dominated by the growth of a CBL enhanced by the increased production of thermal turbulence over the urban area. In these situations, the development of upslope winds may be largely restricted by the UHI induced circulation below the inversion layer.

Closed circulations (smog traps) and elevated polluted layers can develop below an inversion layer in an urban valley as a result of the interaction between the temperature inversion, the UHI and the slope flows.

In urban valleys under the influence of a low-level temperature inversion, different mechanisms of air pollution transport can arise as a result of the interplay between the UHI and the inversion, and depending on the valley width. The persistence of these types of mechanisms can explain the occurrence of severe air pollution episodes in urban valleys.

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# CHARACTERIZATION AND ANALYSIS OF SATELLITE AND GROUND DATA AVAILABLE FOR THE ABURRÁ VALLEY (MEDELLIN METROPOLITAN AREA) AS INPUTS FOR AIR QUALITY MODELS.

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Abstract: The air quality in cities of the Aburrá Valley (Medellín, Colombia; and neighboring cities) is among the worst in Colombia. The topographical and meteorological characteristic of this deep-seated mountain valley generate atmospheric stabilities that trap pollutants for part or most of the day, especially during the biannual transition periods of the Intertropical Convergence Zone (ICZ). In this study, we focus on understanding the temporal dynamics of pollutants (e.g., Nitrogen oxides, Sulphur dioxide, ozone and particulate matter) in this region. The data used were acquired from two different sources: the Monitoring Atmospheric Composition and Climate (MACC) project; and the network of ground-based stations from the Early Warning System of the Metropolitan Area (SIATA, for its initials in Spanish). Time-series, frequency and distributional analyses were performed to characterize and understand the data available for this region in preparation for their use in air quality modelling efforts. Despite differences in resolution and coverage, MACC data captures behavior observed in ground-based data. Nevertheless, the limited spatial resolution of the satellite-based data reinforces the need for additional, strategically placed monitoring stations to capture the air quality dynamics of a region with a highly complex topographical environment.

Keywords: SIATA, MACC, Copernicus, ground-based measurements, Aburrá Valley.

#### INTRODUCTION

With deaths projecting to reach 3.6 million per year in 2050, air pollution will soon overtake contaminated water and poor sanitation as the world's leading environmental cause of premature deaths (Green et al., 2013). The Aburrá Valley, a deep seated canyon that houses the Colombian city of Medellin, experiences periodic episodes of poor air quality. The valley is nestled within highly complex mountainous terrain that heightens its atmospheric stability (Herrera, 2015) and accentuates its poor air quality through thermal inversion episodes (Rendón et al., 2015) that result in low rates of air exchange (Bedoya, 2009).

Although various efforts are being made to understand the problem of poor air quality in the Aburrá Valley (e.g., Baca, 2016; Posada *et al.*, 2016; Zapata *et al.*, 2016), there is no reported evidence of regional scale modelling. Nor is there a systematic evaluation of all the available atmospheric pollutant data, a fundamental first step towards modelling.

This paper presents our efforts in characterizing and understanding the atmospheric contaminant data for the Aburrá Valley, comparing satellite estimates from the Monitoring Atmospheric Composition and Climate (MACC) project; with ground-based data from the network of the Early Warning System for Metropolitan Area (in Spanish SIstema de Alerta Temprana del Área

Metropolitana, SIATA). In exploring the available data, our objectives were: to identify salient dynamics; to assess strengths and weaknesses in the available data, and in so doing develop criteria to suggest the need for more precise and strategic measurements; develop a comparison an analysis framework for evaluating data from different sources as well as modelling results; and to evaluate the suitability of the data for their use in data assimilation of regional models. Different analyses were performed to characterize the available data, which include seasonal and day cycle time distribution, spatial and time correlation and spectral analysis.

#### **METHODS**

The present analyses were conducted on data corresponding to the period between March 31, 2015; and April 30, 2016. This period encompasses a 2016 episode of acutely poor air quality in the Aburrá Valley.

Satellite-based data were obtained from the MACC project (<a href="http://www.gmes-atmosphere.eu/">http://www.gmes-atmosphere.eu/</a>), which is the functioning instrument of the Copernicus Atmosphere Monitoring Service. The data under analysis in this work were a product of the MACC operational near-real time forecast (experiment version g4e2). This data product implemented the IFS model for the meteorological conditions and the C-IFS-CB05 chemistry model to



obtain the concentrations of reactive gases, greenhouse gases, and aerosols. The latter model used the MACCity emissions inventory, and is based on the MACC 4D-Var reanalysis. The spatial resolution is approximately 80 km, with 36 vertical layers that span from 1000 hPa to 100 hPa. For the mentioned reanalysis resolution, four quadrants covered the municipal areas of the Aburrá Valley cities (Figure 1). The corresponding data quadrants were centered at 6.6667°N, 75.9375°W (Q1); 6.6667°N, 75.2344°W (Q2); 5.9649°N, 75.2344°W (Q3); 5.9649°N, 75.9375°W (Q4). MACC data were available with a temporal resolution of 3 hours. Data for nitrogen oxides (NO<sub>x</sub>), Sulphur dioxide (SO<sub>2</sub>), ozone (O<sub>3</sub>), marine and dust aerosols, black carbon, volatile organic compounds, and other available atmospheric species were analyzed. Only O<sub>3</sub> and SO<sub>2</sub> are included in the present abstract due to space, and for comparability with SIATA data (below). In comparisons against ground-based data, only the surface layer (~1000 hPa) was considered. Nevertheless, the individual analyses conducted for all 36 pressure layers for each of the species.

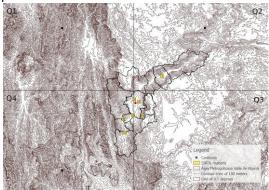


Figure 1. Topographical map of the region under study, showing the political boundaries of the Aburrá Valley cities; the locations within the valley of the SIATA ground-based monitoring stations (yellow boxes); and the MACC data quadrants that cover the Aburrá Valley (four square grid, with the centroid of each a black dot).

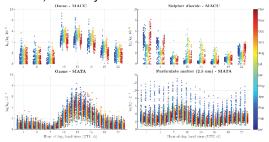
Ground-based data were obtained from the SIATA data web portal (address available upon request). The SIATA project (https://siata.gov.co). operates a network of sensors that monitor, among many other things, meteorological conditions and air quality parameters in the Aburrá Valley. The location of each station used in this study is shown in Figure 1 (yellow boxes). The stations were chosen based on the availability of measurements for PM<sub>2.5</sub> and  $O_3$  for the same period as the MACC data. Data were available with a temporal resolution of 1 hour. Data for all stations for each time point were averaged (discarding absent data points) to obtain a valley-wide average.

Due to the different nature of the data under analysis, we performed at least three different analyses to establish similarities in both qualitative and quantitative perspectives: *Distribution analyses*  - Simple of the probability density functions were constructed from data segregated in day and night. *Frequency analyses* - the data preprocessed with median-substraction, zero-padded (up to 2<sup>15</sup> points) were transformed via Fast Fourier Transform (FFT), and the resulting spectra were normalized to the maximum amplitude. *Pearson correlations* were calculated among the different MACC quadrants, and between each of them and the SIATA data to assess the ability of the MACC data to capture the intra-Valley conditions.

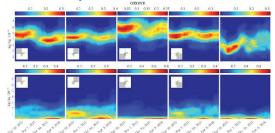
#### FINDINGS AND ARGUMENT

The Aburrá Valley spans roughly 60 km in length, and has an average width of 6 km. The mountains that surround it rise from about 1300 up to 2800 m.a.s.l. As seen in Figure 1, none of the MACC data quadrants contain the valley in its entirety.

Both MACC and SIATA data for ground-level  $O_3$  show that higher values prevail during daytime (10 am to 4 pm) (Figure 2). The highest values are seen during the period March-April, which is associated with a transit of the ICZ over the region, and greater atmospheric stability within the valley. Data for  $SO_2$  shows a monthly dependence of the concentration, as extreme values are found during nighttime in Jan-Mar and Oct-Dec, while high daytime values are seen in Jun-Aug.  $PM_{2.5}$  data reveal extreme values in March, and daily maxima at 08:00 and 20:00.



**Figure 2.** Scatter plots of atmospheric concentration vs. time of day in selected contaminants. Colors correspond to month of the year.



**Figure 3.** Moving histograms for the ozone concentration. Top row presents daytime data; bottom row presents nighttime data. Insets indicate the MACC quadrant being analyzed. Abscissas correspond to the start of the analysis window and ordinates represent concentration bins. The relative frequency of data within each bin is indicated by the color scale indicated above each plot.

Moving histograms for night and day data show the data are clearly bimodally distributed (Figure 3), capturing the diurnal dynamics observed in Figure 2. The results for MACC model and SIATA



ground observations for  $O_3$  agree in the representation of the day/night cycle. Deviations are present as the MACC model tends to overestimate the actual data. It is inferred that MACC data are unable to resolve the valley's topography, as the correlation values (Table 1) between MACC points are considerable higher than the correlation with SIATA data.

Table 1. Correlation coefficients for MACC and SIATA O<sub>3</sub>.

	Q1	Q1	Q3	Q4	SIATA
Q1	1.0	0.89	0.90	0.86	0.70
Q2	0.89	1.0	0.86	0.90	0.72
Q3	0.90	0.86	1.0	0.88	0.77
Q4	0.86	0.90	0.88	1.0	0.74
SIATA	0.70	0.72	0.77	0.74	1,0

Spectral analyses revealed identical frequency components for  $O_3$  in data from both sources (Figure 4). The  $PM_{2.5}$  spectrum presents a very strong low-frequency component behavior compared to the other 2 substances. This can be related to its extreme concentrations during the month of March in contrast to the rest of the year.

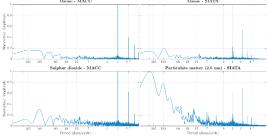
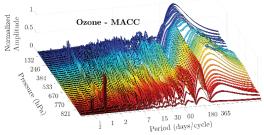


Figure 4. Frequency spectrum for the  $O_3$  for MACC and SIATA,  $PM_{2.5}$  for SIATA and  $SO_2$  for MACC.



**Figure 5.** Frequency spectrum for the 36 layers of the atmosphere that provides MACC

Spectral analyses for all 36 pressure layers of MACC  $O_3$  data (Figure 5) reveal distinct dynamics along the atmospheric column. Higher layers (lower pressures) present stronger low-frequency components, whilst diurnal dynamics dominate the surface layer.

#### **CONCLUSIONS**

With the aim of exploring the atmospheric pollutant data available for the Aburrá Valley, we developed an analysis framework for evaluating data from different sources, and expanded the toolkit for evaluating modelling outputs. Pollutant dynamics captured by MACC data resemble those present in SIATA data, despite the limited overlap

between the MACC data quadrants and the urban areas of the valley. Daily dynamics are in accord with known atmospheric and chemical processes. Discrepancies between the two data sets may be related to the differences in resolution. Focused processing and reanalysis efforts will be needed to increase the resolution of satellite based data, in order of enable detailed model performance assessment (e.g., Xing et al., 2015). Additional works submitted by our group complement efforts towards the implementation of regional and local air quality models, and the identification of areas for increased strategic air quality monitoring.

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## POTENTIAL URBAN POLLUTION IMPACTS ON PROTECTED AREAS IN COLOMBIA THROUGH ATMOSPHERIC TELECONNECTIONS

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Abstract: Urban air contaminants can reach distant ecosystems via atmospheric transport. Deposited contaminants can alter plant physiology, community structure, and ecosystem services. The city of Medellín within the Aburrá Valley (Colombia), presents predominantly poor air quality. It may be a source of contaminants to distant ecosystems. This work explores the prevailing global atmospheric transport dynamics over Northwest South America to identify the ecosystems with the highest risk of detrimental impacts from urban-generated atmospheric pollutants. ERA-Interim data suggest that contaminants escaping the Aburrá Valley will travel predominantly West to the Chocó Biogeographic region, one of the most biodiverse in the world. Qualitative descriptions of satellite-based data agree with the predicted flows. Furthermore, they suggest that the release of contaminants from the Aburrá Valley may be diurnally episodic, owing to the atmospheric dynamics within the valley. As such, we conceptualize the valley, as a point source in space and time that we dubb "The Volcano of the Aburraes", paving the way for the assimilation of valley-centered, ground-based contaminant data into regional transport-chemical models that may afford a more precise estimation of distant ecosystem impacts.

Keywords: Atmospheric teleconnections, ecosystem impacts, air pollution, deposition, Volcano of the Aburraes.

#### INTRODUCTION

The transport of urban atmospheric primary and secondary pollutants towards natural areas represents a threat to ecosystem functions. The Aburrá Valley houses the city of Medellín, constituting the second most populous urban area in Colombia. This work attempts to understand the regional transport dynamics of atmospheric pollutants as a first step towards assessing the impact of urban contaminants on natural ecosystems, paying special attention to the fate of pollutants emanating from the Aburrá Valley.

Human activities are major contributors of reactive nitrogen ( $N_r$ ) species to the atmosphere (Fowler et~al., 2013). Photochemical reactions with  $NO_x$  and  $NH_3$  can lead to the formation of secondary aerosols (Erisman and Schaap, 2004) that may transport  $N_r$  long-distances. Atmospheric transport of nitrogen alters the ocean's nitrogen budget (Duce et~al., 2008). Global deposition of atmospheric reactive nitrogen (Jia et~al., 2016) accounts for over 8% of the planet's reactive nitrogen flow (Fowler et~al., 2013). Deposition of atmospheric  $N_r$  can alters ecosystems (Erisman et~al., 2013), affects community species distribution (Bobbink et~al., 2010; Farrer and Suding, 2016; Maskell et~al., 2010; Simkin et~al., 2016; and Stevens et al., 2004), and in the process, alter ecosystem stability (Koerner et~al., 2016).

Atmospheric  $NO_x$  can lead to the formation of tropospheric ozone ( $O_3$ ). Exposure to ozone can interfere with photosynthesis and result in alterations of community structure (Payne et al.,

2011). Global estimates for losses in agricultural productivity linked to ground-level ozone exposure range from 4-16% (van Dingenen *et al.*, 2009).

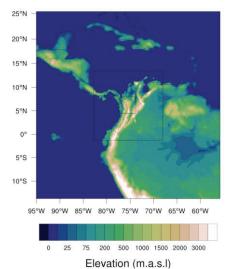
Colombia is one of the 17 megadiverse countries in the world, containing the highest diversity in Bird and Butterfly species, and ranking near the top of the list of diversity of many other taxa. The development plans for the country are linked to the development of its Bioeconomy, where sustainable utilization of its biodiversity and integrated agricultural production systems are seen as major pillars of growth. Evaluating the ecological impacts resulting from long-distance transport of urban-sourced atmospheric pollutants will identify acutely vulnerable areas that may require more than local conservation effort for the preservations of their ecological functions. With this work, we aim to initiate the identification of protected areas that may be affected by distant urban pollution.

#### **METHODS**

As a first approximation to understanding the transport of urban atmospheric contaminants in Colombia, we used data from the ERA-Interim reanalysis to identify the large-scale wind patterns over Northwest South America (NWSA; Figure 1) during a period of one year. We focused on the pressure layer corresponding to 750 hPa, as an approximation to the layer flowing above the mountains that surround the Aburrá Valley (2500-3100 m.a.s.l.). We next constructed a map of protected and vulnerable ecosystems in Colombia to identify the areas downwind of major urban



centres that may be impacted through atmospheric teleconnections.



**Figure 1.** Location of the Northwest South American domain (middle box), which comprises the region within 1.113129°S and 12.43902°N; and 80.12182°W and 68.38552°W.

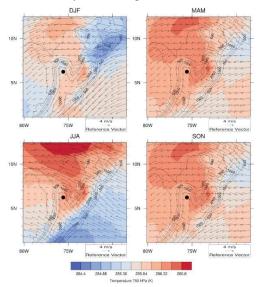
Lastly, we explored qualitatively pollutant data to identify concordance with the predicted flows. We constructed animations of data from the  $\underline{\mathbf{M}}$ onitoring  $\underline{\mathbf{A}}$ tmospheric  $\underline{\mathbf{C}}$ omposition and  $\underline{\mathbf{C}}$ limate (MACC) project, as in (Rodríguez et~al., 2017).

#### FINDINGS AND ARGUMENT

The circulation above the mountains surrounding the Aburrá valley is dominated by the trade winds (Figure 2). Assuming regional representativity for the ERA-Interim results, it could be predicted that the majority of the atmospheric pollution emanating from the Aburrá Valley heads West during the times of transition of the Intertropical Convergence Zone (MAM and SON), and it veers slightly Northward and slightly Southward during the Boreal (JJA) and Austral (DJF) summers, respectively (Figure 2).

The winds flowing above the Aburrá Valley suggest that at various times during the year, ecosystems such as Las Orquídeas National Natural Park (60-100 km NW), the Upper Atrato River (80-130 km SW), and Utría National Natural Park (170-200 km W-SW, on the Pacific coast) could be receiving contaminants emanating from Medellín (Figure 3). Depending on the strength of the flow, atmospheric contaminants may reach the tropical rainforests of the Daríen region (about 250 km NW). These ecosystems are within the Chocó Biogeographic Region, one of the most biodiverse in the world. Due West from the Aburrá Valley along the Western Cordillera lie a series of Paramos (Figure 3), high-altitude ecosystems that function as water providers for large part of the Colombian territory. They are protected under Colombian law as providers of fundamental ecosystem services. The Paramos West of the Aburrá Valley are likely receiving pollutants from

the valley through the atmospheric teleconnections depicted in Figure 2.



**Figure 2.** Long-term seasonal variations of the wind (at 750 hPa) and temperature (at the surface) fields in northwestern South America. Data from the ERA-Interim reanalysis. Black dot indicates the location of the Aburrá Valley (Medellín and neighboring cities).



**Figure 3.** Distribution of National Natural Parks and Paramo ecosystems in relation to major urban centres in Colombia.

constructed animations of concentration data to evaluate concordance with the predicted flows. The concentration landscape of Sulphur dioxide, a proxy for urban atmospheric contamination, highlights the major foci of pollution in Colombia (Figure 4, left). The animations (external link) show a marked diurnal cycle (see also Rodríguez et al., 2017), and episodic releases into the stream of the trade winds (Figure 4, right), which are related to diurnal cycles of human activity, but also to the atmospheric stability (Herrera, 2015) that traps contaminants within the valley for extended periods. Based on this behaviour, we conceptualize the valley as "The Volcano of the Aburraes", a



view that will permit us, based on measured intravalley atmospheric dynamics, ground-based contaminant data and mass balance calculations, assimilate local data (e.g., Fu et al., 2015) into regional transport-chemistry models.

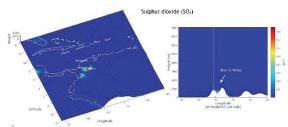


Figure 4. Sulphur dioxide concentration snapshot (June 12, 2015; 10:00) over Northwest South America (left) and the Aburrá Valley (right). Data from MACC. See Rodríguez et al. (2017) for a more detailed description of the contaminant dynamics in the Aburrá Valley. For an animated version of the data, visit <a href="https://www.youtube.com/watch?list=PL7DZTyo1q1YIF4c">https://www.youtube.com/watch?list=PL7DZTyo1q1YIF4c</a> <a href="https://www.youtube.com/watch?list=PL7DZTyo1q1YIF4c">wB0df-Au0Kj1YFz07&v=20hXT-ShGAw</a>.

#### **CONCLUSIONS**

Global circulation patterns over Northwest South America suggest that atmospheric pollutants from the Aburrá Valley have the potential to reach vulnerable ecosystems within the Chocó Bioregion. Higher resolution estimations, via regional transport-chemical models (e.g., LOTOS-EUROS) is urgently needed to identify accutely vulnerable areas. Conceptualization of the valley as a pointsource, dubbed "The Volcano of the Aburraes", will permit the assimilation of local emissions data into regional models, and thus improve the assesment of urban-generated atmospheric pollution on vulnerable ecosystems, and thus inform policies geared toward the preservation of ecosystem services.

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### Challenges and opportunities for Open LOTOS-EUROS model to reproduce the Dynamics for Tropical Andes Domain

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Abstract: In this paper we present the challenges and opportunities to model the chemical dynamics on Tropical Andes Domain through LOTOS-EUROS model, particularly to the understanding of recent air quality crises in Colombia. Improving the capability of modeling the behavior and dynamics of the pollutants in the atmosphere is one of the main goals of the meteorological and air quality community. Few works about the implementation of air quality models on South America have been developed, most of these over Southern South America (South of Brasil and Perú, Argentina and Chile). Through analysis and comparison between the LOTOS-EUROS outputs and data retrieved from ensembles and reanalysis from the Copernicus Project (ECMWF, MACC2), we present the challenges and opportunities for the successful implementation and development of LOTOS-EUROS model as an alternative to model the dynamics of pollutants in the Tropical Andes domain. We also address the challenge to couple the LOTOS-EUROS model with the well demonstrated Meteorological Model WRF and explore their capability to be part of a multiensemble strategy with WRF-Chem module.

Keywords: LOTOS-EUROS Model, WRF model, models coupling, air quality, tropical andes.

#### **INTRODUCTION**

The biggest cities in Latin America keep alarming pollution levels, because they gather the majority of industries and combustion vehicles (Green & Sánchez, 2012). The recent environmental crisis in Colombia has sparked renewed scientific interest several knowledge fields understanding the local and regional air quality dynamics. Efforts have been made with the modelling of the underlying meteorological dynamics through the WRF model over Tropical Andes Domain (Rendón, et al, 2014, 2015, 2016). The use of atmospheric chemistry and transport models centered in the region is incipient at best. The LOTOS-EUROS (LOng Term Ozone Simulation-EURopean Operational Smog) model is an Eulerian chemistry transport model that describes in three dimensions across the troposphere the dynamics of certain groups of pollutants by reproducing the advection, diffusion, emission, deposition, vertical diffusion, mixing and chemistry processes, LOTOS-EUROS allows the calculation of concentrations for ozone, particulate matter (PM), nitrogen dioxide, heavy metals and organic pollutants with a standard model resolution of approximately 36x28 km. (Sauter et al., 2012). The LOTOS-EUROS model has been widely used in different projects around the world, reflecting its capacity. The model is within the framework of the project MACC II,

which is looking to produce the forecast at European continent level in air quality, meteorology and solar radiation (Marécal et al., 2015). The MACC II project uses the network of satellites and sensors denominated COPERNICUS along with LOTOS-EUROS (among other air quality models) to make the predictions of air quality (Schaap et al, 2016). Likewise, the LOTOS-EUROS is used in The Netherlands to predict ozone concentrations and PM in its national territory (Hendriks et al., 2013). The LOTOS-EUROS model has not been only implemented in Europe; it is also part of the project PANDA, which collects a set of models and looks for modeling and predicting pollutants concentrations in the Chinese territory. The model was also implemented in Brazil to monitor and predict Ozone concentrations, Nitrogen Dioxide and PM 2.5 during the 2014 FIFA World Cup. The model was successfully assimilated in 4D-variational and ensemble schemes for the analysis of Eyjafjallajökull volcanic eruption and (Fu et al, 2017; Lu et al, 2016).

In spite of the different success cases, implementation of the LOTOS-EUROS model over the Tropical Andes region faces considerable challenges, principally due to the orography of the region, meteorological dynamics, lack of an accurate emissions inventory and the difficulties in finding sources of data for the initial and boundary conditions.



#### **METHODS**

To model the air quality in the Tropical Andes region, mainly in Colombia we implemented the chemical transport model LOTOS-EUROS. As a chemistry transport model, the LOTOS-EUROS needs multiple inputs data like meteorological dynamics (air velocity, humidity, solar radiation, etc) and emissions of pollutants uses as initial and boundary conditions. To implement the LOTOS-EUROS model over the region, we used data available from different sources. For the meteorology, data were taken from ECMWF database. The natural emissions were taken from MACC 1 database and the repository of emissions is taken from EDGAR. The model was implemented in a standard resolution of 0.25° x 0.25° in the region between -80 to -65 west degrees, and 25 to-10 north degrees. The simulation experiment was set for the period March 24-April 4, 2015. This period corresponds with the contingency in the region owing to the high concentration of pollutants in the atmosphere over the Medellín metropolitan area. Our objective is to evaluate through the statistical analysis the consistency of error of the physical-chemical results in comparison with the data of the Copernicus Project. To compare the error of the model we used four statistical measures applied to the volume mixing ratio of NO<sub>2</sub> and O<sub>3</sub> modeled through LOTOS-EUROS. The analysis is based on eight pairs of modeled and measured observations over the selected domain. The evaluation measurements implemented are: the ratio, the residual, the root mean square (rms), and the average correlation coefficient (Barbu et al., 2009).

#### FINDINGS AND ARGUMENT

The volume mixing ratios of  $NO_2$  and  $O_3$  modeled through LOTOS-EUROS are shown in Figure 1 and 2, respectively. The selected points to compare the LOTOS-EUROS outputs with data from the Copernicus Project are shown in Figure 3. For each point was calculated the four statistical measures to have a spatial representation of the model error. The total statistical measures for the domain are presented in the Table 1.

According to the Table 1, the model tends to overestimate the concentrations both  $NO_2$  and  $O_3$  for the entire domain. For  $NO_2$ , a part of the bias is due to high-modeled concentrations at two points. The other points have a value closer to the regional mean. For  $O_3$  the ratio has a high value for almost all points, presenting a more uniform trend in the region. For both substances, for most points the correlation coefficient is into the range between 0.40 and 0.88, with only a point with a lower value (0.28) and other with a higher value (0.99). The total correlation coefficient for the domain in both substances is considerably high,

this means that the model is able to reproduce the temporal behavior of the two substances with an acceptable performance.

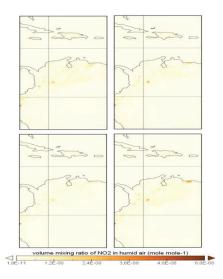


Figure 1. Volume mixing ratio of NO₂ modeled through LOTOS-EUROS for the days March 24, March 28, April 1 and April 4.

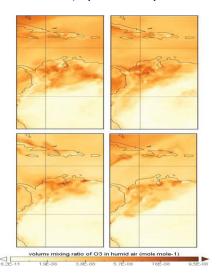


Figure 2. Volume mixing ratio of O₃ modeled through LOTOS-EUROS for the days March 24, March 28, April 1 and April 4.

To have a full representation of the air quality in the region, a higher resolution is needed, due to the fact that the tropical Andes have many important valleys and other forms of relief with a large population (such as the city of Medellín, located inside the Aburrá valley at 6.2° lat. and -75.5° long., marked in red in Figure 3).

Nevertheless, the model basically described the general dynamics for  $NO_2$ ,  $O_3$  and other species over the Tropical Andes region.



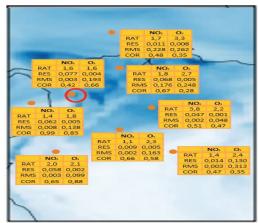


Figure 3. Distributions and statistical measures of the comparison points. The red circle is the Aburrá Valley (Medellín) location.

Table 1. Statistical measures features

Variable	NO <sub>2</sub>	O <sub>3</sub>							
Ratio	1.8	2.1							
Residual	0.003	0.005							
rms	0.053	0.183							
Corr. Coef	0.62	0.65							

The difficulty to increase the resolution of the model relies on the lack of accurate meteorology data and emissions inventories. One alternative of the problem with the meteorological resolution is the coupling with a meteorological model like WRF. WRF is able to perform a representation of the meteorology with higher resolution than the databases available for the region (Rendón et al, 2016). With the coupling with WRF it is possible to run the LOTOS-EUROS model with higher resolution than the current resolution, and to get a complete representation of the pollutants in the region and principally in the main cities. The WRF model also has been used with the Chem module fort the initial evaluation of  $PM_{10}$  concentration over Bogotá city with an acceptable performance (Kumar et al., 2015).

#### **CONCLUSIONS**

LOTOS-EUROS is a capable tool to represent and simulate the dynamics of the pollutants over the Tropical Andes region. Despite the observed errors in magnitudes, the LOTOS-EUROS model captured the temporal dynamics of the substances analyzed. With the current resolution, LOTOS-EUROS is not able to represent precisely the dynamics of the pollutants in certain cities of the region such as Medellín. Although it is possible to increase the resolution of LOTOS-EUROS, it is necessary to have data for initial and boundary conditions of better resolution. Data assimilation for LOTOS-EUROS with data from ground-based stations and other

sources, can improve the accuracy of the model, both for the current scale and for smaller scales.

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## APPLICATION AND CRIATION OF LOCAL CLIMATES ZONES IN BELO HORIZONTE (BRAZIL) USING WUDAPT

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Abstract: This study applied the local climatic zones classification model from the World Urban Data Base and Access Portal Tools project in the city of Belo Horizonte (Brazil). An urban distribution analysis was made for each neighborhood in the 9 city regions, being related to the urban characteristics with the altitudes differences in the study area. This analysis was made from the Google Earth Software, which enabled the Belo Horizonte mapping in the LCZ classification along with the altitude determination of each location. It was observed that the city has a great altitude difference in all its extension and in diverse scales, besides owning many urban aspects. It was also found that there is a need to improve the analysis using LCZs, so that these also have as standardized characteristics the altitudes aspects.

Keywords: LCZ, WUDAPT, classification, urban areas, altitude

#### INTRODUCTION

According to Pacheco et al (2017), during the last decade Brazil has been facing rapid economic growth that has triggered an increase in vehicle fleet and air pollution in urban centers, especially in capitals and their metropolitan areas. The Metropolitan Area of Belo Horizonte (MABH) is the third largest metropolis in Brazil. Belo Horizonte is its main city and the capital of Minas Gerais state. The MABH has 5.7 million inhabitants distributed throughout a surface area of 9500 km<sup>2</sup>, which is divided into 34 cities (IBGE, 2015; Miranda et al., 2011). The region is characterized by a tropical climate with wet (October to March) and dry (April to September) seasons; January and July are the hottest and the coldest months of the year, respectively. The region has a topography characterized by mountains that determine the pollutants circulation.

The urbanization process in Belo Horizonte began to intensify from the 1960s, when started to build skyscrapers, asphalts, among others. This process continues until today, and has expanded to the neighboring cities in MABH. Currently, MABH is the third largest urban agglomeration in Brazil and the 62<sup>nd</sup> largest urban settlement in the world.

In this work, the Local Climate Zones (LCZ) classification system (Stewart and Oke 2012) was applied to the MABH. It *supplies* a standardized description of urban function and

form. The general objective is to perform the Belo Horizonte urban mapping using the standart WUDAPT methodology (Bechtel et al 2015), adapting the LCZ classification to the city altitudinal characteristics.

#### **METHODS**

Using the tutorial to create LCZs, provided by WUDAPT, the urban area of Belo Horizonte was demarcated from a ROI polygon (Created in Google Earth). Through the System for Automated Geoscientific Analysis (SAGA) (Conrad et al. 2015), it was selected an area of interest from 703 km²( lat  $19\,^\circ46'20.00"S$  to  $20\,^\circ00'49"S;$  long  $43\,^\circ49'00"$  W to  $44\,^\circ05'07"W;$  center of the grid is lat  $19\,^\circ.53'37.13"S$   $43\,^\circ57'18.29"W)$  with 12-meter resolution grid (supplyed by the Deutsches Zentrum für Luft- und Raumfahrt (DLR) - German Aerospace Center) was carried out in the ROI polygon of the study area.

From the grid map, an observational analysis was performed on Belo Horizonte neighborhoods and its urban characteristics (for example, building height and distribution, among others). Thus, LCZs were identified in the city of Belo Horizonte.

#### FINDINGS AND ARGUMENT



Belo Horizonte is divided into 9 microregions, and each one has one or two predominant LCZs, as can be seen in table 1:

Region	Prevailing LCZs						
Barreiro	LCZ 3 and 10 - Compact Low Rise and Heavy Industry						
South Center	LCZ 1 and 2 - Compact Mid Rise and High Rise						
East	LCZ 3 - Compact Low Rise						
Northeast	LCZ 3 - Compact Low Rise						
North	LCZ 3 - Compact Low Rise						
Northwest	LCZ 3 - Compact Low Rise						
West	LCZ 3 Compact Low Rise						
Pampulha	LCZ 6 - Open Low Rise						
Venda Nova	LCZ 3 - Compact Low Rise						

Table 1. Regions of Belo Horizonte related with the LCZ classification

The table above was originated from the analysis of 9 tables that identify the urban characteristics of each Belo Horizonte neighborhood. From this second table was made the city mapping, characterizing it with the LCZ classification (Figure 1).



Figure 1. Belo Horizonte maped in LCZ classification
Reference: Aline Nascimento 01/05/2017

Belo Horizonte has in its extension the predominance of LCZ 3 (Compact Low Rise), followed by LCZ 6, 9, A and B (Open Low Rise) in its extremities.

#### **CONCLUSIONS**

The main Belo Horizonte urban characteristics are the presence of houses or buildings with 1 to 2 floors, distributed compactly

among themselves, built from heavy materials such as concrete, brick, and others. Most of the city is in regions of impermeable soil. However, in the extremities of Belo Horizonte there is presence of many places with permeable soil characteristics, abundant arboreal areas and houses with more sparse distributions among themselves. Another important feature of the city is the high altitude difference, both in the greater urban development area and in the natural area. The height difference between the highest and lowest places in the city is approximately 800 meters.

However, for the more detailed determination of Belo Horizonte urban topography, it is important to create LCZs that consider the altitude differences concomitantly with the urban site characteristics. In figures 2 and 3 it is possible to observe different urban aspects in places with great altitude differences.



Figure 2. Region South - Serra do Curral



Figure 3. Region South - Buritis

#### **ACKNOWLEDGMENT**

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## EFFECTS OF URBANIZATION ON THE URBAN HEAT ISLAND IN THE METROPOLITAN AREA OF VITÓRIA, BRAZIL

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Abstract Abstract: In this work, it was evaluated the effect of urbanization on the heat island formation in the Metropolitan Area of Vitória (MAV), Espírito Santo State, located in the Southeastern Brazilian Region, through the mathematical modeling of the atmosphere with the WRF coupled with the UCM model. For this, it was evaluated the difference between a real simulation for the period from May 26 to 27, 2011 in the MAV, and the control and hypothetical simulation, in which the urbanized areas were replaced by the vegetation type equivalent to the code 13 of WRF (evergreen broadleaf). Among the results, relevant changes were observed in the production of sensible heat flux and temperature at 15z. Another important characteristic was the increment of the wind intensity, due to the presence of the city, and also an increase in horizontal wind divergence, which leads to a rise in the downward component over the city.

Keywords: land use, land cover, WRF / UCM, Metropolitan Area Vitória, sensible heat.

#### INTRODUCTION

Changes in land use and coverage, especially in cities, have an impact on the local climate due to variations in physical processes that govern energy, momentum, and the matter exchange between Earth's surface and atmosphere (OKE, 1974). Thus, studies of urbanization impacts on the climate of cities are very important. This has motivated the development of a large number of scientific studies investigating the heat island formation (MARQUES FILHO et al., 2009), local circulation (FREITAS et al., 2007), energy balance (ARNFIELD, 2003), and mathematical modeling and changes of land use and coverage (BHATI and MOHAN, 2016).

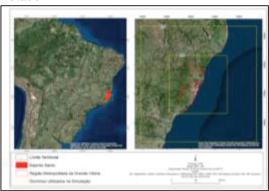
In this sense, this work evaluated the effect of urbanization on the heat island formation in the Metropolitan Area of Vitória (MAV), Espírito Santo State, located in the Southeastern Brazilian Region, through the mathematical modeling of the atmosphere with WRF (Weather Research & Forecasting Model) (SKAMAROCK, et al., 2008) coupled with the UCM model (Urban Canopy Model) (KUSAKA et al, 2001). The MAV has an area of 2,311 km2 and population density of 730 inhabitants/km2. It consists of 7 municipalities, 4 of which form an urban conglomerate (Vitória, Serra, Vila Velha and Cariacica) plus Viana, Fundão and Guarapari (Figure 1). Currently it concentrates 48.01% of the Espírito Santo population and has 80% of the large companies located in the state, representing 48% of the state's GDP (IBGE, 2015).

#### **METHODS**

In this work, the WRF model coupled to the UCM was used. UCM is used to represent urban surfaces,

including their geometry which is represented by canyons in long streets, with various types of surfaces (roof, walls and roads) to introduce different sensible heat flows, in addition to the thermal and mechanical effects.

Figure 1: Study area and domains used in the simulation  $% \left( 1\right) =\left( 1\right) \left( 1$ 



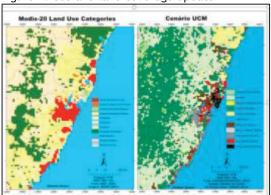
Elaboration: Wesley Correa

Regarding the classification of land use and coverage, in some models, this data is out of date or inaccurate for several regions of the world (SCHICKER, 2011; CHENG et al., 2013). Therefore, in this research, it was necessary to update it for the whole d2 domain through the equivalence of the Brazilian system with the Moderate Resolution Spectroradiometer Imaging System (Globion, 2015) and later for the USGS. The mapping process to update land use and coverage was performed in the software ArcGIS 10.1 with the use of aerial photos of 2014, provided by the company Hiparc Geotecnologia Ltda., at the scale of 1: 5000 and pixel spatial resolution of 0.25 cm. After the



mapping process, the input files for the WRF in ASCII format were generated using the gdal complement and editing the geographic data control files. After upgrading, in order to meet the WRF-UCM characteristics, the USGS-33 classification was used with three distinct urbanization types: low residential density, high residential density and commercial/industrial area (Figure 2).

Figure 2: Use and land coverage update



Elaboration: the authors

The simulation was initialized with data from the meteorological variables provided by the National Centers for Environmental Prediction (NCEP-FNL). The used configuration was of two nested domains with the two-way nesting option, where d02 domain encompasses MAV. The simulation period was from May 25 to 30, 2011. The parameterization options used can be seen in Table 1.

Table 1: Parameterization options used in WRF (3.5.1 version) for d01 and d02 domains.

(3.3.1 Version) for do and do	z domanis.				
WRF Setting and physics options	Value				
Horizontal resolution	5 km	1 km			
Column/row	49	121			
Vertical levels	21				
Microphysics	Single-Mor	ment 3-class			
Long wave physics	RRTM				
Short wave physics	Dhudia				
Surface Layer	MM5				
Land Surface	Noah Land Surface Model				
Planetary Boundary layer	Noah land surface				
PBL scheme	BouLac PB				
Cumulus scheme	Betts- Miller- None Janjic				

Elaboration: the authors

The simulation performance was evaluated by comparison with observational data from the Eurico de Aguiar Salles Airport meteorological station,

based on the methodologies suggested by Emery et al. (2001).

In order to evaluate the effect of urbanization on the formation of heat island in the MAV, the parameters of air temperature, wind speed and direction, sensible and latent heat were analyzed through the difference between the real simulation for the study area, control simulation and hypothetical simulation. In hypothetical scenario urbanized areas were replaced by the vegetation type equivalent to the code 13 of WRF (evergreen broadleaf).

#### FINDINGS AND ARGUMENT

The results of the difference between the real simulation (real city) and the hypothetical scenario (without the presence of the city) are presented below. In this work were only presented results for the afternoon of 05/26/2011 and dawn of 05/27/2011.

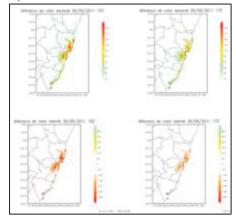
In Figure 3 it is possible to observe the difference between the sensible and latent heat flux for the 05/26/2011 at 15 and 17Z. A sensible heat difference of 190 W/m2 was observed at 15 and 17z, especially in the eastern part of the study area. This indicates a great heat transfer during the day, which is associated with areas of high residential and commercial/industrial density, that leads to greater heating and local circulation. In relation to the latent heat, differences up to -330 W/m2 can be observed in same areas, indicating that, during the day, evaporation is much smaller with the presence of the city, even if it is very close to the ocean.

The difference between the simulated air temperature with the presence of the city and the hypothetical scenario is presented in Figure 4 at 15 and 17z. It is possible to observe a difference up to 2.7 °C in air temperature for the proposed scenarios, especially in areas of high residential and commercial/industrial density, which is associated with high heat transfer and low humidity.

In figure 5, the difference of the wind field and divergence for 27/05 at 0 and 03z is shown. In relation to wind speed, the difference of 1.34 to 3.0 m/s is observed, mainly in more densely constructed areas. Changes in wind field can contribute to changes in other parameters, such as temperature advection, impacting the sensible heat flux, as observed by Freitas and Silva (2000). The difference between the scenarios for horizontal wind divergence field (Figure 5) shows a very similar pattern to that observed for the differences of wind field at the same level. In general, there is a divergence increase at levels closer to the surface which leads to an intensification in air subsidence.

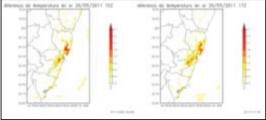


Figure 3: Sensible and latent heat flux difference  $(W/m^2)$ 



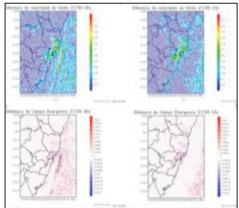
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Figure 4: Air temperature difference (°C)



Elaboration: the authors

Figure 5: Surface wind field difference and divergence for the second day simulation at 00z (left) and 03Z (right) (m/s)



Elaboration: the authors

#### CONCLUSIONS

The present work showed that WRF/UCM model is an important tool for the study of the impact of the city in local climate. It was observed that the urban heat island is more intense in the eastern portion of the study area, especially in those of high residential and commercial/industrial density, with great heat transfer and higher temperatures at 15z. Another important characteristic was the increment

of the wind intensity, due to the presence of the city, and also an increase in horizontal wind divergence, which leads to a rise in the downward component over the city.

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# EVALUATION OF WEATHER CONDITIONS SIMULATED BY WRF-MODEL DURING CONSECUTIVE DAYS WITH HIGH OZONE AND PARTICULATE MATTER CONCENTRATIONS IN THE METROPOLITAN AREA OF RIO DE JANEIRO

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Abstract: Air quality monitoring stations often record ozone (O3) and particulate matter (PM10) concentration levels above the values proposed by the World Health Organization (WHO) in the Metropolitan Area of Rio de Janeiro (MARJ). The MARJ has 19 towns, with a population about of 12.5 million people, present the second largest vehicle fleet and industrial concentration in Brazil. Sometimes, the sum of several weather conditions and high emissions of air pollutants may be favorable to ozone formation and high concentacion to PM10, during consecutive days in a region. In this context, this study examined the influence of weather conditions on three periods when high ozone and PM10 concentrations were registered on consecutive days in the metropolitan area. The study used the Weather Research and Forecasting (WRF) mesoscale numerical model for simulation this of meteorological conditions and variables favorable for maintenance of high concentrations of ozone and PM10, verifying that the model simulated well the influence to South Atlantic Subtropical High (SASH), the penetration time and the influence of the sea breeze and the occurrence of calmwinds, during the night and morning. Through statistical analysis between simulated and observed data, it was observed that, in general, the model underestimated the air temperature and overestimated the relative humidity, but the model simulating well these two variables.

Keywords: Ozone. PM10. MARJ. WRF.



## Use of the observational nudging and the updated soil use and occupation in the performance of the WRF model

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Abstract: The problem of using parameters such as soil coverage, provided by the USGS is that they are available with the last update date in 1993. To solve this problem the main objective is to evaluate the influence of the update data on land use and land cover, with the observational nudging to evaluate the performance of the WRF model over the Greater Victoria Metropolitan Region (RMGV). It worked specifically for a small area of 120 km x 120 km covering the entire RMGV, using the use and coverage of Brazilian land classified in 24 categories suggested by the USGS. And finally the nudging was taken with the surface meteorological records of the Airport Station. In the evaluation the modeling performance of the direction and speed of the wind and the temperature, improvement in every month.

Keywords: WRF, Influence of land use and occupation, Data assimilation.

#### INTRODUCTION

When the numerical prediction model has more accurate spatial resolution, it betters represents urban airflow and air pollution. That is why, for the application in studies of air quality it is necessary accurate meteorological fields to make the correct modeling of the transport and chemical processes involved in the atmosphere. For this purpose, the Metropolitan Region of Greater Victoria (RMGV) uses the numerical model of the WRF mesoscale.

Geographic parameters entered within the WRF are commonly used by the United States Geological Survey (USGS) with half-degree spatial resolution. The USGS land use and land cover data used in the WRF are based on AVHRR satellite data (April 1992 to March 1993) using the approximate 1km resolution (Schicker 2011, Sertel 2009). However, this data is outdated and may lead to incorrect errors or estimates in future modeling. The meteorological reanalysis parameters provided by the National Center for Atmospheric Research (NCAR) have half-grid space resolution every six hours (ARW, 2014).

Using parameters such as soil cover of past dates has the problem of variations in time, which can be the product of vegetation removal, urban and suburban area increase, changes in agriculture (type of planting), loss of glacial areas, among others. They alter the effects of radiation forcing and have a potential impact on global and regional climate. Thus, the inclusion of data from superficial observations that may help in the prediction of modeling. Since the use of data

assimilation means forcing the input data by providing an initial value closer to reality for modeling.

However, in the RMGV, the first works with the WRF in the air quality laboratory of the Federal do Espirito Santo University (UFES) did not make specifications of the geographic data, nor even the assimilation of data from superficial observations to improve the simulations.

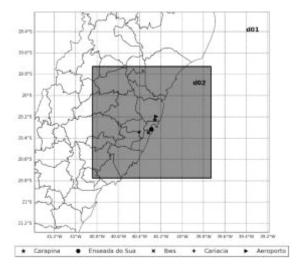
In this context, the objective of this work is to evaluate the influence of input data specification regarding land use and land cover, together with the assimilation of meteorological data (direct observations) to evaluate the performance of the WRF model for Greater Metropolitan Region (RMGV).

#### **METHODS**

Weather Research and Forecasting (WRF) was developed to be flexible, with portable code efficient in parallel computing environments (ARW, 2014). Figure 1 shows the modeling scope for each domain.

Figure 1: Location of the study area and nesting used. Brazil - Espirito Santo.





Typically, spatial analysis is performed with a Geographic Information System (GIS). In this question, we worked with arcGIS for each step of the process of obtaining more accurate maps.

Focused specifically on a small area of 120km x 120km that covers the entire RMGV, this being the area of interest. The information on the use and occupation of the Earth initially has the following information: projection system - Universal Transversal of Mercator UTM), Datum - 84, Zone -24 south. The use and land cover for the RMGV was updated using information from the 2007/2008 period provided by the State Institute of the Environment of Espírito Santo Subsequently, a reclassification of land use and coverage information was made from orthophotos of 2014 provided by Hiparc Geotecnologia Ltda, with scale 1: 5000 and spatial resolution of the pixel of 0.25 cm. As there is no direct equivalence between the USGS and IBGE classification, the equivalence of IBGE was adopted first with the MODIS system (Globion 2015) and then USGS.

Table 1: Grouping of USGS categories of land use and coverage and approximate equivalence for the MODIS-IBGP system (Liang et al., 2005) and equivalence with the classes used by the Brazilian system (GLOBION, 2015).

Classe - USGS	Classe - IGBP	Classe - Brasil  Extração mineral, área edi- ficada, estradas  Pastagem				
<ol> <li>Urben and Built-up Land</li> </ol>	Urban and Built-up					
<ol> <li>Dryland Cropland and Pasture</li> </ol>	Croplands					
<ol> <li>Cropland/Grassland Mosaic</li> </ol>	Croplands or Grasslands	Cultivo agrícola				
8. Shrubland	Closed Shrublands	Campo rupestre, macega				
<ol> <li>Decidnous Broadleaf</li> <li>Forest</li> </ol>	Deciclious Broadless For- rest	Restinga				
<ol> <li>Deciduous Needleleaf</li> <li>Forest</li> </ol>	Deciduous Needleleaf Fo- rest	Refigrestamento - Serin-				
<ol> <li>Evergreen Needlelenf</li> <li>Forest</li> </ol>	Evergreen Needlehaf Fo- rest	Reflorestamento - euca- lipto - pinos				
15. Mixed Forest	Mixed Forest	Mata nativa				
16. Water Bodies	Water Bodies	Massa de água				
17. Herbaceous Wetland	Permanent Wetlands	Brejo				
<ol> <li>Burren or Sparsely Vegetated</li> </ol>	Barren or Sparsely Vegeta- ted	Solo exposto, afforamento rochaso				

The geographic data generated is exported in ASCII format, preserving the characteristics of each image.

Observational nudging within the WRF is done using the OBSGRID program which uses input data from the METGRID outputs and surface observations' data with temporal logging every 3 hours.

As seen in Table 02 the general specifications for the rounds, WRF version 3.6.1 was used, reanalysis data obtained from the NCEP-FNL model with frequency intervals every six hours with approximate horizontal resolution of 0.5 degrees by 0.5 degrees (Latitude x longitude) with vertical resolution 27 levels ranging from 1000 to 0.27 hPa, differently separated according to the proximity to ground level (NCEP 2003). The Nudging Coefficients used are: G = 6E-4 s<sup>-1</sup>, radius = 180 km time step of 40 minutes.

Table-02: General specifications for the rounds.

Parâmetro	Domínio d01	Domínio D02				
	Geográfico					
Pixeis em "x"	49	121				
Pixeis em "y"	49	121				
Niveis verticais	21	21				
Espaço em m	5000	1000				
	Fisicn					
Microfisica	Single-moment 3-class	Single-moment 3-class				
Radiação	Dudhia Scheme	Dudhia Scheme				
Camada superficial	Monin Obukhov Scheme	Monin Obukhov Scheme				
Superficie terrestre	Noah land-surface model	Noah land-surface model				
CLA	Bougeault-Lacarrere Scheme	Bougeault-Lacarrere Scheme				
Cúmulos	Betts-Miller-Janjic scheme	Sem parametrização				

The statistical analysis will be performed based on the indicators suggested by (Emery et al., 2001), to make a more sensitive and comprehensive analysis of the modeling results will be used the Benchmarks. These are based on several studies that point out that it is difficult to reach these indicators (Borge 2008, Zhang 2014, Reboredo 2014), even Emery et. Al., (2001), mainly for the direction of the wind.



In order to illustrate the effect of relief and land use updates, the 10/07/2010 was selected randomly.

The changes between the simulations for the RMGV can be better observed, which shows the average, minimum and maximum wind velocity at the position of the monitoring stations.

Figure 2: Metric performance for all stations for wind speed on the right and wind direction on the right, standard USGS round.

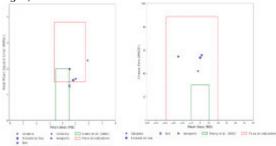
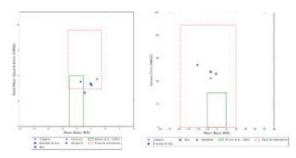


Figure 3: Metric performance for all seasons for wind speed on the right and wind direction on the right, rotated with the influence of nudging.



It can be observed that the results are quite similar, with few distinctions, as seen in Figures 2 and 3. It can be seen that all results are quite similar, with a single marked difference that the highest MAGE value without the Use of nudging. In general, there was little improvement in the indicators, as in the comparison with data from the Suá Inlet where the simulation with the use of nudging was within the dashed range in comparison to the other simulations.

Figure 4: Wind chamber at 2m for domain d02 at 12:00 hours, for the standard USGS modeling.

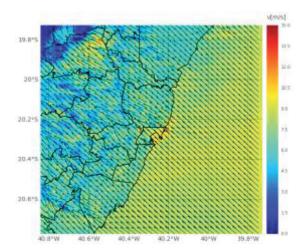
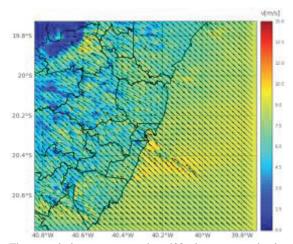


Figure 5: Wind camp at 2m for domain d02 to 12:00 hours, for modeling with the influence of nudging.



The wind directions to the d02 domain, with the influence of nudging, improves the modeling, showing the influence of this in the mountainous part of the state (North - West). Decreasing overestimates and adjusting slightly the wind direction. The accumulated monthly rainfall for the year 2010, March is the month with the highest accumulated rainfall and January the lowest. When modeling is influenced by the assimilation of data in addition to the use of IBGE data it increases the estimation of precipitation, being the least predicted when the influence of nudging is used.

#### **CONCLUSIONS**

The objective of this work was to update the specification data of the soil use and cover, evaluating the influence of these parameters on the WRF simulation on the RGMV. The results



obtained indicate an improvement in the statistical indicators, especially for the airport station, which is the most suitable for measuring the meteorological variables of the region, the only one that is in accordance with the guidelines of the World Meteorological Organization and has no building or High vegetation in the immediate vicinity. The other stations are included in the urban network, with proximity to buildings and high vegetation (trees). In general, the best results were obtained with the use of nudging for d02.

Future Work specific to the RMGV, evaluate the performance of topographic parameterization, perform the assimilation of radio probing data or satellite measurement campaigns reports, use alternative methods to perform nudging (grid-nudging and spectral-nudging).

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# Session 9 Air Quality Measurements and Observational Studies



#### AIR QUALITY MONITORING AND DATA AVAILABILITY IN BRAZIL

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Abstract: The air pollution has been one of the most important causes for human diseases, affecting mainly elderly and children. Many studies has been focusing the relation between air quality and respiratory problems, and althouth the negatives effects are already proved, air quality is not faced as an important problem to be solved in many countries. In Brazil, the air quality monitoring is under responsability of the government of each state. Due to several points regarding the air quality management, from the 26 states, only 10 can perform the monitoring. Taking into account, and with the target of better inform the population, to assit the policy maker and provide data for research, the Institute of Energy and Environment, in collaboration with the States Environment Agencies and, has been working to make the air quality data be more easily accessed. On an online platform (<a href="www.qualidadedoar.org.br">www.qualidadedoar.org.br</a>), all official air quality data of the country are presented in interactive graphics, where anyone can compare different air quality moniroting stations and observing the variation over the years. Furthermore, it is important to point out that the data are available for download. Considering the importance of the air quality, the next step of the plataform is providing hourly data.

**Keywords:** air quality monitoring, data availability, air pollution

#### INTRODUCTION

Exposure to air pollution is the cause of many injuries to human health, very often associated to aggravation of respiratory, cardiovascular and neurological dieses, it affects mainly children and elderly (Bravo et al, 2016; Segalin et al, 2016; Conceição et al, 2001). Lin et al (1999) identified an increase of 20% in emergency room visits for children associated to respiratory diseases, coinciding with high pollution episodes in the Metropolitan Area of Sao Paulo. Regarding the effect on elderly, Pinheiro et al (2014), in a 10-years analysis showed that an increase of 10  $\mu g/m^3$  can lead to an increase in the relative risk of death related to respiratory disease.

Even considering that air pollution has an important impact on human health, Brazil still has been facing the challenge of monitoring the air quality. Due to several national management issues, only 9 states perform the air quality monitoring, see Figure 1. Furthermore, most of them also face difficulties on publishing their data and even the diagnostic of their monitoring network.

Considering this scenario, in an effort with the State Environmental Agencies, the Institute of Energy and Environment (a Brazilian nonprofit Organization located in São Paulo) compiled the first document entitled: "The 1st Air Quality Monitoring in Brazil" (IEMA, 2014, in Portuguese). The main objective of this work was organizing and disseminate information about the configurations of the monitoring networks in operation, under direct or indirect management responsibility by the public authority, as well as the data generated by it. In 2015, this document was adapted to an online

platform filling a national-scale environmental information gap.

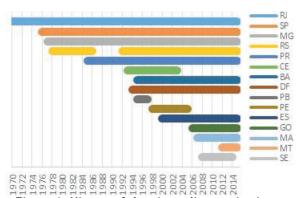


Figure 1. History of the air quality monitoring networks operated by the National Environmental Agencies.

#### **METHODS**

The first effort of this initiative focused on the identification of which states was performing the air quality monitoring and how they publish such information (format, content, level of detail, etc). After then, only states with representative data (regarding the time and spatial series), also the ones only with private network stations. This part of the work showed that not all the relevant information was available on the medias used on the research (internet, reports, etc). Therefore, a new effort started: the direct engagement with the State Environmental Agencies. This partnership corroborated to the published data validation by the own agencies, such as correcting data already



published, also incorporating data series not published yet.

Currently, the divulgation of the environmental agencies data is consolidated on the air quality platform (www.qualidadedoar.org.br).

#### FINDINGS AND ARGUMENT

IEMA provides all official air quality data available from Environmental Agencies on its platform, given the station location, year and pollutant, as shown on Figure 2.

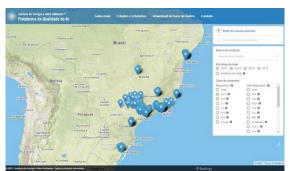


Figure 2. Location of all the air quality stations (environmental agencies) in Brazil and their respective time series and pollutant.

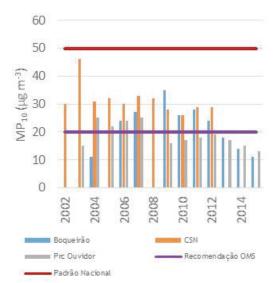


Figure 3. PM<sub>10</sub> time variation over 2002 to 2015 for three different station in Parana state.

One of the products available is the interactive graphics that the user can choose a pollutant an analyse its variation over the time, selecting as different stations. An example is presented on Figure 3 for the annual arithmetic mean of particulate matter 10  $\mu m$  (PM10) from 2002 until 2015 for three different stations from Parana state. The National air quality standard and the standard recommended by the Wolrd Health Organization

andare also presented on the graphics. Besides providing the means, the graphic options has the number of exceending air quality standards for the same time series. Furthermore, the series of historycal data is also available for download on the same website.

It is important to point out that different from the Environmental Agency of Sao Paulo State, which has an online platform for its data wit also interative graphics for user, the other states does not have it, for different reasons regarding management. This difficulties encoraged IEMA to help the other states on publishing their data in an accessible way for the public.

#### **CONCLUSIONS**

The monitoring air quality network just covers some areas of a few Brazilian States, and it performance over the time is very often compromised due to the difficulties on keeping the maintenance of equipment or even missing qualified staff. This is one of the consequences of the low priority given to environmental-urban policies and what affects the air quality management. Furthermore, other challenge faced by the most Environmental Agencies is the communication of the data produced, mainly on making them available online and even on publishing analytical air quality report Considering this scenario, IEMA has been working not only in collaboration with the Environmental Agencies, but also supporting them to publish their work to all kind of public. In this effort, focusing on provide more detailed information about air quality, the next step for the platform is to provide the hourly data for all monitoring air quality station in Brazil.

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#### VERTICAL PROFILES OF PM2.5 AND BC IN BOGOTÁ

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This research explores vertical profiles of fine particulate and black carbon of the lower atmosphere in Bogota, Colombia. We used low cost sensors and a tethered metrological balloon to obtain high time resolution measurements up to 300 m in height of fine particulate, black carbon, temperature and relative humidity at several sites in the city at 7 00 am. Data was processed to correct black carbon measurements for the loading effect and reduce noise in all measurements. Later, we compared said measurements with values obtained from simulations done using Bogotá's air quality modeling system based on CMAQ. Preliminary measurements show concentrations up to 15 µg/m3 and 110 µg/m3 of BC and PM2.5 respectively as high as 300 m.



## Correlation study between air quality data and the Lidar system in Cubatao, Sao Paulo

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Abstract: We present here the results of two methods with a scanning multiwavelength elastic lidar system and Beta Ray method (CETESB) realized in an industrial area. The objective is a comparer of these two methods to identify fixed sources of aerosol and to monitor plume dispersion. The results of the two aligned techniques indicate that can provide information on the concentration, spatial and temporal distribution of aerosol.

Keywords: LIDAR, Remote Sensing, Pollutants, Aerosol, PM10.

#### INTRODUCTION

Cubatao is a city located in state of Sao Paulo, Brazil. It is placed on a narrow costalplain surrounded by mountains on south, west, east and by the sea to the south. The region hold one of the oldest and largest industrial complex of Brazil. Because there was no guidance plan for the installation of industrial, industry sites have been established in the Serra do Mar State Park. Due to the local topography and proximity of the ocean, wind direction and velocity show daily changes that affect air quality, and frequent events of high pollutants concentration in the industrial area are recorded.

A significant number of events of high levels of pollutants, are recorded by the local authority (CETESB), which operates 2 air quality monitoring stations in the industrial area.

#### **METHODS**

It was used for the present work a three wavelength elastic backscatter system operated with a Nd: YAG laser (CFR 450, Quantel SA) at 355 nm, 532 nm and 1064 nm, transmitting pulses of  $7 \pm 2$  ns of duration at A fixed repetition rate of 20 Hz and a divergence less than 0.3 mrad. The system also has a receiver used to collect backscattered laser light, a 150 mm diameter Dall-Kirkham telescope with an effective focal length of 1000 mm.

For the construction of a comparison line, data were also used from the QUALAR - State System of Information on Air Quality of CETESB, through which data on pollutants are available throughout the state territory by manual and automatic networks, these are available in Different formats. In the case of this work, among all the pollutants monitored by

CETESB were selected: NOX, O3, MP10 to make an analogy with the LIDAR system.

The data extracted from the automatic networks of the QUALAR system are time data of the date of the campaign.

#### FINDINGS AND ARGUMENT

A campaign was conducted for data collection in August 2016 in the city of Cubatão / SP. The collection site was close to a CETESB station (LAT 23° 51 '08.06s - LON 46°23'26.40s) and the purpose was to monitor the spatial and temporal distribution of the aerosols in the region and to correlate these results with pollutant graphs (PM $_{10}$ , NO $_{x}$  and O $_{3}$ ) obtained by CETESB's QUALAR System from a stations located ~ 2km and 4km from where the LIDAR system was installed.

The stations of the CETESB that were used are the stations Centro and Vale do Mogi.

The data demonstrate a considerable amount of particulate matter in the study region. In figure 1A, we have a graphical representation of the backscatter of the particles with wavelength of 355 nm, we noticed a moderate concentration of aerosols. In Fig. 1B, with a wavelength of 532 nm, in it can be considered as a larger grouping of particles, which occurs in the case that the larger the wavelength is larger than its backscatter. In figure 1C we work with the wavelength of 1064 nm, we observe a greater agglomeration of aerosols, which indicates a greater occurrence of aerosols of large particles. The as an overlay (georeferencing) of the LIDAR graphics on the image of the area in google earth (figure 1A, 1B and 1C)



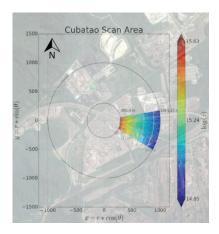


Figure 1A: Plot of 355 nm Google earth V 7.1.8.3036. (January 26, 2017). Cubatao, Brazil. 23°50'57.71"S, 46°23'19.80"W, Eye alt 6.24 km. Digital Globe 2016.

http://www.earth.google.com [January 17, 2017].

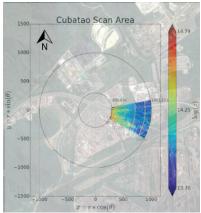


Figure 1B: Plot of 532 nm

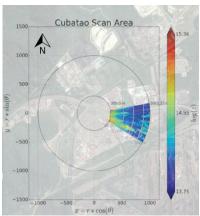


Figure 1A: Plot of 1064 nm

Figures 2A and 2B are taken from QUALAR and show concentrations of  $NO_x$  and  $O_3$  (Figure 2A) and  $MP_{10}$  and  $O_3$  (Figure 2B) on the campaign day in Cubatão.

Figure 2A shows that on the day of the data collection CETESB station - Vale do Mogi - recorded its highest peak around 14h (Brasília time), at this time this increase of Ozone maybe due to the greater amount of atoms of free Nitrogen and also by the high influence of the solar rays. Figure 2B shows the concentrations of  $NO_x$  and  $PM_{10}$ , it is noticeable that there is a symmetry between the data obtained, because when there is an increase of  $NO_x$  the concentrations of  $MP_{10}$  are high.

The high concentrations of  $NO_x$ , could be related to the fertilizer plant that is in the campaign area, once fertilizer manufacturing processes can generate emission sources of atmospheric effluents such as loading and feeding of raw material; The reactor; The granulation, drying and curing of the products. These sources emit pollutants such as particulatematter (PM),  $SO_x$ ,  $NO_x$ ,  $NO_x$ ,  $NO_x$ , and  $NO_x$  HF. [2]

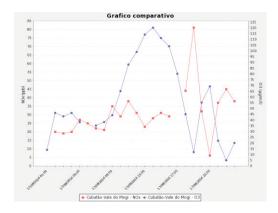


Figure 2A: CETESB station - Vale do Mogi.Comparative chart  $NO_{\rm x}$  and  $O_{\rm 3}$ . Hourly data 08-17-2016.

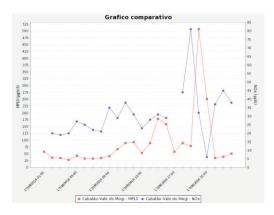


Figure 2B:CETESB station - Vale do Mogi.Comparative chart  $MP_{10}$ and $NO_x$ . Hourly data 08-17-2016.



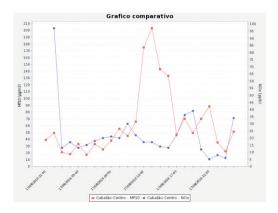


Figure 2C :CETESB station - Centro.Comparative chart  $PM_{10}$  and  $NO_x$ . Hourly data 08-17-2016.

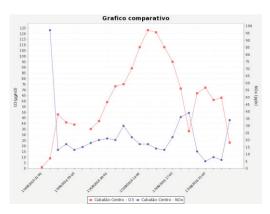


Figure 2D: CETESB station - Centro. Comparative chart O₃andNO<sub>x</sub>. Hourly data 08-17-2016.

Figure 2C shows the relationship between NOx and PM10, although it follows a similarity to that of the Vale do Mogi, there are some factors that may interfere with the PM10, such as the high circulation of cars. Figure 2D shows a relationship between ozone and NOx different from that expected, because NOx is one of the major precursors of tropospheric ozone, if its concentration decreases the ozone should follow the same trend.

#### **CONCLUSIONS**

The results obtained by the Lidar system indicate that the region studied has a high concentration of aerosols, as expected, since it is an industrial area with a high flow of vehicles.

Comparing these data with those of CETESB automatic stations, we believe that there is a high probability of the presence of larger particulates, starting at 10um.

The incompatibilities of the data with the theory show that there is a great possibility of transport and confinement of aerosols in the region.

New campaigns will be carried out to optimize the results obtained in the present study.

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## AIR QUALITY ASSESSMENT AND DESIGN OF THE MONITORING NETWORK OF CONGONHAS, MG, BRAZIL

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Abstract: In order to fill knowledge gaps about air quality and meteorological conditions in the Congonhas, MG, Brazil, an intensive air quality study was performed, including the characterization of the study area, assimilation and analysis of meteorological data, using surface data analysis and WRF modeling, conducting the atmospheric emissions inventory and applying the CMAQ model for the calculation of atmospheric concentrations of pollutants. Regarding the results of CMAQ, particulate matter (PM) were identified as a most relevant impact. The major emissions of PM are provenient from open pit iron ore minings, industrial emissions and resuspension of particles from the paved roads, in urban centers. With the collection of information produced, Congonhas Air Quality Network was designed, consisting of 16 stations that will provide continuous monitoring of the air quality and meteorological conditions.

Keywords: air quality, monitoring, network design, modelling, emission inventory.

#### INTRODUCTION

Congonhas city is located in Minas Gerais state, which among other attributes presents an important historical and artistic heritage, including the Sanctuary of Bom Jesus de Matosinhos, a world cultural heritage (UNESCO, 2017). The region of Congonhas has an important iron ore mining and steelworks park, which has significant sources of air pollutants, interspersed by urban centers such as Conselheiro Lafaiete, Ouro Branco and the city of Congonhas, which also generate atmospheric pollutants.

These features make the urban areas of this region more susceptible to significant changes in air quality. There are frequent manifestations of the Congonhas inhabitants regarding the occurrence of air pollution events, especially in the city of Congonhas. In addition, there are occurrences of acute episodes of air pollution by particulate matter (visible dust cloud). The study area does not have systematic monitoring of air quality, with adequate coverage and able to inform, with accuracy, the levels of pollutants to which resident communities are exposed.

Regarding this lack of information about air quality in Congonhas, the Ministério Público de Minas Gerais (MPMG), in partnership with Ferrous Resources do Brasil, requested the present study, in order to: diagnose air quality in the Congonhas region, recognize the main sources of air pollutants and their contributions to air quality changes, and finally to develop an optimized air quality monitoring network project.

This project was supported by MPMG, Secretaria de Meio Ambiente de Congonhas, Fundação Estadual do Meio Ambiente (FEAM) and companies located in the study area.

#### **METHODS**

The study area (60x60 km, LL = 586861, 7706243; UR = 647715, 7765901, 23K, WGS84) was characterized as a computational domain subdivided in cells of 1 km. Figure 1 shows the delimitation of the study area for the air quality monitoring network design and the computational domains used for the WRF (Skamarock et al, 2008) and CMAQ (Byun and Ching, 1999) models.

The detailed inventory of atmospheric emissions was produced using the techniques recommended by the USEPA (2017) covering different types of emission sources, including industries (mining and steel making), urban emissions (vehicular traffic, residencial and commercial), natural sources and wildfires. The inventory considered information from the issuing sources according to their emission and production conditions for the year 2011. Emission rates of  $PM_{10},\,SO_2,\,CO,\,NO_x$  and VOC were assimiled by EcoSoft Atmos application database (Santolim et al., 2010). Natural emissions were calculated using the MEGAN model (Guenter, et al., 2006). Wildfires were evaluated using data available in INPE (2011) database.

Physical and meteorological conditions that occur in the Congonhas were studied to provide adequate support for computation of the emissions inventory,



as well as the pollutants dispersion analysis. In addition, WRF model was applied to analyze the historical data of available meteorological measurements.

The WRF simulations were driven by GFS data with 1° spatial resolution and 6h 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. Average concentrations obtained in Congonhas were used for initial conditions (ICONs) and boundary conditions (BCONs) for the inner domain.

The simulation considers the entire year of 2009, hourly. Calculated air concentrations were used to evaluate the potential air quality impacts on the study area and as input to the algorithm of Figures of Merit and Spheres of Influence used for the air quality monitoring network design.

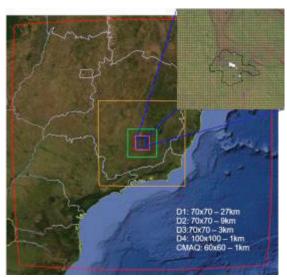


Figure 1. - Modelling domais for WRF and CMAQ

CMAQ was also used to assign the responsibilities of the emitting sources to the  $PM_{10}$  concentrations in environment. The contribution of each emitting sources group to the air quality changes was estimated based on the concentrations of  $PM_{10}$  calculated by the CMAQ. Contributions of the main groups of pollutant sources in relation to air quality were calculated for different sectors of the study area. In this way, it was possible to analyze the synergistic impacts of the emission sources and the contribution portion by company or group of sources, allowing the generation of a ranking of responsibilities for the alteration of air quality by sectors of interest.

From the results generated by the modeling carried out, the Air Quality Monitoring Network of Congonhas Region (AQMN) was designed. In this process, the most frequently affected areas and associated to the sites with the greatest interest in monitoring were defined, generating the Figures of Merit (FOM). For each candidate site to host an air quality monitoring station, the Influence Spheres (SOI) were generated, and these represent the predefined coverage efficiency for the measurement network (Santolim, 1991).

#### FINDINGS AND ARGUMENT

As described by the emission rates of pollutants (Table 1), the most relevant amounts of pollutants are emitted by the industries. However, it should be noted that in specific cases small-scale emitters can significantly alter the air quality of their immediate vicinity. In Congonhas, urban paved roads present very high silt content, due to deposition of materials brought by vehicles that travel on unpaved roads, mainly in mining operations (Congonhas, 2011).

The results obtained with CMAQ application corroborate with the environmental perception of the population. In general, the air quality of the study area is altered by particles and the calculated concentrations indicate even the potential extrapolation of the air quality standards established by CONAMA 03/1990, Federal Rule (Figure 2) in specific areas of the study area. In general, these sites are located in the immediate surroundings of the main sources of air pollutants.

It is identified that the major contributions to air quality change are the industrial activities of the region, with main focus on unpaved traffic ways and areas subject to PM wind erosion inside iron ore mines. The urban roads exert strong influence on the air quality change, reaching the main receivers considered in this study due to their proximity. Notably, PM emissions in urban roads come from the process of resuspension of particles deposited on road surfaces.

AQMN was designed considering the use of proper number of monitors and stations needed to provide adequate space coverage of priority areas for monitoring (Figure 3).

Table 1. Emission rates of air pollutants, 2011, g/s, in brackets the proportions of each group

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Emissions Group	PM <sub>10</sub>	SO <sub>2</sub>	NO <sub>X</sub>	СО	COV
Industrial	468.4	478.8	468.9	3121.8	137.4
	(92.9%)	(99.9%)	(97.3%)	(98.0%)	(78.7%)
Urban	34.7	0.4	12.5	55.8	36.4
	(6.9%)	(0.1%)	(2.6%)	(1.8%)	(20.9%)
Wildfire	1.0	0.1	0.3	9.4	0.7
	(0.2%)	(0.0%)	(0.1%)	(0.1%)	(0.4%)
Total	504,1	479,3	481,7	3187,0	174,5



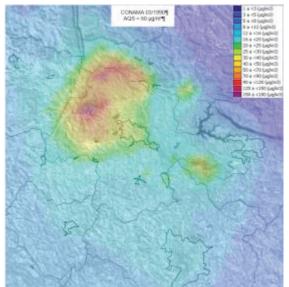


Figure 2. Annual averages of PM<sub>10</sub>

According to the technique applied, the monitoring network is optimized by undertaking the minimum resources necessary for adequate monitoring at study area, rationalizing the way of applying them, maximizing the spatial monitoring coverage.

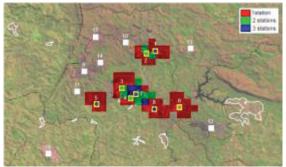


Figure 3. Location of Stations and PM<sub>10</sub> Spheres of Influence - Congonhas AQN

The AQMN project will integrate 8 air quality stations in addition to the meteorological stations associated with the main industrial developments in the region (Table 2).

Station	TSP	PM <sub>10</sub>	CO	HC	NO <sub>x</sub>	SO <sub>2</sub>	03	BTX	WD	WS	RN	AP	SR	AT	RH
1. Pires	Х	Х							Х	Х	Х	Χ	Х	Х	X
2. Motas	Х	Х													
<ol><li>Casa de Pedra</li></ol>	Х	Х							Х	Х					
4. Basílica	Х	Х			X	Х	Χ		Х	Х					
<ol><li>Plataforma</li></ol>	Х	Х													
6. Lobo Leite	Х	Х	Х	Х	X	Х	Χ	Х	Х	Х				Х	
7. Matriz	Х	Х													
8. Jardim Profeta	Х	Х													
9. MetWNW									X	Х	Х	Χ	Х	Х	Х
10. MetN									X	Х	Х	Χ	Х	Х	Х
11. Viga									Х	X	Х	Х	Х	Х	Х
12. Ouro Branco									Х	Х	Х	Χ	Х	Х	Х
<ol> <li>Miguel Burnier</li> </ol>									Х	Х	Х	Χ	Х	Х	Х
14. Engenho									Х	Х	Х	Χ	Χ	Х	Х
15. Fábrica									X	X	Χ	Х	Х	Χ	Х
16. Jeceaba									X	Х	Х	Х	Х	X	Х

#### **CONCLUSIONS**

The activities in Congonhas region (industries and urban areas) pressures the air resource. The characterization of emitting sources in the region, the assimilation of meteorological data and the simulation of air quality were very important to fill lacks of information about the air quality in the region. The AQMN as designed, will provide uninterrupted monitoring of air quality and meteorological conditions of the region, and can generate indicators to evaluate the performance of implemented air quality control plans, supporting decision makers.

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## METHODOLOGICAL PROPOSAL: EVALUATION OF BIOMASS BURNING CONTRIBUTION TO ATMOSPHERIC POLLUTION IN THE URBAN AREA OF MANAUS

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Abstract: Manaus city, located in Central Amazon region, is an important study area for analyze and understand of the impact of biomass burning on air quality and local population health in relation to particulate matter <2.5µm (PM2.5) and volatile organic compounds (VOCs), once Amazon region is passing through intense process of change of land use associated mainly to biomass burning. Here, a methodological proposal is presented to evaluate the sazonality of biomass burning tracers in urban air of Manaus in one year (June-2017 to June-2018). The focus is the organic compounds in PM2.5 and VOCs associating them with possible regions that they come from. Analyzes will be carried out in gas chromatography with derivatization technique, identification of compounds signatures and analysis of dispersion and trajectory of particles with modeling. Therefore, we seek to understand the impact of biomass burning from different regions in air quality in Manaus during one year, assisting in public policy decision making of air quality management for the prevention, combat and reduction of pollutant emissions.

Keywords: Amazon, WRF-Chem, HYSPLIT, principal components, backtrajectories.

#### **INTRODUCTION**

In Amazon, the adoption of economic policies to meet the growing demand for the use of natural resources, fossil fuels, expansion and intensification of the agricultural for food production has been intensifying the process of land use change and contributing to air pollution. Considering the magnitude of deforestation associated with biomass burning and the efficiency of atmospheric transport processes, the Amazon region annually contributes with emissions of large amounts of pollutants as carbon moxide (CO), volatile organic compounds (COVs), particulate matter (PM<2.5µm), between others compoundsto atmosphere, impacting in air quality and affecting the health of the population living in the region (Longo et al., 2010, Martin et al., 2010, Artaxo et al., 2013).

Studies in Amazon region show that biomass burning impacts on interannual variability of greenhouse gases, particulate matter, volatile organic compounds (locally and at long distances from the far region) and also show that there is an increase in ambulatory care for respiratory diseases in some cities of the region (for example,

Manaus) associated with exposure to MP2.5 and VOCs from biomass burning. (Artaxo et al., 2013, Alves et al., 2015, Andrade et al., 2017). Recently, in dry period of 2015 and 2016 due to the strong El Niño event, in terms of number of fires in the Amazon and smoke pollution, it was one of the most serious episodes in the history observed in Manaus, according to Data from the National Institute for Space Research (INPE).

In Manaus, unlike other cities such as São Paulo, continuous monitoring of pollutant gases, VOCs and PM2.5 on the surface are scarce, and measurements are only taken from sporadic campaigns aided by aircraft, like the campaigns Amazon Boundary Layer Experiment (ABLE-2 1985/87), Tropical Forest and Fire Emissions Experiment (TROFFEE 2004) and Green Ocean Amazon (GoAmazon 2014/15) (see Martin et al., 2010). In this context, few studies have evaluated the contribution of biomass burning in the variability of these pollutants in the atmosphere of Manaus urban area at different seasons of the year.

Therefore, the present study show the methodological proposal that will be applicate to



understand the impact of biomass burning of different regions in air quality of Manaus in one year (June-2017 to June 2018), with focus in the biomass burning tracers in PM2.5 and VOCs. The results of this project will be useful as a basis information that will help in public policies for the city's air quality management.

#### **METHODS**

Following are the steps of sampling, chemical analysis, statistical analysis, trajectory and dispersion particle modeling.

<u>Samplings:</u> The sampling of VOCs, MP2.5 and CO will be carried out in the urban area of Manaus, at the Superior School of Technology of the State University of Amazonas (EST-UEA) (3rd 5'32 "S and 60°1'4" W ). The sampling period will be from June 2017 to June 2018, monday to friday, every 12 hours, with a total of 240 samples.

PM2.5: The High Volume sampler for PM2.5 will be used, with a flow rate of 1.13 m³.min⁻¹ with less than 1% deviation in 24 hours. Quartz filters will be used from Pall Corporation model Tissuquartz ™ Filters 2500 QAT-UP 7204 with 99.9% particle retention. Prior to field sampling, the quartz filters will be preheated to 550°C for 12 hours. Every 10 field samples will be made 1 field blank. Analysis of PM2.5 samples will be performed using gas chromatography with flame ionization detector and mass spectrometry (GC-FID-MS), associated with the derivatization technique and based on the method described by Surrat et al. (2010).

**VOCs:** Compact and portable sampler with a constant flow pump (100 mL.min<sup>-1</sup>) will be used with thermal desorption tubes having as adsorbent material the Tenax TA Carbograph 5TD and that are specifically for applications of tracking of volatile organic compounds and semi-volatiles from the air, being a hydrophobic material suitable for sampling under humid conditions. The analysis of VOC samples will be performed using gas chromatography techniques with flame ionization detector and mass spectrometer (GC-FID-MS) in the Agilent 7890B equipment.

CO: Carbon monoxide data will be obtained from the airpointer® air quality station which has continuous monitoring every 1 minute. The station follows the methodology recommended by the US Environmental Protection Agency (EPA). It uses, for the quantification of carbon monoxide, the principle of measurement Non Dispersive InfraRed and Gas Filter Correlation, with a minimum limit of detection of 0.04 ppm, accuracy of ± 0.1 ppm and sample flow rate of 500 mL.min

<u>data:</u> Biomass burning and <u>meteorological</u>
Biomass burning data will come from the
Burned Program of the National Institute of Space
Research (INPE), which continuously monitors fires

in Brazil through satellite measurements every three hours, every day of the year. A spatial analysis of the daily biomass burning data will be performed using the Kernel technique that is based on methods of interpolation in relation to the distance of each event in order to identify the point intensity (frequency) of the number of fires in the region. The meteorological data (air temperature, precipitation, relative humidity, solar radiation, wind speed and direction) will be from the automatic meteorological stations of the Climate Change Network of the Amazon - REMCLAM that cover the entire city of Manaus. The data is generated continuously with a time resolution of 5 minutes.

Statistical analysis: In the first step, descriptive statistical analyze (mean, standard deviation, variance and boxplot) will be used to evaluate the distribution and variability of the data in different time scales, allowing to describe and understand the central tendency, dispersion and distribution of the concentration of biomass burning tracers and the meteorological variables. In the second step, the influence of fires and meteorological variables on the concentrations of biomass burning tracers in the atmosphere during the year will be evaluated. For this, the correlation analysis will be used, which shows the intensity of the relationship between the two studied variables. The third step will be to apply the principal component analysis (PCA) to identify the signatures of biomass burning tracers presents in the atmosphere throughout the year. This PCA analysis will help to identify the regions of origin and sources of organic compounds, in which groups of compounds with similar variabilities indicate common sources, similar formation or transport processes that are contributing to the measured concentrations.

<u>Trajectory and dispersion particle</u> <u>modeling:</u> Case studies of trajectories and dispersion will be carried out from simulations to help identify the origin regions of organic compounds biomass burning tracers groups in the different seasons of the year obtained in the PCA. The HYSPLIT NOAA model, an atmospheric transport and dispersion models most used in the atmospheric sciences, with input data of the Global Data Assimilation System (GDAS), with 0.5° spatial resolution (Stein et al., 2015).

Associated with the HYSPLIT model, dispersion simulations will be carried out using the Weather Research and Forecasting model coupled with the chemical module (WRF-Chem version 3.6.1) and the Brazilian Biomass Burning Emission biomass emission model (3BEM) (Grell et al., 2005, Longo et al., 2010). The simulations for the study period will allow the evaluation of pollutants dispersion from long-distance burnings in a near real situation in the atmosphere, since it relates both physical and chemical processes. The physical



parameters and the initial boundary conditions of the chemical compounds of the model will be based in the study of Medeiros et al. (2017). The simulations will be defined for three domains: domain 1 with resolution of 27km covering all regions of Brazil; domain 2, with a resolution of 9 km, covering the Legal Amazon and the northeast region of Brazil; domain 3, with resolution of 3 km, covering the metropolitan region of Manaus (MRM). The meteorological input data of the model for the study period will be obtained Climate Forecast System Reanalysis of the National Center for Environmental Prediction (NCEP) with spatial resolution of 0.5° and temporal resolution of 6 hours

#### FINDINGS AND ARGUMENT

- It is expected that there will be a seasonal variability of the biomass burning tracers. In the dry period (July to November), due to intense biomass burning activity in the Amazon associated with the prevailing winds of east and northeast, higher concentrations are expected with a high contribution of biomass burning in MRM and from long distances (Brazilian east and southern region of the north and northeast region) on PM2.5 and VOCs in the urban area of Manaus. On the other hand, in the rainy season smaller concentrations are expected due to the reactions with hydroxyl radicals, wet deposition, lower number of fires, less contribution of the MRM fires emissions and predominance of the contribution from long distances due to the seasonal biomass burning;
- Understand the correlation of the variability of the biomass burning tracers with the meteorological variables and carbon monoxide;
- Identify the signatures of biomass burning tracers (levoglucosan and others) that occur in the study period, through clustering analysis, characterizing them for the different regions of origin associated with the backtrajectories and dispersion analysis;

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# AVALIATION OF CONCENTRATION, SIZE DISTRIBUTION AND CHEMICAL CHARACTERISTICS OF FINE ATMOSPHERIC PARTICULATE MATTER IN THE CENTRAL REGION OF THE STATE OF SÃO PAULO

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Abstract: This study presents physical and chemical analysis of particulate matter (PM) smaller than 2.5 μm presented in Araraquara city atmospheric air. Evidenced the relation between the fires places, air trajectory, concentration, size distribution and chemical analysis of particulate matter sampled by a cascade impactor and an optical monitor. The ionic composition of the particulate matter was analyzed for different particles size. The chemical and physical characterization of the pollutant sampled, evidence the harmful effects to health and climate relate to the increase of biomass burning in industrial processes as energy source.

Keywords: particulate matter, air pollution, chemical analysis, sampling, monitoring, sources.

#### INTRODUCTION

Currently Brazil is the largest producer of sugar cane (635 million tons) and is responsible for one third of the global harvest, with a planted area of 9,0 Mha in 2014/2015, 90% of the cultivated area are in the Mid-South region, with approximately 157 active sugar cane distilleries (CONAB, 2015). The growing demand of ethanol associated with a future projected expansion and the excess of sugar cane bagasse produced is used more often as a biofuel, cause concerns about the potencial of environment impacts in this region. The prospect of increasing use of bioenergy in many countries has brought international debate concerns about environment impacts, poverty, deforestation and biodiversity reduction, and health problems due to water quality and air pollution emission. (Moraes, M.A.F.D. et al. 2015).

According to França et al. (2012) is necessary to expand the scientific knowledge about the impacts of the growth of ethanol production in Brazil and generate inventory of Greenhouse gases and emission of aerosols associated with this activity. Whether biomass burning is in agricultural activities to facilitate harvest with the burning of the external leaves, or the burning of the sugar cane bagasse in industrial processes to generate energy and heat, is one of the most important sources of pollutant gases and particulates for atmosphere (Urban. R.C. et. at., 2016). The use of sugar cane bagasse as a biofuel in distilleries and industries intensified, and the emission from the

burning of this fuel extend to the local population, regional and global (Ibrahim Al-Naiema et al., 2015).

In order to evaluate such changes, characterization of particulate matter emissions has been and will continue to be studied to determinate its size distribution, concentration and its ionic composition (Oliveira, P.L. et al., 2013). Emitted particle from the burning of biomass has variegated composition, including organic, inorganic, as well elemental carbon. According to Oliveira, P.L. et al., (2013) the variation of size range of particulate matter is related with the different emission sources and its chemical composition. Considering the chemical processes that occurs in the atmosphere, in addition to combustion which favor the formation of fine particulate matter. As some of these elements may come from specific sources, knowledge of the particulate matter distribution combined with the concentration of these elements in the different size ranges is relevant because of the possibility of indicating sources and residence time in the atmosphere, in addition to being able to predict effects due to toxicity (Oliveira, P.L. et al., 2013).

The aim of this study was to evaluate the local atmosphere quality of an important agroindustrial region in the countryside of the State of São Paulo through the sampling of particulate pollutants, considering the number of fires places and the air mass trajectories. It was analyzed the



concentration, particulate matter size distribution and the composition of trace elements present in these pollutants, as well how the distribution of these elements as a function of the particulate size.

#### **METHODS**

The study was performed out in the city of Araraquara located in the central region of the State of São Paulo, Brazil. It is located at geographic coordinates 21°47′37"(South latitude) e 48°10′52" (West longitude). The particulate material sampling was conducted using optical monitor DataRam (DR4) and Impactador sampler of cascade of eight stages. For the comparative study distribution particle size concentrations of ions present in the samples were analyzed the filters of eight stages of the impactador corresponding to the fractional size distribution (0 to 10 µm). The solutions were submitted to chromatographic determination. The ionic species analyzed were: sodium (Na+), ammonium  $(NH_4^+)$ , potassium  $(K^+)$ , magnesium  $(Mg_2^+)$ , calcium  $(Ca_2^+)$ , fluoride  $(F^-)$ , acetate (H<sub>3</sub>CCOO), Formate (HCOO), chloride (Cl), nitrite  $(NO_2)$ , nitrate  $(NO_3)$ , phosphate  $(PO_4^2)$ , sulfate  $(C_2O_4^2).$  $(SO_4^{2-})$  and oxalate Ionic species concentrations were determined by ion exchange chromatography using the ion chromatograph Thermo Scientific ICS 5000.

#### FINDINGS AND ARGUMENT

Figure 1 shows the size distribution and composition of particulate matter sampled. The average particle size distribution was 0.1 to 0.4  $\mu$ m and reached minimum value 0.0473  $\mu$ m.

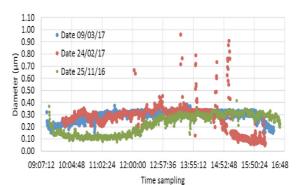


Figure 1 - Distribution of size of the particles

In the Figure 2 can be observed the particles concentration that was obtained with optical monitor (These datas were confirmed with cascate impactor). In this figure, its possible to confirm that high particles concentration are allocated in the low size diameter.

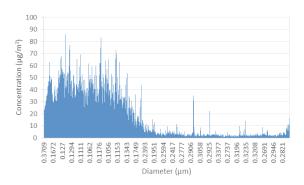


Figure 2 - Concentration of the particles

The Figure 3 shows the chemical analyses od particle colleted in filters. The presence of particles in this size range can have as a primary source to burning of biomass used as industrial fuel or even the open burning of biomass near the area sampled or both for transport of air masses of distant regions. The results of concentration and size distribution were obtained with the optical monitor and confirmed by the impactador, which have larger quantities of particles to the smallest diameter ranges in all sampling days.

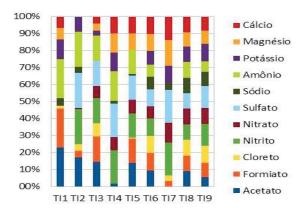


Figure 3 -Chemical Analysis present in the filters of different size of particle

The concentration reached values close to 90 µg/m3 with 0.085 µm diameter, with the largest concentration for diameters smaller than 0.1 µm. Evaluating the fire of burned (https://prodwwwqueimadas.dgi.inpe.br), the presence of sugar distilleries in the State (Unica2017) e trajectories of air masses (www.arl.noaa.gov/HYSPLIT) is possible pick up a relationship between the results with the emission sources. Evaluating the fire places in the central region and the State, it was found that a large number exist in the North and Northeast region in 02/2017.

In the 11/2016 period the greatest amount of fires places was in the Northeast and Northwest and Northeast regions 03/2017. The vast majority of



plants that use biomass as fuel are located in the Northwest, North and Northeast of the state. Evaluating the air mass trajectories in the period from 11/2016 these came from the Northeast regions, in 02/2017 from the North and Northeast region passing specifically by some distilleries and regions with large number of industries. To 03/2017 the masses of air from the Northeast region the same regions. From the analysis of anions present in the filters of different stages of impactador showed the highest concentrations of acetate, formate and ammonium to the larger particles TI1 (9-10 µm), Figure 1. A greater range of analytes for the smaller particles TI8 (0.4 - 0.7µm) and TI9 (0-0.4 µm). Nitrate, sulphate and potassium in stages with particles with diameter less than 1 µm. In the study of Souza, M.L. (2016) made in the same region reported that the nitrate and sulfate are important components of aerosols present in the region of study and related to the burning of sugarcane. The same influence was found for potassium, nitrate and sulfate in 0.4 µm size fraction. According to Souza (2016), the concentration of potassium measured on the day influenced by the biomass burning was about four times higher in comparison to the day that it was not affected by the burning, whereas the concentrations of nitrate and sulfate were about 2 Times on the impacted day.

#### **CONCLUSIONS**

The high particles concentration with diameter low that  $0.05 \mu m$  were observed in 25/11/16.

In the anions analysis were observed the higher analytes quantity in the low particles diameters. In the low diameters (below 1  $\mu m)$  were observed high anions concentration of Sulfate, Nitrite, Nitrate and Chlorate. For the cations observed high concentration of Sodium, Potassium and Magnesium.

These analyses are important to predict the possible source of emissions of the particle material and changes of chemical atmospheric.

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# HYDROCARBONS (C<sub>6</sub>-C<sub>11</sub>) CONCENTRATIONS AROND A PETROCHEMICAL COMPLEX OF THE GREATER ABC, SÃO PAULO, BRAZIL.

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Abstract: Hydrocarbons ( $C_6$ - $C_{11}$ ) are mainly composed of the exhaust of the engine of vehicles as well as of industrial processes and precursors in the photochemical process of tropospheric ozone formation ( $O_3$ ). The Region of the Greater ABC presents a singularity in addition to an important vehicular fleet also has a strong industrial character, with a presence of the Greater ABC Petrochemical Complex, in the division of the cities of Mauá and Santo André. This complex presents a peculiarity in relation to the others distributed by Brazil, with a single of a densely occupied residential and urban area. In Brazil, despite the knowledge about adverse health effects, there is no standard quality standard for HC. The objective of this work was to determine the concentrations of HC and evaluate the potentials of formation of  $O_3$  (OFP), from their concentrations, in an urban and industrial area. The emissions are quantified through the technique of gas chromatography with FID detector (Flame lonization Detector). This work contributes to the identification of the most significant HCs in the study area and contributes to the development of  $O_3$  in the region, identifying cis-2-hexene, m+p-xylene, toluene and 1,2,4-trimethylbenzene as the of higher concentration and main precursors of  $O_3$  in the area of the Petrochemical Complex.

Keywords: Hydrocarbons, Petrochemical Complex, Air quality, Ozone formation Potent

#### INTRODUCTION

Hydrocarbons (HCs) in the urban and industrial atmosphere mainly originate from motor vehicle exhausts and other combustion processes utilizing fossil fuels, petroleum storage and distribution, solvent usage and other industrial processes (Cetin et al., 2003).

Petroleum refineries and petrochemical plants are generally large industrial installations. Their operation is associated with the emission of various organic compounds into the atmosphere, mainly originating from the production processes, the storage tanks and the waste areas (Kalabokas et al., 2001). In urban and industrialized areas the benzene, toluene and xylenes constitute more than 60% of the Volatile Organic Compounds (VOC) (TIWARI et al., 2010). Despite the knowledge of the adverse effects of these compounds, there are no air quality standards defined for these compounds in Brazil to control emissions (Junqueira et al., 2005).

The region of Greater ABC is located in a strategic area for the development of studies of atmospheric pollution, due to its high degree of industrialization, urbanization and flow. However, there are still few studies on air pollution in the ABC region.

In this context, there is a need to better understand the emission sources and means of HC dispersion in the atmosphere. The objective of this work was to determine the concentrations of HC and to evaluate the potentials of formation of  $O_3$  (OFP), from their concentrations, in an urban and industrial area. In this way, the work will contribute to the understanding of which are the most relevant HCs in the study area and the contribution of local sources to the formation of  $O_3$ .

#### **METHODS**

#### 2.1. Study Area

Although it is part of the Metropolitan Region of São Paulo (MASP), the Region of Grande ABC has singularities, such as the industrial character, with the presence of the Petrochemical Complex, on the border of the counties of Santo André and Mauá. The Capuava Refinery (RECAP), and 14 other industries constitute this petrochemical complex. Also included in the region are important road traffic routes, such as State Avenue and Costa and Silva President Avenue, a link between the cities of Grande ABC (Mauá, Santo André and São Caetano do Sul) and different regions of São Paulo. The first avenue is located about 5 km northwest of Polo, with a flow of about 12,000 vehicles per hour, the second is located parallel to Capuava Petrochemical Complex (CPC) and Mário Covas Rodoanel, which is about 9 km from the Polo and contains heavy traffic of heavy vehicles.

#### 2.2. Sampling of Air

Air sampling for HC analysis was performed by TENAX TA tubes (polymer resin specifically designed



for the retention of volatile and semi-volatile compounds). The air inlet to the tubes is made with a vacuum pump, with a constant flow at low pressure.

Air samples were collected on August 19, 2016 every 1 hour, from 8:00 am to 6:00 pm, in two points after a post-frontal meteorological condition:

P1 - Federal University of ABC, which is located on States Avenue and is about 5 km from the petrochemical center in the northwest direction (Figure X);

P2 - Beneraldo de Toledo State School, located in the Capuava neighborhood, in Santo André, SP and is about 800 m from the front entrance of the petrochemical complex, located at Presidente Costa e Silva Avenue.

### 2.3.Analysis of hydrocarbons by gas chromatography

The samples are analyzed in the Laboratory of Analysis of Atmospheric Processes (LAPAT), at the IAG / USP, using the gas chromatography with FID detector. A Perkin Elmer chromatograph was used with two chromatographic columns and two flames ionization detectors (CG / FID model Clarus 500) coupled to a thermal desorption module. The dual system contains two FID detectors. The detector is a device that quantizes and the chromatographic column qualifies the components separated by it. In the FID detector the sample is burnt in a hydrogen flame, and an electric current is generated that is proportional to the concentration of the analytic, then the current passes through a signal converter and is recorded (DOMINUTTI et al., 2016). In this study the two analytical columns used is: PLOT (Porous Layer Open Tubular) column for the more volatile HC and BP-1 methyl silicone column for the less volatile HC.

#### FINDINGS AND ARGUMENT

#### 3.1. Concentrations of hydrocarbons

In this study, the concentrations for 37 HC were found, being 54% aromatic, 28% alkanes and 18% alkenes. In Figures 1 and 2, it is possible to observe the mean concentrations at each sampling time. The HCs with the highest P1 concentration were cis-2-hexene, 1,2,4-trimethylbenzene, cyclohexane and n-heptane; In P2 were for cis-2-hexene, 1,2,4-trimethylbenzene, cyclohexane and Methyl Cyclopentane. The highest values are observed in P1 in the morning (08: 00-10: 00), and then the concentrations have a lower average, and then rise again in the late afternoon (15: 00-18: 30), Already in P2 the concentrations stay high by the morning and afternoon (08: 40-16: 00).

Figure 1 - Concentration of HC in Point 1

P1

2 Add
9 50,50

1,2,4-trimethylbenzene

Styrene

Methyl Toluene

N-heptane

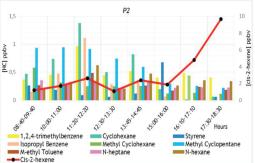
N-heptane

N-undecane

N-undecane

N-undecane

Figure 2 - Concentration of HC in Point 2



### 3.2 Concentrations of aromatic HC: toluene, ethylbenzene and xylenes.

The aromatic HC benzene, toluene, ethylbenzene and xylenes were evaluated separately for their importance as primary pollutants from industrial and vehicular emissions. The BTEX are HC of great relevance in this study because of their high concentrations at both sampling points (Figure 3), mainly toluene. Figure 4 shows that in P2 the concentrations found are higher. M+p-xylene reacts photochemically, its concentration decreases at the end of the morning (10:00 am to 11:00 p.m.) in the presence of sunlight and starts to rise again in the early afternoon (14:00 p.m. to 3:00 p.m.). Maximum concentration on this day in the period from 17: 30-18: 30, as can be seen in P1. However, in P2 the concentration of m+p-xylene remains above 0,5 ppbv in the same period (11: 00-15: 00), that is, even reacting, it maintains with average concentrations equal to the times where the action of sunlight is no longer present.

Figure 3 - Concentration of aromatic HC in P1

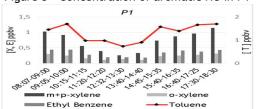
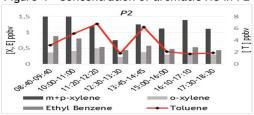




Figure 4 - Concentration of aromatic HC in P2



The xylenes/ethylbenzene (X/E) ratios were estimated to estimate the photochemical age of the plume, this is possible because ethylbenzene has a long shelf life (about 1.6 days), being less reactive, as opposed to xylenes that Are more reactive (life time between 11-20h). In P1 and P2 the ratios were 2.17 and 2.00 respectively, indicating that the feathers are young and the sources of emission were close to the sampling sites.

#### 3.4. Ozone Formation Potential (OFP)

The complex relationship of ozone dependence with its precursors, with radiation and with the influence exerted by meteorological conditions, another important factor that makes the process of ozone control difficult is the large amount of different HCs that are constantly emitted into the atmosphere, each reacting at different rates and with different reaction mechanisms. Because of this, HCs may differ significantly in their effects on ozone formation. These differences in the effects of ozone formation are refer to as "reactivity" of VOCs (MARTINS, 2006). The MIR scale proposed by Carter (1994) was create from simulations in the SAPRAC-07 model for 39 different scenarios and has reactivity factors for VOCs. Therefore, to evaluate the importance of HCs for the formation of O3 in the study area, and thus to be able to choose which compounds have the greatest O<sub>3</sub> formation potential (OFP). The amount of O 3 formed for each gram of HC  $(gO_3/gHC)$  (Alvim et al., 2011) was calculate from the HC concentrations.

HCs with higher PFO can be observed in figures 5 and 6, the graphs relate the concentration of each HC and its PFO. At P1 although the compounds had a relatively low concentration, about 1.2 ppbv, the PFOs were high. Cis-2-hexene, m + p-xylene and 1,2,4-trimethylbenzene are the compounds with the highest OFP. For P2 HC with higher OFP were cis-2-hexene, toluene, m+p-xylene and 1,2,4-trimethylbenzene.

Figure 5 - Ozone Formation Potential (OFP) in P1

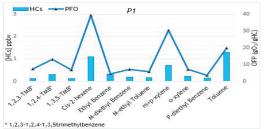
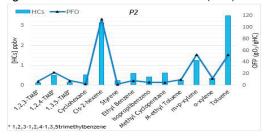


Figure 6 - Ozone Formation Potential (OFP) in P2



#### **CONCLUSIONS**

From the evaluation of HC concentrations in the study area, it was possible to identify which compounds are most relevant in the local pollution scenario, such as cis-2-hexene, 1,2,4-trimethylbenzene, cyclohexane, n-heptane And methylcyclopentane; Of the aromatic HCs which are primary pollutants were toluene and m + p-xylene. Compounds that contribute actively to O 3 pollution have been identified as cis-2-hexene, m + p-xylene, toluene and 1,2,4-trimethylbenzene.

We recommend that more studies be done to analyze more compounds under different meteorological conditions in order to increase the knowledge of the pollution in this area

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### FORMATION OF SECONDARY INORGANIC AEROSOL IN SÃO PAULO

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Abstract: This work studies the equilibrium composition of the secondary inorganic aerosol in the metropolitan region of São Paulo, formed in the atmosphere from the primary emission of gaseous compounds, mainly related to the burning of fuels in vehicles, in addition to trying to understand the composition of the inorganic aerosol in function of the variation of relative humidity and temperature, through a thermodynamic equilibrium program called ISORROPIA, which solves the chemical equilibrium calculations between inorganic species with rigorous modules of high efficiency for use in regional or global models. The data used were from August 2016 and were collected on the IAG-USP terrace, and the x-ray analysis was used to determine the inorganic elementary constitution. The samples were collected with a cascade impactor which resulted in a different mass distribution for different relative humidity, being very clear the hygroscopic properties of the aerosol, in addition another analysis showed that the highest concentrations of chemical compounds in the air are linked with the presence of ammonium salts.

Keywords: Formação, aerosol secundário, São Paulo.

#### INTRODUCTION

The fine particulate material (aerodynamic diameter less than 2.5 microns) is composed of carbonaceous species (organic and elemental carbon) and inorganic species and water. This work studies the equilibrium composition of the secondary inorganic aerosol formed in the atmosphere from the primary emission of gaseous compounds. The secondary inorganic aerosol in São Paulo consists mainly of sulfate, ammonium and nitrate from gaseous compounds emitted by the sources of fuel combustion in the vehicle fleet. The analysis presented here deals with the description of the inorganic balance aerosol composition as a function of relative humidity and temperature variation. Ammonia is an alkaline species, playing an important role in neutralizing atmospheric acidity, in addition to being directly linked with the formation of NH4, which salt is involved with the formation of secondary inorganic aerosol. NH3 is considered a toxic pollutant that has mostly natural sources primarily bound to the soil, but automobile exhaust systems can function as a direct source of ammonia in urban areas, especially with respect to the use

of three-way catalysts. The present study aims to provide a better understanding of the distribution of nitrogen species in relation to other compounds present in the atmosphere. For the equilibrium solution between the possible phases of the aerosol is being used the thermodynamic aerosol model ISORROPIA, which solves the calculations of chemical equilibrium between inorganic species with rigorous modules of high efficiency for use in regional or global models.

#### **METHODS**

The present work had the objective of analyzing the constituent elements of air by analyzing the distribution of nitrogen species in fine particulate matter (PM2.5) through an equilibrium model. The model of thermodynamic equilibrium of the aerosol was carried out using the Isorropia Model (Nenes et al., 1998; Fountoukis & Nenes, 2007), where from the data of aerosol precursor compounds (such as NH3, HNO3, HCl, H2SO4, Na, organic precursors) - or a subset of them, and under environmental conditions of temperature and relative humidity, the number of phases that develop in the aerosol and the chemical composition in the different phases are calculated.



ISORROPIA considers that the system consists of the solid, liquid and gas phases as a function of local relative humidity. In the solid phase the following considered: species are NaHSO4, NH4HSO4, Na2SO4, NaCl, (NH4)2SO4, (NH4)3H(SO4)2, NH4NO3, NH4Cl, NaNO3, KHSO4, KNO3, K2SO4, KCl, CaSO4, Ca(NO3)2. MgSO4. CaCl2, MgCl2. Mg(NO3)2. In the liquid phase: Na+, NH4+, H+, OH-, HSO4-, SO42-, NO3-, Cl-, H2O, HNO3(aq), HCl(aq), NH3(aq), Ca2+, K+, Mg2+. And in the gas phase: HNO3, HCl, NH3, H2O. The sulfates can be either completely or partially neutralized by the amount of ammonium, soil species and sodium. There is also the possibility of complete neutralization of sulfuric acid by soil and sodium species or by soil species only. Thus, the problem is divided into sub-cases in which different possible species exist. Division of the entire range of aerosol species concentrations into sub-domains is performed based on the molar ratios, where the sulfate ratios determine which salts can be formed. particulate matter data were collected by the MOUDI Cascade Impactor on the IAG - USP terrace, at the Butantã campus, in August 2016. It collects particulate matter at different stages (Table 1) on polycarbonate impacting surfaces. These samples for each stage of the MOUDI were analyzed for their mass concentration and also for the determination of the elemental composition from X-Ray Fluorescence The ammonia concentration data were obtained by monitoring with a PICARRO G2103 Analyzer equipment. The meteorological parameters were obtained from the weather station of IAG-USP, located in Água Funda.

Stage	D(50) (μm)	Concentration (µg/m³) Day/Night	
AF	< 0,020	4,5 (2)	2,5(0,2)
S10	0,056	5,0 (2)	4,0(0,5)
S9	0,10	6,5 (5)	4,9(1)
S8	0,18	6,2 (2)	6,2(2)
S7	0,32	7,2 (3)	7,6(2)

Table 1: Particulate material collected at each MOUDI stage with diameters D50. The values of the blue column represent the daytime period and those of the red column represent the nighttime period.

#### FINDINGS AND ARGUMENT

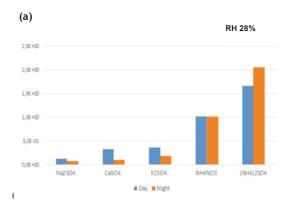
(a) Stage Na (μg/m³) Mg (µg/m³) S (μg/m<sup>3</sup>) 4E10-2 2E10-2 0,6 0 0,3 (0,1) (8E10<sup>-2</sup>) (0,1)(0,4)0,1 (6E10<sup>-</sup> **S10** 0,3 (0,1) 10-3(0,1) (9E10-2) (0,2) 10-3 0,8 0,3 (0,6) 0,3 (0,2) 0,3 (0,2) (10-2) (0,5)8F10-2 3F10-3 **S8** 0,4 (0,1) 0 1,7 (1) 2 (0,6) (0,1) $(10^{-2})$ 0,3 (0,2) 0,1 (0,2) 2E10<sup>-2</sup> 2,8 (2) 4 (2)

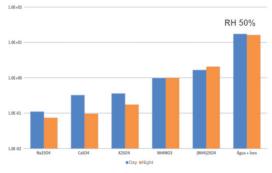
(	(b)							
	Stage	Cl (μg/m³)		K (μg/m³)		Ca (μg/m³)		
	AF	0	0	0,2 (0,1)	0,1 (0,1)	0,1 (6E10 <sup>-2</sup> )	0,1 (3E10 <sup>-2</sup> )	
	\$10	0	0,1 (10-3)	8E10 <sup>-2</sup> (6E10 <sup>-2</sup> )	0,1 (0,1)	10 <sup>-3</sup> (10 <sup>-3</sup> )	10-3 (10-2)	
	<b>S9</b>	0	10-3 (10-3)	0,3 (0,2)	0,2 (0,1)	10-2 (10-2)	10-3 (10-2)	
	\$8	0	10-3 (10-2)	0,4 (0,2)	0,3 (0,2)	3E10 <sup>-3</sup>	10 <sup>-3</sup> (10 <sup>-3</sup> )	
	\$7	2E10 <sup>-2</sup> (10 <sup>-2</sup> )	2E10 <sup>-2</sup> (10 <sup>-2</sup> )	0,3 (0,2)	0,3 (0,2)	3E10 <sup>-2</sup> (10 <sup>-2</sup> )	10-2 (10-2)	



Table 2 (a and b): Results of the elemental composition from X-ray Fluorescence analysis for MOUDI data from August 2016. The values represent the mean and the standard deviation. The columns in blue represent the daytime values and the red ones show the night time period.

data From these (table 2), the simulations were done with ISORROPIA, and the results are presented here referring to the AF stage in the Cascade Impact. The results presented here refer to the last stage of the Cascade Impactor, the After Filter. These particles are those that can reach the respiratory tract.





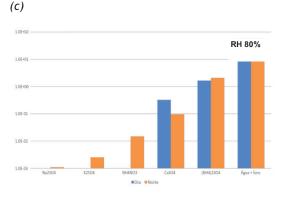


Figure 3: Constituents of particulate matter less than 0.02 micron for different relative humidity. (a) RH=28%; (b) RH=50%; (c) RH =80%. The simulations for the day were made with a temperature of 20.5°C and 15.5°C for night. The values in blue represent the daytime period and in red the night time period is represented. Concentration values on the y-axis (µg/m3)

#### CONCLUSIONS

According to Isorropia model, when RH is low, less than 50%, all inorganic aerosols found in the atmosphere are in the solid state. with ammonium sulfate ammonium nitrate being the major compounds for São Paulo aerosol. For simulations (b) and (c) the amount of water in the atmosphere is enough that the aerosols present are mostly liquids. Again, the major compounds are related to the presence of ammonium salts. This study contributes to the description of mechanisms of formation of secondary inorganic aerosols and their hygroscopicity properties.

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## THE IMPORTANCE OF TEST RIG QUALIFICATION TO OBTAIN RELIABLE DATA

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Abstract: The reliability of data obtained experimentally is of paramount importance in the industrial and scientific branches in any work area and is no different with the air filtration. The objective of this work is to show the importance of the qualification of an air filtration test rig to ensure greater representativity of the data. The qualification consists mostly of simple and rapid tests such as zero particle count and air leak tests and a few more complicated tests, such as air velocity uniformity and aerosol concentration tests inside the sampling duct, particle size selector accuracy test and particle counter calibration for particle concentration, which require some specific materials and equipment. As a result of the qualification, the effort made to ensure that the test rig works properly and that the equipment works in the same way individually is very beneficial.

Keywords: Test rig qualification, Air filtration, Filter media, Aerosol neutralization.

#### INTRODUCTION

The air filtration industry has great complexity, as it is a single branch managed by different standards in different locations (BENNET, 2012), as it happens in North America with the ASHARAE 52.2 (2007) and Europe with the EN 779 (2012). Small changes in experimental parameters are sufficient to produce different results (EPA, 2009).

In both the industrial and scientific fields, the reliability of the data and the results obtained are extremely important. One way to ensure greater reliability is the qualification of the test rig used for the filtration tests (SACHINIDOU AND WANG, 2015). This qualification consists of the survey of all equipment used and functional tests.

The objective of this work is to illustrate how the qualification of a filter media testing system should occur, as well as to point out some possible improvements in this process and its importance.

#### **METHODS**

The qualification was carried out in the filter media test rig at the Environmental Control Laboratory of the Chemical Engineering Department of the Federal University of São Carlos. However, the equipment used is not the focus of this work. The qualification is.

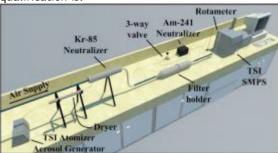


Figure 1. Filter media test rig.

Among the equipment of the test rig shown in Figure 1, it is worth noting the SMPS, Scanning Mobility Particle Sizer Spectrometer, which consists of a Particle Size Selector and a Particle Counter. In addition, other equipment is used during filter media testing. They are pressure drop meters, temperature, relative humidity and atmospheric pressure.

The qualification should be performed in order to ensure that the equipment works properly, both individually and together in the system. The tests were performed in accordance with CEN/TC195, a workgroup of the European Committee for Normatization that is working in a new standard for nanoparticles filtration (CEN, 2016).

The tests performed were:

- Particle counter zero count test: a high efficiency filter (HEPA) must be installed directly on the instrument input and one minute counting should be performed. The maximum limit of the total counts per minute should be 10 particles.
- Particle Size Selector Accuracy Test: The calibration of the particle size measurements is made to check its reliability on the analysis of particle size, which can be done using reference materials samplings.
- Qualification of neutralization: This test verify the effectiveness of the neutralizer. In this case, were performed aerosol samplings without neutralizer on the test rig, with the usual neutralizers and with a certified x-ray neutralizer to compare the results and check if the neutralizer of the test rig is working. But the effectiveness was not tested yet, because there was no electret filter at the time of the qualification. In addition, other



tests can be done for different neutralizer types, such as a corona discharger neutralizer.

- Response time of the aerosol generator: The objective of the test is to measure the time that it takes for the aerosol concentration going from the bottom level to the steady state level and the time interval for the aerosol going back to the background level. This test was performed using a simple stopwatch.
- Zero particles count and system air leakage tests: The zero particles count test checks the particles upstream the filter without aerosol generation. The purity of the air and system leakage test checks the particles downstream the filter with aerosol generator off. The maximum limit of the total counts per minute should be 10 particles.
- 100% efficiency test: For this test, a HEPA filter, class H13 according to EN 1882 (2009), was used, and four 60 second sampling tests were used for each sampling point. For this tests the efficiency should be higher than 99% for the most penetrant particle size (MPPS).
- Pressure drop check: The pressure drop should be checked using Wire Mesh, which is considered as a highly uniform filter medium. In this way the pressure drop of the filter medium must be easily repeatable.

In addition to the tests performed, it is also suggested to perform tests of uniformity of velocity and uniformity of the aerosol concentration inside the sampling duct. However, it was not possible in this test system due to its dimensions. Also it is necessary the calibration of the particle counter as the concentration of particles, compared with the data of a certified electrometer. This test was also not possible because the equipment was not available.

#### FINDINGS AND ARGUMENT

The results for the particle counter zero count test, test rig zero count test and test rig air leakage test are at the Table 1.

Table 1. Zero counts and air leakage tests results.

Qualification	Number of	Particles				
Test	Samples	Counted				
Particle						
counter zero	10	0				
count test						
Test rig zero	10	0				
count test	10	O				
Test rig air	10	0				
leakage test	10	U				

These are the simplest and quickest tests to do. They show if the particle counter and test rig are dirty and also if the airflow inside the system may be contaminated with atmospheric air. It is suggested that these tests be performed every time,

at least a 60-second sampling, before testing begins in the test rig.

The particle size selector accuracy test was performed with standard size particles, more precisely PSL (Polystyrene Latex Spheres) of mean size of 98nm. The values sampled must have a difference less than 5% in relation to the reference value. The results are contained at the Table 2.

Table 2. Particle Size Selector Accuracy Test results.

Sampling	Mean diameter sampled (nm)	Difference with the reference value (%)
1	98.985	1.005
2	99.547	1.579
3	97.079	0.940

This test is important to ensure that the values measured by the particle selector are within normal range and should be performed every 6 months. Neutralization of the aerosol is very important in obtaining the results. It is the responsibility of the neutralization to organize the electric charges of the particles for the SMPS to make the correct

the particles for the SMPS to make the correct reading. The results of the neutralization qualification are contained in Figure 2.

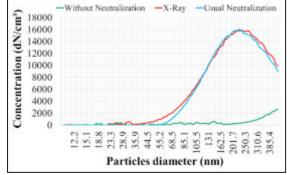


Figure 2. Qualification os neutralization results.

At first, it is possible to observe the influence of the aerosol neutralization on the obtained data. It is therefore extremely important to make sure that the neutralization in the system is working properly. In this particular case, it can be observed that the neutralization is similar to the neutralization of a certified equipment. The neutralization effectiveness check should be done every year.

The 100% efficiency test was done with particles generated from DEHS and a HEPA filter media. Table 3 shows the most penetrating particle size, filtration efficiency for this size and global overall filtration efficiency for each test performed.

This test should be performed to make sure that the test rig works well with absolute filters.



Table 3. 100% efficiency test results.

MPPS (nm):	145.9	135.8	216.7
MPPS filtration efficiency (%)	99.973	99.873	99.914
Global filtration efficiency (%)	99.997	99.992	99.990

Other qualification tests were: the aerosol generation response time test, where the time the aerosol was taken to reach a steady state level when the generator was switched on and off; the pressure drop check with a highly homogeneous filter media Wire Mesh. The response time found in this test rig was 90 seconds and it is important to ensure that errors are minimized with respect to the constancy of the particle generation. The pressure drop obtained with Wire Mesh was 59 Pa for a filtration velocity of 5 cm/s (Politecnico di Torino found a value of 57 Pa for example). This test is important to make sure that the manometer used is working correctly.

From the tests of uniformity of velocity and concentration inside the sample duct, which in this case were not possible due to the small internal diameter and the lack of instruments that fit this factor, are also very important to ensure representative samplings of aerosol. In large ducts, these tests are performed by positioning the velocity measurement instrument or the sampling nozzle at various points inside to determine its variation. In the case of small dimensions, it is suggested a calculation of the properties of the flow, In order to have an idea of the behavior of the fluid.

#### **CONCLUSIONS**

The qualification of a filtration test rig is a fundamental procedure for error minimization and risk prevention that can mask the obtained data. There are many simple and fast execution tests to ensure a great reliability of the data, because the qualification tests guarantee the proper functioning of the equipment individually and also their operation together in the test rig.

An important point to note is the difference between reliability and repeatability of the data. As previously mentioned, small changes in experimental parameters or in the test rig lead to different results. The qualification does not guarantee repeatability of data unless the parameters are maintained and the rig test is exactly the same.

A more practical example is about the neutralization of the aerosol, as already seen is fundamental in the filtration process, and can affect the filtration efficiency depending on its effectiveness. With the qualification it is possible to

determine if this equipment is at its best performance for a radioactive neutralizer or to determine the best working configuration for a corona neutralizer.

One suggestion for qualification tests is the differentiation between test rigs, regarding size and shape, as some tests do not fit into ducts with small dimensions. Another alternative would be to standardize filtration test rigs that use filter media, thus ensuring repeatability of data at different locations. However, this last suggestion is more difficult to occur due to the logistics of standardization and to involve businesses.

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#### Study of diurnal pattern of air quality using Cluster Analysis

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Abstract: This study aims to investigate temporal patterns of air pollution in Piracicaba (São Paulo State, Brazil), during the years of 2014 and 2015. It was used a multivariate statistical analysis on air pollution datasets. Hierarchical Agglomerative Cluster Analysis (HACA) was applied to find a diurnal pattern. Five Clusters were found, grouping the hours of the day according to six pollutant concentration ( $O_3$ , NO, NO<sub>2</sub>, NO<sub>x</sub>,  $PM_{10}$  and  $PM_{2.5}$ ). Meteorological factors influenced the air pollution concentration differently, according to each period of the day. Higher  $PM_{2.5}$  and  $PM_{10}$  concentrations were found in the evenings, while higher  $O_3$  concentrations were found in the afternoons. The peaks of NO, NO<sub>2</sub> and NO<sub>x</sub> concentrations were obtained during mornings and evenings, which correspond to periods of the day with high traffic of vehicles.

Keywords: Cluster analysis, air quality data, diurnal pattern.

#### **INTRODUCTION**

Air pollution is a recognized problem because it impacts human health, well-being, fauna, flora and the environment. There are several studies that associate air pollutants with respiratory and cardiovascular problems (Matyasovszky et al., 2011, Breitner et al., 2014, Rodopoulou et al., 2015). On the other hand, there is an interest to evaluate air pollution and its association with time, in order to identify patterns (Latif et al., 2014, Targino and Krecl, 2016). Toh, Lim and Glasow (2013) analyzed the meteorological effects on diurnal, monthly and seasonal variations of  $O_3$  and  $PM_{10}$  concentrations in Tanah Rata city, in Malaysia.

Cluster analysis (CA) has been used for identifying groups of elements in several studies. In some cases, this analysis is used for grouping air mass trajectories (Borge et al., 2007, Wang et al., 2010). In others, it is used for grouping monitoring stations (Pavón-Domínguez et al. 2014, Huang et al., 2015). There are studies that used CA for grouping time periods, as days or hours, in order to identify a temporal pattern of air quality.

Targino and Krecl (2016) used cluster analysis for grouping days with similar profiles of meteorological variables, and after that, they identified the relation between these profiles and the diurnal pattern of Black Carbon (BC). Finally, they concluded that BC could be related to local waste burning and intense motorized traffic. In Boston, during 2004 and 2009, Austin et al. (2012), classified days in groups based on the profile of pollutant concentrations (gases and particulates). The k-means algorithm was used in the cluster analysis.

Latif et al. (2014) analyzed seven air pollutants (NO,  $NO_2$ ,  $NO_x$ ,  $O_3$ ,  $PM_{10}$ , total hydrocarbon and CH<sub>4</sub>) in the city of Jerantut, Malasia. In this study, the objective was evaluating the relation between daily, monthly and yearly tendencies with local

influence. Using cluster analysis, they observed that traffic emissions were the main contributor to air pollution in the region and that during the peak hours of traffic flow (during 7 to 9h and 17 to19h), the air pollutant concentration was the highest.

Cluster analysis was used here to group hours, in order to assess trends in pollutant concentration in Piracicaba, São Paulo, Brazil. The main objective is to identify a diurnal pattern for all air pollutants collected in Piracicaba.

#### **METHODS**

#### Location of sampling and Data collection

The air quality data of this study was collected in Piracicaba, which is located in São Paulo State, in Brazil. This city has an area of 1.378.069 Km² and an estimated population, in 2016, of 394.000 inhabitants (IBGE, 2010).

The air quality data used here was collected between January 2014 and December 2015 by CETESB's (the Environmental Company of the State of São Paulo, Brazil) automatic station in Piracicaba. The data obtained online, at the QUALAR platform (QUALAR, 2017).

The data were divided into two groups: meteorological and pollutants. The meteorological data were temperature (temp) [°C], relative humidity (RH) [%] and wind speed (WS) [m/s]. The air pollution data, in  $\mu g/m^3$ , were ozone (O<sub>3</sub>), nitrogen oxide (NO), nitrogen dioxide (NO<sub>2</sub>), oxides of nitrogen (NO<sub>x</sub>) and particulate matter (PM<sub>10</sub> and PM<sub>2.5</sub>) concentrations.

#### Statistical analysis

Hierarchical Agglomerative Cluster Analysis (HACA) was applied to the datasets. HACA was implemented using Ward's method, while the Euclidean distance was used to measure similarities. Ward's method is an agglomerative process where each point is 1 cluster at first and,



then, it iteratively combines the points in order to minimize the sum of squared error (Han and Kamber, 2006; Austin et al., 2012).

All analyses were performed using R v3.1.3 and Excel 2007.

#### FINDINGS AND ARGUMENT

First, the hourly average was calculated for each variable. For the six air pollutants  $(O_3, NO, NO_2,$ NOx, PM<sub>10</sub> and PM<sub>2.5</sub>), HACA was applied. The result of HACA is presented in a dendogram (Figure 1). The temporal pattern shows 5 groups, detailed in Table 1. Cluster 1 groups dawn hours. Cluster 2 corresponds to early morning, while Cluster 3 evening, consists, mainly, of late corresponding the stability to air mass (temperature inversion)(Schnelle and Brown, 2002, Latif et al., 2014). Cluster 4 groups morning (11-12h) and evening (18h) hours. Finally, Group 5 corresponds to the afternoon (13-17h), when the temperature, and consequently UVB, is sufficiently substantial to initiate photochemical reactions and subsequent non-photosensitive reactions (Vallero, 2008, Baird, 2011).

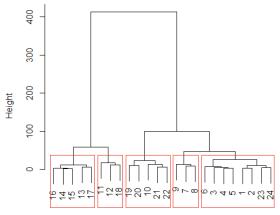


Figure 1.Dendogram of diurnal temporal pattern based on average concentration of six variables (PM<sub>10</sub>, PM<sub>2.5</sub>, NO, NO<sub>2</sub>, NO<sub>x</sub> and O<sub>3</sub>)

Table1.Cluster of hours obtained by HACA

Cluster	Hours	Period predominant
1	23,24,1,2,3,4,5,6	Dawn
2	7,8,9	Morning
3	10,19,20,21,22	Evening
4	11,12,18	Morning
5	13,14,15,16,17	Afternoon

Table 2 shows the results of descriptive statistics (mean, standard deviation, minimum and maximum) for all air pollutant in each cluster. Notice that Cluster 3 presents higher  $PM_{10}$  concentration, when the temperature is lower,

while, Cluster 5 shows lower  $PM_{10}$  concentration, when the temperature is higher. So,  $PM_{10}$  shows a peak in the evening and minimum in the afternoon, when temperature increases, and relative humidity decreases (Figure 2). This indicates that physical processes, such as dilution with free tropospheric air, can decrease  $PM_{10}$  concentration (Schnelle and Brown, 2002, Vallero, 2008). A similar phenomenon occurs with  $PM_{2.5}$ .

Table 2. Descriptive analysis by cluster

	Mean						
Cluster	PM <sub>10</sub>	PM <sub>2.5</sub>	NO	NO <sub>2</sub>	NO <sub>x</sub>	O <sub>3</sub>	
1	38.5	16.0	3.9	20.2	14.0	24.4	
2	35.8	13.7	15.4	20.9	23.7	19.9	
3	39.9	15.1	4.9	25.9	17.8	45.8	
4	37.5	13.7	3.5	16.5	11.6	69.2	
5	31.2	11.7	1.4	10.5	6.8	88.5	
		Star	ndard D	eviatio	on		
Cluster	PM <sub>10</sub>	PM <sub>2.5</sub>	NO	NO <sub>2</sub>	NO <sub>x</sub>	O <sub>3</sub>	
1	2.3	0.5	1.0	3.0	1.8	4.5	
2	0.8	1.5	3.4	0.5	3.0	6.5	
3	1.1	1.1	2.6	4.5	0.9	8.1	
4	1.3	0.7	1.5	5.0	2.5	8.5	
5	1.3	0.4	0.3	2.4	1.4	3.0	
			Minim	num			
Cluster	PM <sub>10</sub>	PM <sub>2.5</sub>	NO	NO <sub>2</sub>	NO <sub>x</sub>	O <sub>3</sub>	
1	35.6	15.2	3.1	17.1	11.8	17.6	
2	35.0	12.6	11.6	20.3	20.3	15.0	
3	38.6	14.0	3.5	18.4	16.8	37.0	
4	36.1	12.9	2.4	12.1	8.9	59.4	
5	29.8	11.2	1.2	8.6	5.5	85.0	
			Maxin	num	,		
Cluster	PM <sub>10</sub>	PM <sub>2.5</sub>	NO	NO <sub>2</sub>	NO <sub>x</sub>	O <sub>3</sub>	
1	41.8	16.4	6.1	25.3	17.1	31.5	
2	36.7	15.5	18.0	21.3	26.0	27.3	
3	41.1	16.7	9.6	29.5	19.0	58.3	
4	38.7	14.1	5.2	21.9	13.6	75.2	
5	32.8	12.2	1,7	14.6	9.2	91.7	

 $NO_2$  presents a peak of mean in Cluster 3 (evening), and NO and  $NO_x$  shows a peak of mean in Cluster 2 (morning). These peaks are associated with rush hour traffic of vehicles, in the evening and morning, respectively (Schnelle and Bronw, 2002, Latif et al., 2014).

Cluster 5 (afternoon) shows a higher concentration of  $O_3$ , exactly when higher temperatures occur (Figure 2). The  $O_3$  formation involves the photochemical reaction of  $NO_x$  (Sillman, 1999, Baird, 2011).



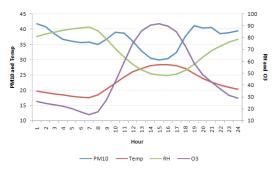


Figure 2. Diurnal pattern for average concentration of  $PM_{10}$  (PM10), temperature (Temp), relative humidity (RH) and  $O_3$  (O3)

#### **CONCLUSIONS**

This study shows the diurnal pattern of major air pollutants at a Piracicaba station, in São Paulo State, Brazil. Meteorological factors influence air pollution concentration, according to the hours of the day. A future policy focusing on managing Piracicaba air quality will be more effective if we know the changes in pollutant concentration. So, these results aid to evaluate the air pollution condition, and then, propose actions to reduce the emission of these pollutants. As a suggestion for future works, this analysis may be applied to datasets from different places and to other air pollutants and meteorological variables.

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## Quantity of inhalable particulate matter (PM10) in the city center of Sao Carlos, Sao Paulo state, Brazil.

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Abstract: Inhalable particulate matter with aerodynamic diameter smaller than 10µm (PM10) have long been considered as air pollutants associated with health issues. They penetrate into the upper respiratory tract, causing respiratory problems such as asthma. The aim of this study was to measure the amount of PM10 particles in the atmospheric air of the city center of Sao Carlos in the period 2014 to 2017 compared with a 1997 to 2006 sampling period. The samplings were collected daily in the first stage (2014-2015) and in the second stage (2015-2017) the samplings were performed on alternate days during the week, for periods of 23h and 30 minutes. The equipment used was the high volume sampler (Hi-vol). The amount of PM10 particulate matter was reduced from 70.03  $\mu$ g/m³(1997-2006) to 31.90  $\mu$ g/m³ (2014-2017), that is, an effort to reduce this inhaled particulate.

Keywords: Coarse particulate matter(PM10), the high volume sampler.

#### INTRODUCTION

The basic use of natural air resource is to maintain life. All other uses are subject to the maintenance of the quality of the air to avoid a strongly deterioration of health and well-being of humans (DERISIO, 2012). The world lives today with a major concern about the increase the air pollution. Big cities are taking measures to reduce the concentration of dust and breathable particles in the atmosphere (ABRASEG.2016). People have a false impression that only large cities have problems of air pollution. In the Campinas region (state of Sao Paulo), a city like Santa Gertrudes, population of 24,737 with a (IBGE.2016) is currently experiencing serious pollution problems, due to the ceramic industries. increase that greatly concentration of particulate matter in the air are the burning of materials and sugar cane in the region. The particulate matter of aerodynamic diameter smaller than 10µm, which is also known as PM10, is composed of primary particles, formed from mechanical processes such as combustion ash, natural biogenic emissions and resuspension of dust from the soil by winds (FREITAS and SOLCI, 2009). The particles of PM10, when inhaled, can reach the lower respiratory system. The aim of this study was to measure the amount of PM10 particles in the atmospheric air of the city center of Sao Carlos of the period 2014-2017 and comparison with 1997-2006 sampling period.

#### 1. Area of study

The city of Sao Carlos is located near the geographical center of the state of Sao Paulo, at 47°31' West longitude and 22°00' South latitude

coordinate limits, with 830m of average altitude. With a population of 240,000 inhabitants and 1.137,332 km2 area (IBGE 2016), the local weather is temperate, characterized by the alternation of dry winters and rainy summers, with an average annual temperature of 21.2°C and 1512mm of annual average precipitation. Figure 1 shows the map of the state of Sao Paulo, city of Sao Carlos, study site and sampling point.

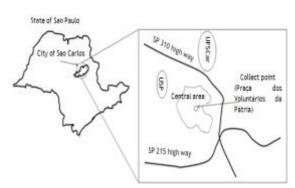


Figure 1. Map the location of the city of Sao Carlos in Sao Paulo

#### **METHODS**

#### 2. Sampling

The place of collection of the PM10 was the Praça dos Voluntários da Pátria, which is the place where there is a large circulation of vehicles and pedestrians and it houses the greater number of services of the city, meaning that the population in it are subject to inhalation of particulate matter from a variety of sources.



For the collection of the coarse particulate matter PM10, the equipment used was the high volume sampler (figure2).

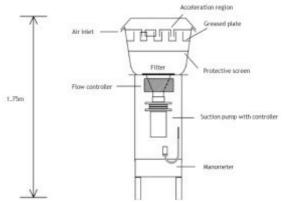


Figure 2. High Volume Sampler

The process of sampling the PM10 particulate matter was performed in the square municipal market. Figure 3 ahows the flowchart of the process of collection of particulate matter PM10.

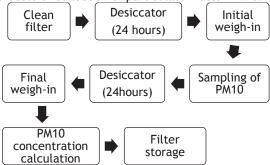


Figure 3. Prepared by the author, 2017

The equation used to calculate the concentration

PM10 is: 
$$CPM10 = 10^6 \frac{Mt}{Vr}$$
 [µg/m3],

where: Mt is diference betwen final weigh-in and initial weigh-in, and Vr is real volume to sample.

#### FINDINGS AND ARGUMENT

In Figures 4 and 5, an increase the influence of relative humidity on PM10 particulate matter. In Figure 4 (daily sampling) it is observed that the relative humidity of the air had strong influence in the rainy period, which goes from November to March, indicating that the higher the relative humidity the lower the PM10 concentration. This time( 2014-2015), the highest concentration was recorded in August-2014 (39.58  $\mu g/m^3$ ), precisely the month in which sugar cane was burned in the region and had a strong influence on the increase in the amount of PM10 particulate matter, which extended up to September.

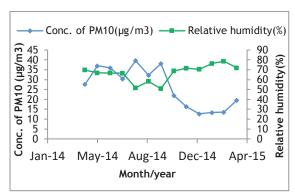


Figure 4. Influence of relative humidity on the conc. of PM10-2014/2015

In Figure 5 (alternate days sampling), it was also observed in the rainy season a decrease PM10 concentration with the increase in relative humidity. And the highest concentrations were registered in the months of August-2015 (29.38  $\mu g/m^3$ ) and September-2016 (31.90  $\mu g/m^3$ ). According to POZZA(2005), particulates such as potassium (K), zinc (Zn) and copper (Cu) were detected in the PM10 particulate material sampled in the city center of São Carlos from sugarcane burning. There is strong evidence of the element sulfur (S) in the region of Araraquara. From the traced profile of vehicular emissions, it was verified that this element is characteristic from diesel fuel used by motor vehicles that circulate in that city.

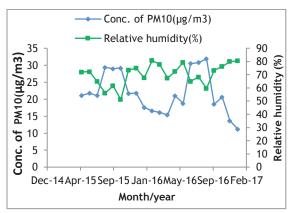


Figure 5. Influence of relative humidity on the conc. of PM10-2015/2017

In both periods (2014-2015 and 2015-2017), low PM10 concentration means high relative humidity. For example, when the relative humidity of the air is very low or very high, there may be respiratory problems. With very low humidity (less than 30%), allergies, sinusitis, asthma and other diseases tend to aggravate. Even when the relative humidity of the air is very high, fungi, molds and dust mites can arise.



In Figure 6, it is observed that the during the sampling period of 1997-2006 (CELLİ et al. ,2006), the samplings were performed on alternate days during the week.

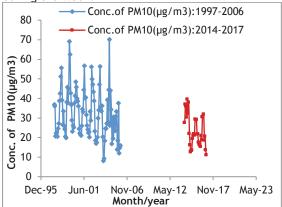


Figure 6. Comparison of PM10 sampling data for the 1997-2006 and 2014 -2017 periods

The concentrations in the monthly average reached very high values but, at that time, the city population was smaller of (210,986 inhabitants), with less vehicles in circulation and less industries in operation. But on the other hand, there was less rigour in the inspection of polluting sources, which consequently allowed industries to emit more pollutants to the atmosphere without worrying about the environment. Today, inspection and legislation are more stringent, which makes industries more concerned about the environment and thus ensuring the well-being of all who enjoy a healthy environment. It is still observed in the same figure that in the period of 2014-2017, that the amount of the airborne pollutant PM10 decreased in the center of the city. But the highest concentrations of PM10 continued to be recorded in the months of August and September, that is, it is still burning sugar cane in those months that put at risk the life of the local community.

#### **CONCLUSIONS**

It was observed in this comparison of the amount of PM10 inhalable particulate matter between the periods of 1997-2006 and 2014-2017 that the amount of PM10 in the atmospheric air of the city has been decreasing, a variation of 37.10% over the past period. This is a sign that industries and other polluting agents are worrying more about the quality of the air around them and consequently is a benefit to all who enjoy it.

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### PM<sub>2.5</sub> CHEMICAL CHARACTERIZATION IN AN URBAN AND INDUSTRIALIZED REGION IN VITÓRIA - ES.

**Abstract:** The goal of this work is to chemically characterize fine particulate matter ( $PM_{2.5}$ ) in a single receptor located in an urban and industrialized region in Vitória, Espírito Santo for application in a source apportionment study with a high degree of colinearity sources. Samples were collected using the MiniVol Sampler for analysis by Energy-dispersive X-ray spectroscopy for metals (Na to U) and Ion Chromatography for water soluble ions ( $SO_4^2$ ,  $NO_3$ ,  $NH_4$ , Na, Cl). Sulphates, sodium, nitrates, chlorine are the major components of  $PM_{2.5}$  in samples collected in a receptor located near the industrial park of the RMGV. The results suggest that sulphates and nitrates can be originated by gas precursors from industrial sources. Sodium and chlorine are emitted by sea spray dust.

Keywords: PM<sub>2.5</sub>, sulfates, EDX, IC, source apportionment.

#### INTRODUCTION

For the last few years, there has been increasing publicly concern about Particulate Matter (PM) pollution around the Metropolitan Region of Grande Vitória (RMGV) (de Melo, 2015) because its effects on visibility (Hyslop, 2009), climate change (Kondratyev et al., 2006) and effects on public health (Nascimento, 2015).

Fine particles ( $PM_{2.5}$ ) can be emitted directly from combustion sources, but can also be formed in the atmosphere by gas to particle conversion from gas phase precursors such as  $SO_2$  or NOx, which are mostly industrial emissions (Finlayson-Pitts & Pitts, 2000). Nitrate ( $NO_3$ -), ammonium ( $NH_4$ +) and sulphate ( $SO_4$ <sup>2</sup>-) are important components of  $PM_{2.5}$  in urban and industrialized regions like the RMGV. These components are also known as secondary inorganic aerosols (SIA).

SIAs have been listed as one of the major pollutants in air quality standards (EPA, 2008) and the direct strategy to reduce the level of SIAs is to control industrial emissions of precursors. This may be an effective method overall to reduce pollution. Therefore, it is important to understand the dynamics of SIA in the urban atmosphere of RMGV to better apply policies to control industrial pollution.

The Emissions Inventory of the RMGV (IEMA, 2011) presents that  $SO_2$  emissions are dominated by industrial sources (representing 80% from the total emission 3,169.50 kg/h). As result,  $SO_4^{2-}$  can be formed in the atmosphere due to  $SO_2$  oxidation trough the presence of  $OH^+$ ,  $O_3$  or reactions in the aqueous phase, considering high levels of humidity in the coastal area of RMGV.

To date, only a few researchers have focused on the chemical characteristics, transportation and source apportionment of atmospheric fine particulate matter across the RMGV (Maioli, 2011; Nascimento, 2015).

The most recent studies related to the determination of source contribution have used hybrid models that combine the characteristics of dispersion models and receptor models to identify sources such as Chemical Transport Models (CTM) like Models- 3 Community Multiscale Air Quality (CMAQ). These models may be adopted to compensate the limitations of the receptor models (Kwok et al., 2013, Napelenok et al., 2014) and nonlinearities in the transformation of pollutants. Among the methods currently in existence are: Particulate Matter Source Apportionment Technology (PSAT) (Wagstrom et al., 2008), Tagged Species Source Apportionment (TSSA) (Wang et al., 2009), The Integrated Source Apportionment Method (ISAM) (Kwok et al., 2013), and various approaches to sensitivity analysis of sources and receptors (Koo et al., 2009).

The CMAQ Integrated Source Apportionment Method (ISAM) is a tool implemented in the most current version of the CMAQ model, version 5.0.2 to track contributions from source groups, specific regions of the modeling domain or chemical precursors to the levels of Concentration and deposition of pollutants (O<sub>3</sub> and PM<sub>2.5</sub>). The CMAQ ISAM has specific mechanisms to treat the formation of secondary particles and the ability to identify the contribution of emitting sources.

Based on this context, this work intends to present the chemical characterization of the  $PM_{2.5}$  collected in a specific receptor that will be used to evaluate the application of the CMAQ ISAM in determining the



contribution of  $PM_{2.5}$  sources in an urban and industrialized region of the RMGV. To reach this objective, the work will focus on the evaluation of compounds in an ionic form to separate source contributions from industrial emissions with high degree of collinearity.

#### **METHODS**

PM<sub>2.5</sub> samples were collected every 48 hours using MiniVol sampler from AirMetrics in one of the air pollutants monitoring station (Clube Ítalo) of the Automatic Air Monitoring Network from Grande Vitória (RAMQAr) (Figure 1). 33 samples were collected from 10/22/2016 to 12/19/2016 and analyzed by Energy-dispersive X-ray spectroscopy (EDX) for metals (Na to U) and Ion Chromatography (IC) for water soluble ions (SO<sub>4</sub><sup>2-</sup>, NO<sub>3</sub>-, NH<sub>4</sub>+, Na+, Cl-).

Samples were collected in a TEFLON filter (PTFE Whatman n° 7592-104) for EDX analysis and quartz filters (QMA - Whatman n° 1851-865) for IC analysis. Filters were equilibrated in a controlled room (T: 20 - 23 °C  $\pm$ 2 °C and RH: 30% e 40%  $\pm$ 5% ) for pre-and post-weighted.

It was used a spectrometer Shimadzu brand (EDX-800/'m) with the analysis system (software) PCEDX Analysis System (Shimadzu, Japan) for EDX analysis and Metrohm 930 Compact IC Flex Oven/SeS/PP/Deg for IC analysis



Figure 1. Location of the receptor used for  $PM_{2.5}$  sampling campaign. The receptor is located in a region that receives directly  $PM_{2.5}$  industrial contribution.

#### FINDINGS AND ARGUMENT

The results of IC analysis (Figure 2) shows that sulfates (2.68  $\pm$  0.54  $\mu g/m^3$ ) are the major components of PM<sub>2.5</sub> in the ionic form, followed by sodium (2.00  $\pm$  1.05  $\mu g/m^3$ ), nitrates (1.68  $\pm$  0.88  $\mu g/m^3$ ) and chlorine (1.67  $\pm$  0.61  $\mu g/m^3$ ). The result is expected due to high levels of SO<sub>2</sub> monitored at

the RAMQAr. Also, due to the proximity of the ocean, sodium and chlorine were observed in significant concentrations.

Nitrates are in significant concentrations and must be mainly originated by industrial sources. It was not found any significant level of ammonium in the samples analyzed.

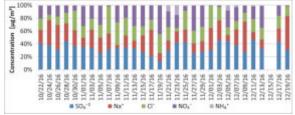


Figure 2. Water soluble ions present in PM2.5 samples collected at Clube Italo air monitoring station from october 22 to december 19/2016.

The EDX results (Figure 3) shows that Cl  $(3.51 \pm 0.92 \, \mu g/m^3)$ , Na  $(1.98 \pm 0.50 \, \mu g/m^3)$ , S  $(1.58 \pm 0.65 \, \mu g/m^3)$  and Fe  $(0.59 \pm 0.24 \, \mu g/m^3)$  are the major components of PM<sub>2.5</sub>. Sodium and chlorine are emitted by sea spray aerosol. Sulphur can also be emitted by sea spray or industrial sources and Iron is more related to industrial sources.

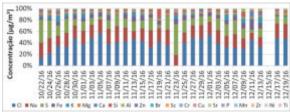


Figure 3. Metals present in  $PM_{2.5}$  samples collected at Clube Italo air monitoring station from october 22 to december 19/2016.

#### **CONCLUSIONS**

Sulphates, sodium, nitrates, chlorine are the major components of  $PM_{2.5}$  in samples collected in a receptor located near the industrial park of the RMGV.

The results suggest that sulphates and nitrates can be originated by gas precursors from industrial sources. Sodium and chlorine are emitted by sea spray dust.



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### IMPACT OF FINE PARTICULATE MATTER AND BLACK CARBON ON HUMAN HEALTH IN SÃO PAULO

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Abstract: An expressive source of emission of pollutants in urban areas is the burning of fossil fuels and biofuels. According to WHO (WHO, 2015) more than 7 million people worldwide are affected by air pollution, both indoor and outdoor and short and long term exposures PM2.5 and its Black Carbon component, are associated with a wide range of impacts on human health when it is inhaled. The objective of the study is to measure the impact of components on morbidity and mortality due to diseases of the respiratory system. The data consist of the concentrations of MP2.5 and its elemental composition, subjected to the analyzes of Reflectance for the determination of the concentration of Carbon Black, and daily data of deaths and hospitalizations due to diseases of the respiratory system were obtained from the Service platform (SIC) of the Ministry of Health. The correlation values obtained among BC and PM2.5 and health data show that there are indications of relationship between them, but they are strongly associated with other factors such as Influence of meteorological variables.

Keywords: Polluition, Particulate Matter, Black Carbon

#### **INTRODUCTION**

Black Carbon is a component of fine particulate matter (diameter smaller than 2.5 µm). Its main source is the incomplete combustion of fossil fuels, biofuels and biomass. It absorbs short-wavelength energy from the atmosphere by changing the radiative energy balance of the climate system. In addition another consequence is its harmfulness to human health, since it is associated with health problems. Due to these and other factors, it is essential to emphasize the study of this component, so that we can work on strategies to reduce Black Carbon in the atmosphere. The objective of this work is to evaluate the impact of Fine Particulate Matter (PM2.5), specifically its Black Carbon concentration, on morbidity and mortality due to respiratory diseases.

#### **METHODS**

The data base was collected in the years of 2007 and 2008, during the sampling experiment carried out in the scope of the project: "Evaluation of air quality in six Brazilian Metropolitan Regions", coordinated by the Faculty of Medicine of the University of São Paulo. The samples from São Paulo aerosol were collected at the Medical School of the University of São Paulo and weighed for the determination of the mass concentration and subjected to the analysis of the Reflectance for determination of the Black Carbon concentration.

On the other hand, daily data of deaths and hospitalizations due to respiratory diseases were obtained from the Citizen Information Service (SIC) platform of the Ministry of Health. The air pollution data was correlated with health data and emphasis was placed on two risk groups: children (0 to 14 years) and the elderly (over 60 years). Pollution events and their correlation with number of deaths were analyzed considering different lags of time.

#### FINDINGS AND ARGUMENT

Figure 1 shows the histogram of deaths together with the temporal values of concentration of PM2.5 and BC in São Paulo in the years of 2007 and 2008. Table 1 shows correlations between a concentration of PM2.5, BC and number of deaths due to respiratory diseases, with lags of 1 to 3 days. Table 2 shows the same data by age group (children and elderly).



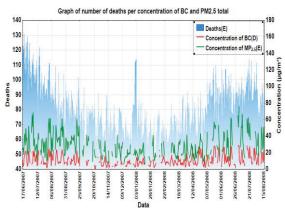


Figure 1. Histogram of number of deaths and temporal variability of PM2.5, and Black Carbon in the years 2007 and 2008.

Table 1. Correlations between mean mortality and mean concentration of PM2.5 and Black Carbon with lags of 1 to 3 days, in the years 2007 and 2008.

	Present	Lag	1	Lag	2	Lag	3
	Day	day		days		days	
BC	0,28	0,25		0,27		0,28	
MP	0,35	0,34		0,32		0,34	

Table 2: Correlations between mean mortality data and mean concentration of PM2.5 and Black Carbon in the years 2007 and 2008.

Correlation	PM(µg/m³)	BC(µg/m³)
Children's Deaths	0,42	0,48
Elderly's Deaths	0,85	0,71
Total	0,83	0,70
Statistical Significance	5%	5%

#### **CONCLUSIONS**

The results of the correlation indexes obtained between BC and health data, especially for the population over 65 years, indicate that there may be a relation of causality among these variables, but it is needed to perform a more detailed analysis including other confusing variables as meteorological and seasonal factors.

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# EVALUATION OF THE AIR QUALITY OF THE AMAZONAS NEIGHBORHOOD, ITABIRA - MG, DURING THE MONTHS OF OCTOBER AND NOVEMBER 2016

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Abstract: This paper presents the first monitoring study on environmental air quality results in Amazonas Neighborhood. The work performed including sampling of particle concentration and black carbon concentration data determined for each of PM 10 and PM 2.5 particulate. Research results show that the Amazonas neighborhood of Itabira, despite all the retrospect of the city, presented good air quality for October and November 2016. Itabira is recognized for its poor quality, but with this work, it is possible understand that the air quality is not the same in all of city scope.

Keywords: Particulate Matter, Air Quality, Black Carbon, Mining Cities.

#### INTRODUCTION

Air pollution in recent years has been increasingly identified as a serious public health problem in the world. Industries and motor vehicles are generally regarded as the main sources of emissions associated with air pollution in large urban centers. In the city of Itabira (Minas Gerais), air quality is also a problem.

The city, like any major urban center, already suffers from several sources of particulate matter, such as incomplete combustion of vehicles, burning of biomass, industrial processes and resuspension of street dust. Itabira, meanwhile, hosts one of the country's largest open-pit mining complexes, which according to Braga (2007) is the most relevant source of inhaled particulate matter emissions. Almeida (1999), in his study, found higher values for particulate matter close to mining stations, than those found in the urban area. Those values even exceeded Brazilian legal standards. Reis (2000) stated that the villages, located near Itabira's iron mines, had high levels of ore particles suspended in the air, Reis also expounded that half of the city had respiratory problems. Silva (2004) in his research, through questionnaires, showed the discomfort of local society facing the problems of air pollution. Souza (2007) discussed several protests, through inhabitants, in the 1990s on environmental issues including the poor air quality of Itabira. In most recent studies, such as Devlin and Tubino (2012) and Wasylycia-Leis, Fitzpatrick and Fonseca (2014), also addresses poor air quality, reaffirming the above annoyances mentioned.

This work has the objective of evaluating the air quality in the Amazonas neighborhood in Itabira, through Particulate Matter (PM) and Black Carbon (BC) measure, serving as a marker for other work involving air quality in the region.

#### **METHODS**

A sampler operated to collect coarse and fine particles at an average flow rate 16.7 1/min, this equipment collected the particulate material by inertial impaction in two fractions separately. The holder that supports the filters will have two compartments. In the first one, a filter was used (with eight µm pores diameter), for PM<sub>10</sub> and in the second a filter, (with eight µm pores diameter), for PM2.5. The hole equipment was placed in a private property in Amazonas, neighborhood. It was far from trees, highways, places with vegetation cover in the ground, free from obstacles, safe from the action of curious and with available electrical energy (GODOY, 2001). With the necessary care, 40 Nuclepore polycarbonate filters (47 mm diameter) were sampled, between October and November 2016, 20 for fine and 20 for coarse matter.

The sampled filters were weighed before and after collection and by difference, the deposited mass was obtained. With the mass obtained, the volume of air sampled and controlled, and by knowing the filter area, it was possible to determine the concentration of the particulate collected in fine and coarse fractions of each inlet filter. The filter masses were obtained by a micro-analytical scale, XP micro and ultra-micro, of the Mettler Toledo brand, with nominal precision of 1µg. Before each weighing, the filters were left for 24 hours in aluminum boxes, for air conditioning and exposed to alpha (polonium) sources, to neutralize the electric charges present on their surface, which can alter the weighing results (GODOY, 2001).

The measure of black carbon by reflectance takes advantage of this property by absorbing light in the visible region. In this analysis, was used the M43D SmokeStain Reflectometer, from the Diffusions



Systems brand. The black carbon mass present in the sample was calculated from the calibration curve calculated by Loureiro (1994).

#### FINDINGS AND ARGUMENT

With the data collection of mass and reflectance, along the time, sampled volume, and by knowing the area of each filter it was possible to determine the concentration of particulates, Black Carbon and average in  $\mu g/m^3$ , shown in Table 1.

Table 1. Black Carbon and Particulate Matter concentrations

	Concentrations					
	Fine	Coarse	РМ	BCFine	BCCoarse	
Sample			μg/m	3		
ITB-01	8,56	12,72	21,29	1,11	0,19	
ITB-02	10,92	11,01	21,93	1,11	0,14	
ITB-03	5,30	7,79	13,09	0,63	0,09	
ITB-04	6,98	14,14	21,12	0,97	0,18	
ITB-05	4,51	8,37	12,89	0,71	0,13	
ITB-06	6,43	13,28	19,71	1,01	0,18	
ITB-07	8,63	14,69	23,32	1,24	0,19	
ITB-08	15,28	16,02	31,30	2,24	0,28	
ITB-09	10,16	14,75	24,91	1,00	0,15	
ITB-10	6,97	8,44	15,41	1,02	0,18	
ITB-11	7,79	13,29	21,07	1,29	0,20	
ITB-12	5,33	11,12	16,45	0,87	0,13	
ITB-13	12,15	14,08	26,24	1,36	0,21	
ITB-14	2,99	6,25	9,24	0,39	0,08	
ITB-15	5,91	9,52	15,44	1,42	0,16	
ITB-16	6,97	11,13	18,10	1,02	0,14	
ITB-17	4,57	7,86	12,43	0,53	0,08	
ITB-18	3,15	5,81	8,97	0,51	0,08	
ITB-19	3,92	6,04	9,96	0,71	0,09	
ITB-20	7,14	8,35	15,49	1,04	0,15	
AVG	6,97	11,06	17,28	1,02	0,15	

Observing Table 1, for the Amazonas neighborhood and for the sampling period, the data presented a good air quality, considering the Brazilian Legal Patterns stated at Conama Resolution number 3. Figure 1 shows a PM Concentration graphic. In Blue PM<sub>2.5</sub> and in red PM<sub>10</sub>.



Figure 1. PM Concentration at Bairro Amazonas

Figure 2 shows a comparative graph between the values found for black carbon and particulate matter, for the fine and coarse fractions. Black carbon, as shown is more apparent in the fine fraction, where there is a certain tendency between the factors, whereas in the coarse fraction, there is no such tendency.

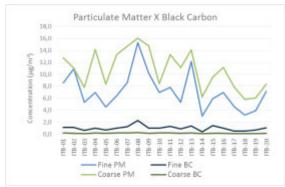


Figure 2. Particulate Matter and Black Carbon Concentration at Bairro Amazonas

Black carbon is more related to smaller particles than larger particles. Confirming this tendency, BC represents 15% of the fine fraction mass, while it only represents 1% of the gross fraction and 6% of all particulate matter.

#### **CONCLUSIONS**

The Amazonas neighborhood in Itabira, despite all the retrospect of the city, presented good air quality for the sampled period. It must be taken into account that the sampling period was very short, this work results should not be expanded to all city regions and seasons, until new points are sampled. Although Itabira city be recognized for its poor air quality, this work shows that the poor quality is not the same in all of city scope. Now it will be able to focus the sampler fields only in the most alarming areas of the city.



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## DETERMINATION OF GASEOUS AMMONIA BY IMPINGER SOLUTION: A CASE OF STUDY IN LAVRAS, MG, BRASIL.

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Abstract: Ammonia is characterized as the only source of aerosol particles expected to grow, in terms of emission rate, throughout the 21st century. The NH<sub>3</sub> emissions, have been increasing in the last decade, on a global scale, accompanying the increase in the agricultural activities, as a result of increasing demand for food production. The goal of the present study is to verify the levels of atmospheric ammonia present in Lavras, southern region of the state of Minas Gerais. Two equipment will be used for the samplings: the gas sampler - APV TRIGAS (which works by the "impinger" method), and the Meteorological Station - WatchDog. Data of ammonia concentrations, solar radiation, air humidity, temperature, dew point, wind speed and direction, and atmospheric pressure will be produced at the end of the experiment. This study integrates a larger project "Evaluation of ammonia emissions levels, released in a sugar cane culture, fertilized with urea, in Lavras/MG - Brazil", and its main objective is to serve as a database for future assessment of nitrogen sources in a agricultural background, and also encompassing one of the main factors responsible for the emission of NH<sub>3</sub> into the atmosphere.

Keywords: air pollution, atmospheric emissions, ammonia, impinger

#### INTRODUCTION

Ammonia is the most abundant alkaline gas in the atmosphere, and plays an important role in secondary atmospheric pollutants formation. Due to its low residence time, ammonia is promptly converted in fine airborne particles by atmospheric acids. As ammonium salts, such particles remain in the atmosphere for several days or weeks. Therefore, NH3 is responsible for a significant fraction of the reactive nitrogen and their environmental fate, and also transported over long distances (hundreds of kilometers) (COMMITTEE ON THE ENVIRONMENT AND NATURAL RESOURCES, 2000; SEINFELD; WILEY, 2006).

Recent studies indicate that ammonia emission levels have been increasing in the last decade on a global scale, accompanying the increase in the agricultural activities, as a result of increasing demand for food production (BEHERA et al., 2013; ZHU et al., 2015). Ammonia is characterized as the only source of aerosol

particles expected to grow (in terms of emission rate) throughout the 21st century, with releases of anthropogenic origin expected to double in year 2100 (ZHU et al., 2015).

The main source of ammonia emissions into the atmosphere is agriculture, responsible for the vast majority of total NH<sub>3</sub> emissions. The use of nitrogen-containing fertilizers, and intensive livestock farming are the major sources. Other sources also adds to atmospheric emissions of NH<sub>3</sub>, among them it is important to highlight vehicular emissions, industrial processes, biomass burning, volatilization from soils and oceans, and plant and microbial decomposition (BEHERA et al., 2013; PAULOT et al., 2014; ZHU et al., 2015).

Global estimative of reactive nitrogen emissions shows that 63% of NH<sub>3</sub> emissions originate from anthropogenic food production processes (PAULOT et al., 2014). Thus, given a scenario with no regulation of the current production

system allied with a food demand steep increase in the near future, the emission of NH<sub>3</sub> will increase throughout time. This perspective highlights the impacts of NH<sub>3</sub> excesses in the environment. Despite the current trend towards an increase in atmospheric ammonia, in some regions of the world, such as the European Union, this trend is still mixed. This discrepency is mainly due to the decrease in the number of livestock and better practices in handling and application of fertilizers (EUROPEAN ENVIRONMENT AGENCY, 2016; ZHU et al., 2015).

The heterogeneity of agricultural activities and the complex gas-particle reactions associated with a limited number of studies related to gaseous ammonia are the main aspects that reative nitrogen hinders assessments. Furthermore, the current NH3 inventories are not entirely reliable, given the high uncertanties envolved in such estimatives (COMMITTEE ON THE ENVIRONMENT AND NATURAL RESOURCES, 2000; ZHU et al., 2015). This summarizes the importance of further studies related to reactive nitrogen species and biogeoghemical nitrogen cycle, with emphasis in atmospheric ammonia.

There is no regulation for ammonia emissions in Brazil, and the number of studies on reactive nitrogen species are scarce. The present study seeks to verify the atmosphere ammonia concentrations ammonia, in Lavras/ MG, with the following objectives:

(I) Determination of the levels of ammonia in a urban area with rural background; (ii) estimate the atmospheric emission of reactive nitrogen, and (iii) the impacts on the deposition, and cycling of nitrogen; (iv) serve as a database for future monitoring and inventories studies; and (v) assist in narrowing uncertainties associated with ammonia sources.

#### **METHODS**

The study will be developed at Federal University of Lavras - UFLA, located in the municipality of Lavras / MG, according to UTM coordinates (N) 7,641,028,962; UTM (E) 502.816,286 - SIRGAS 2000, and with an altitude of 1,038 meters.

Two equipment will be used for the samplings: the gas sampler - APV TRIGAS, and the Meteorological Station - WatchDog. The sampling site has the following characteristics: 20 meters away from trees, buildings or other large obstacles, no airflow obstruction around, and away from furnaces or incinerators.

The Meteorological Station - WatchDog, will be allocated next to the APV TRIGAS gas sampler, and will continuously monitor the following parameters: solar radiation; temperature; wind speed and direction; humidity; dew point; rainfall and atmospheric pressure.

The gas sampler - APV TRIGAS, works by bubbling a known volume of gas, through an absorber solution, in order to retain the gas for later analysis.

The equipment (APV TRIGAS) consists of: funnel of capture, gas distributor (glass manifold), 3 sets of vial-bubblers, filter for retention of particles and droplets, 3 critical holes (hypodermic needles), vacuum pump, gasometer, hour meter, timer, and vacuum gauge.

The air flow through the "APV TRIGAS" occurs as follows: the capture funnel, is the place where the air will enter the sampling train, it aims to reduce the passage of water droplets inside the equipment. The air then, passes into a glass manifold, that divides the stream into three parts. Each of these three flows is routed to a bubbler flask, the inner tube (bubbler itself) having a pipetted beak. In these flasks, the specific reagents (absorber solutions) act and retain the polluting gases, with the rest of the sample gas continuing to circulate in the equipment.

After retention of the desired gases in the absorber solutions, the air passes through filters of particles and droplets, and then, it is sent to the critical holes. Critical holes are devices that control the sampling rate continuously. For this project, hypodermic needles will be used as critical holes. They will be calibrated in the UFLA's atmospheric effluent laboratory before the sampling start, according to the specifications in the "APV TRIGAS" operating manual. In this work three hypodermic needles will be used: OC 350, with flow rate of 2 l / min, OC 483 - 0.2 l / min and OC 482 - 0.2 l / min.

After finished monitoring, the samples will be transferred to a container sealed with cover, and stored in a place with ice. That following, in the laboratory of UFLA atmospheric effluents, the samples will be frozen until the time of analysis.

The analyzes of ammonia concentration, will be performed by following two different methodologies. Half of the samples will go to the Department of Atmospheric Sciences at the University of São Paulo. The samples will be filtered (MILLIPORE, MILLEX 0.22  $\mu$ m) and frozen up to 15 days until chromatographic analysis.

Ion chromatography (Metrohm model 851) will be used to evaluate the  $NH_3$ , with anionic column Metrosep ASupp5 (250 mm 4 mm) Metrosep column C2 150 (150 4 mm). Analytical quantification will be performed using an external calibration curve from the standards concentrations for ammonia. The detection limits for  $NH_4^+$  is lower than 1.0 mmol  $L^{-1}$ .

The other half of the samples will be analyzed at the Federal University of Lavras - UFLA, to perform the analysis by means of colorimetry,

using the indophenol method, with the aid of spectrophotometer, equipped with cells with an optical path length of 1 cm, capable of measuring the absorbance at 540 nm and 630 nm.

#### PRELIMINARY AND EXPECTED RESULTS

In this first short campaign, six sampling were carried out between 04/06/2017 and 04/07/2017. These campaigns were performed at the Federal University of Lavras - UFLA, in the vecinity of the sanitary and environmental engineering laboratory, according to the following coordinates UTM 502589.00 m E, 7652445.00 m S, zone 23 k, and altitude of 922 meters.

All the blank samples had a sampling time of two hours. For the absorber solution 10 ml deionized water was used in each of the 3 flask vials. Sampling began on the morning of 04/06/2017, and ended at the afternoon of the following day. We obtained 24 blank samples divided by 4 sampling batchs, each batch had 3 flask vials. Throughout the first day it was observed a sunny day with high temperatures (>26.7C), following by a second rainny day (04/07/2017).

On the second day, 2 sampling batchs were performed using 20 ml of sulfuric acid (0.1N) as an absorber solution during afternoon and evening. A total of 12 acid samples were obtained on this short campaign.

All the 24 blank samples and 12 acid solutions were frozen until further analysis. The six sampling batchs carried out between 04/06/2017 and 04/07/2017, are shown in the following table

Table 1 -- Short campaign summary: blank samples (1 through 4) and acid samples (5 and 6) carried out in Lavras, MG on April, 6th and 7th 2017.

N	Sampling volume	Temperature	Pressure	Sampling flow
1ª	10 ml	27.2° C	749.2 mm Hg	288 liters
2ª	10 ml	29.4° C	749.1 mm Hg	288 liters
3ª	10 ml	26.7° C	748.9 mm Hg	288 liters
4ª	20 ml	27.3° C	748.9 mm Hg	288 liters
5ª	20 ml	25.1° C	748.8 mm Hg	288 liters
6ª	20 ml	22.8° C	748.9 mm Hg	288 liters

This short campaign is a preliminar study of environmental ammonia concentrations in Lavras, MG. This first campaign will integrate several others in the following project: "Evaluation of ammonia emissions levels, released in a sugar cane culture, fertilized with urea, in Lavras/MG - Brazil", which will evaluate

nitrogen species emissions (NOx and NH<sub>3</sub>) from agricultural farms in the vicinity of Lavras, MG throughout 2017 and 2018. The future sampling sites are present in the Federal University of Lavras, where the plantation is periodically fertilized.

By the end of November, 2017 data regarding nitrogen species and meteorological data of a season-long fertilized sugarcane crop will be evaluated in order to estimate the impact of agricultural activities on the nitrogen biogeochemical cycle in the southern region of Minas Gerais, Brazil.

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## Analysis of Itabira atmospheric particulates by fluorescence spectroscopy

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Abstract: This paper presents first results of the monitoring study on ambient air quality in Itabira, an iron mining town. A fluorescence analysis was done to determine and quantify the elements present in PM10 and PM 2,5 atmospheric particulates. The results of the study showed that despite containing heavy metals such as As and Pb their concentrations are lower than international standard levels during the sampling period. Through this study, it was concluded that most of the particulates come from the soil resuspension.

Keywords: Iron ore-Fluorescence spectroscopy-Particulate matter-Air quality

#### INTRODUCTION

The mining activity is an atmospheric polluter because it involves activities such as excavation and explosions. Ore losses can occur during tractors, trucks and train transport on the way to the place where the processing steps will be carried out. Dust emanating from the haul roads contributes considerably to the particulate matter content in the atmosphere.

In Itabira city, mines as well as the deposits are in the open so the mined materials are exposed the to wind and weather, producing more particulate matter. Besides that, the mines are located within the urban perimeter, so the inhabitants are directly exposed. According Singh and Perwez (2015), open-cast mining is more deteriorating to air quality than underground mining.

Braga et al. (2007), concludes in his study that in Itabira, the most relevant source of inhaled particulate is the open-pit-iron ore mining.

The study also indicated that measures should be adopted to minimize the emission of mining pollutants and also suggest chemical and toxical analysis to determine the particles elements to clarify the role of each emitting source of PM10 that degrade air quality in Itabira. Reis (2000) stated that the villages located near Itabira iron mines showed higher concentrations of ore particles in the air and half of the city's population was confronted with respiratory problems.

Therefore, air quality monitoring and assessment are required to prevent and minimize the deterioration of air quality due to mining and other anthropogenic activities, as found by Singh and Sharma (1991) and Sharma and Singh (1992).

The main objective of this study is to determinate and quantify the elements in the fine

(PM2.5) and (PM10 -PM2.5) air particulates using x-ray fluorescence spectroscopy technique.

#### **METHODS**

The particulate material was collected in a small volume sequential sampler (AFG), this device collects the particulate material by inertial impaction in two separate fraction. Particles with a diameter up to 2.5  $\mu m$  were collected by filters with pore mesh of 0.4  $\mu m$  and coarse particles with diameters between 2.5 and 10  $\mu m$  were collected by filters with a 8  $\mu m$  mesh. The air monitoring last for 40 days.

The filters were analysed by x-ray fluorescence spectroscopy using a Rigaku, RIX 300 X-ray spectrometer. The analysis were made at LAPAt at the university of São Paulo (USP) to determine the concentration of the elements such as Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, As, Se, Br, Rb, Sr, Zr, Mo, Cd, Sb and Pb.

#### FINDINGS AND ARGUMENT

Analysis by X-ray Fluorescence allowed to determine which elements are present in air particulates. Figure 1 shows the major trace elements present in the fine and coarse particulates, respectively.

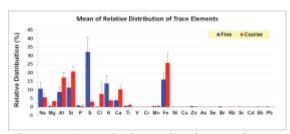


Figure 1. Mean of relative distribution of trace elements.



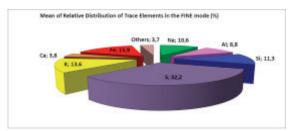


Figure 2. Mean of relative distribution of trace elements in the fine mode (%).

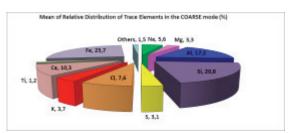


Figure 3. Mean of relative distribution of trace elements in the coarse mode (%).

Figure 2 shows elements of higher concentration in the fine mode and figure 3 elements of higher concentration in the coarse mode.

It was noticed that the elements present in the fine mode are the same as those of the coarse, except for Mg and Ti that only appear in the coarse mode. Al, Ca, Si and Fe concentrations are higher in the fine fraction and Na, S, K are higher in the coarse mode.

Although some elements have high concentration, none of them exceeded the limit value of any international standard (EU, 2008). Heavy metals such as Cu, As, Cd and Pb had a mean concentration in the fine mode of 0.7767; 0.1306; 0.1761 and 2.2731 ng.m<sup>-3</sup>, respectively and 1.2100; 0.1336; 0.1597 and 0.1231 ng.m<sup>-3</sup> in the coarse mode. None of them also presented value above the standard limit. According to Dee et al. (1973), the concentration level of pollutants found below the National Ambient Air Quality Standards are not correctly interpreted as fair and acceptable air quality, but sometimes the concentrations are sufficiently high to pose serious environmental and health problems. For this reason, further studies will be necessary to evaluate the effects of particulates on the health of Itabira inhabitants.

Roeser and Roeser (2010) and Da Costa (2003) analysed "Quadrilatero ferrifero" soil, the region where Itabira is located. The soil in this region has a great amount of Hematite (Fe<sub>2</sub>O<sub>3</sub>), magnetite (Fe<sub>0</sub>O.Fe<sub>2</sub>O<sub>3</sub>), dolomite (CaMg (CO<sub>3</sub>)<sub>2</sub>) (FeS<sub>2</sub>), pyrite (FeS<sub>2</sub>), Chalcopyrite (CuFeS<sub>2</sub>), arsenopyrite (FeAsS), Amphobolic Itabirito containing Fe, P, SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, CaO, MgO. Most of these elements present in the soil of the region correspond to the particles collected in Itabira, which leads to the belief that

these particulates are mainly due to resuspension of the soil dust.

#### **CONCLUSIONS**

In the last years, air pollution has been identified as a serious public health problem in the world. The concentration, as well as the composition of atmospheric particulates, are directly related to respiratory diseases, in the city of Itabira.

The problem related to low air quality has been increasingly emphasized, even more, because this city has an extensive iron ore mining activity and there are a few studies about it, so little is known about the amount and chemical composition of particles. For this reason, atmospheric particulates were collected in the Amazonas neighborhood near a mine during 40 days. The particulates were analyzed by fluorescence spectroscopy. Through this initial study, it was noted that the composition of the atmospheric particles contained metals present in the soil of this region, then this result suggests that those particles came from soil resuspension, not so much from vehicles pollution.

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### ASSESSMENT OF DAILY AND ANNUAL CONCENTRATIONS OF PM<sub>10</sub> IN THE CITY OF FLORIANÓPOLIS

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Abstract: To investigate the air quality in the city of Florianópolis (state of Santa Catarina, Brazil), sampling for PM<sub>10</sub> was performed using a high-volume sampler. The monitoring was conducted between November 8, 2011 to June 6, 2016 with a total of 225 samples. The annual and daily concentrations were compared to Brazilian (CONAMA 003/1990, State of São Paulo) and international (WHO, U.S. EPA and EU) air quality standards. The highest daily concentration of PM<sub>10</sub> was 87 μg m<sup>-3</sup> observed in 2011. This result is lower than the current limit of 150 μg m<sup>-3</sup> set for Brazil and the U.S. EPA; however, it is higher than that recommended by the WHO, the final target of the São Paulo state and the EU standard (i.e., 50 μg m<sup>-3</sup>). In contrast, EU standard allows 35 exceedances each year for 24-h concentrations of PM<sub>10</sub>. The historical average of PM<sub>10</sub> concentration was 24 μg m<sup>-3</sup> (annual range from 20-32 μg m<sup>-3</sup>). Therefore, annual means violate in all years the WHO guidelines and the target value of the state of São Paulo of 20 μg m<sup>-3</sup>. The maximum annual average established by CONAMA 003/1990 of 50 μg m<sup>-3</sup> was exceeded, as the EU standard of 40 μg m<sup>-3</sup>. Furthermore, the temporal profile of the PM<sub>10</sub> concentrations was investigated. According to upto-date air quality standards in Brazil, the air quality in Florianópolis complies with the permissible limits for PM<sub>10</sub>.

*Keywords*: air pollution, inhalable particulate matter ( $PM_{10}$ ), monitoring, air quality standards.

#### INTRODUCTION

The air pollution particularly due to particulate matter with aerodynamic diameter less than 10  $\mu$ m (PM<sub>10</sub>) is a global issue that can directly affect the human health and the environment. Airborne particulate matter (PM) is a pollutant composed of solid and liquid droplets (dust, soot, oil, metal and pollen) that can remain in suspension for long periods in the atmosphere due to its diminutive size, usually less than 100  $\mu$ m. PM originates in several human activities, with emphasis on industrial and vehicular emissions (COSTA et al, 2009). Additionally, PM can also be emitted by natural sources, such as volcanic eruptions and resuspension of soil material because of wind action (COLLS; TIWARY, 2010).

Extensive studies have established linkage between the size of the particles and the type and intensity of adverse effect caused in humans. Fine particles (PM<sub>2.5</sub>) have been more strongly associated with mortality and morbidity, whereas coarse particles (PM<sub>2.5-10</sub>) have been related to respiratory hospital admissions (MINGUILLÓN et al, 2008). The adverse characteristics associated with PM<sub>10</sub> involves both the shape and mean aerodynamic diameter particle, as the chemical composition. Besides, it is clearly understood that the air quality of a certain site depends not only on emission sources, but also more decisively on meteorological elements with multifaceted characteristics present at several spatial and temporal scales (JUNENG et al, 2011).

Undoubtedly, monitoring is a fundamental pragmatic tool for the management of air pollution. Many monitoring activities are performed for compliance purposes. In this regard, current

Brazilian federal legislation on air quality is established by Resolution CONAMA N° 003/1990 (CONAMA, 1990), which includes ambient air limits for  $PM_{10}$ . Moreover, in Brazil, the Decree N° 59.113 of the State of São Paulo (São Paulo, 2013) stands out, because had its limits updated based on World Health Organization guidelines (WHO, 2006) and European Union EU regulatory framework (European Commission, 2008).

This work reports a comparison of both short-term (daily) and long-term (annual average) concentrations of  $PM_{10}$  monitored between 2011 and 2016 in the city Florianópolis with air quality standards. Moreover, we explored the temporal variability of the  $PM_{10}$  concentrations over the months of monitoring.

#### **METHODS**

The study occurred at the Federal University of Santa Catarina, located in Florianópolis (Santa Catarina, Brazil, 27°36'02.2"S, 48°31'05.7"W). PM<sub>10</sub> samples were collected using a high-volume sampler (Energética Qualidade do Ar, Brazil) equipped with PM<sub>10</sub> cutting head to collect the target pollutant on a glass fiber filter (GE Healthcare/Whatman, 0.6 µm pore size; 20.3 cm x 25.4 cm). The sampling procedures followed the guidelines of the Brazilian standard ABNT NBR 13412/1995 (ABNT, 1995). The net mass gain of the pollutant was obtained using an electronic micro balance (AY220; Shimadzu, Japan) accuracy. Consequently, concentrations were determined by gravimetric analysis due to the ratio of the mass retained on the filters and the air volume drawn by the equipment during sampling. Results were corrected to the standard condition (298 K and 1013 mbar).



Meteorological data (i.e., temperature and atmospheric pressure) was obtained from the LEPTEN weather station (www.lepten.ufsc.br), which is located  $\approx 300$  m from the study area. A total of 225 samples were collected between October 2011 and June 2016.

The criteria used for comparison purposes were Resolution CONAMA N° 003/1990; final goal set in Decree N°. 59,113 for the state of São Paulo; National Ambient Air Quality Standards (NAAQS) for the United States of America (U.S. EPA, 2012); WHO guidelines (WHO, 2006) and European Union standard (European Commission, 2008). The target and maximum values set under these legislations can be found in the next section.

#### FINDINGS AND ARGUMENT

Figure 1 shows the comparison between the daily concentrations of  $PM_{10}$  during 5 years of monitoring with air quality standards used as reference. Discontinuity of  $PM_{10}$  measurement line (in red) indicates gaps in the monitoring due to equipment maintenance. The maximum average daily concentration of  $PM_{10}$  was 87  $\mu g$  m<sup>-3</sup> recorded in September 13, 2011.

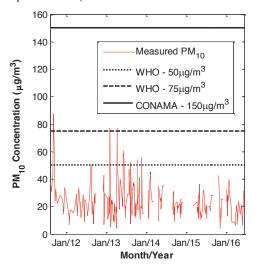


Figure 1. Measured daily concentrations of  $PM_{10}$  and comparison with air quality standards.

The daily limit of 150  $\mu g \ m^{-3}$  for  $PM_{10}$  which is set by Resolution CONAMA N° 003/1990 was not exceeded for the monitoring site. Besides, U.S. EPA states that the primary and secondary standards for  $PM_{10}$  should not exceed 150  $\mu g \ m^{-3}$  more than once per year for an average over 3 years. Thus, the North American standard for  $PM_{10}$  was not violated either. The WHO guidelines and the EU standard (50  $\mu g \ m^{-3}$ ) allow the daily concentration to exceed the limit by up to 35 occasions during one year. However, in the period of investigation  $PM_{10}$  daily concentrations exceed the threshold in 9 occasions. WHO interim target-3 (IT-3) of 75  $\mu g \ m^{-3}$  for 24-h concentrations was exceeded three times from 2011

to 2016. The distribution of  $PM_{10}$  annual averages is presented in Figure 2. For all years, the limit established by WHO and the final goal set by Decree N° 59.113 for State of São Paulo of 20  $\mu g.m^{-3}$  was reached. Conversely, the CONAMA N° 003/1990 and EU standards were not exceeded. From to 2011 to 2016 the annual averages of  $PM_{10}$  were 32  $\mu g~m^{-3}$ , 22  $\mu g~m^{-3}$ , 26  $\mu g~m^{-3}$ , 23  $\mu g~m^{-3}$ , 20  $\mu g~m^{-3}$ , and 20  $\mu g.m^{-3}$ , respectively. The historical average of the period (i.e., 2011-2016) was 24  $\mu g~m^{-3}$ . Most of upper outliers occurred in 2013.

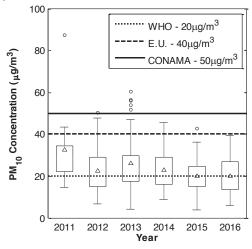


Figure 2. Annual average concentrations of  $PM_{10}$ .

To demonstrate the widespread profile of  $PM_{10}$  concentrations among the months, we can observe the changes in median values in Figure 3. This monthly analysis shows the highest variation and median value for August (winter). There are relatively different monthly concentration patterns with the narrowest total range observed in March (summer with typically higher precipitation amounts than other seasons). This indicates that meteorological parameters play a significant role.

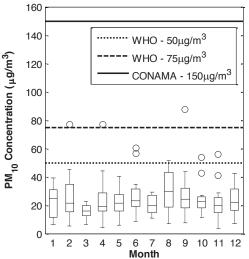


Figure 3. Monthly variability of  $PM_{10}$  concentrations.





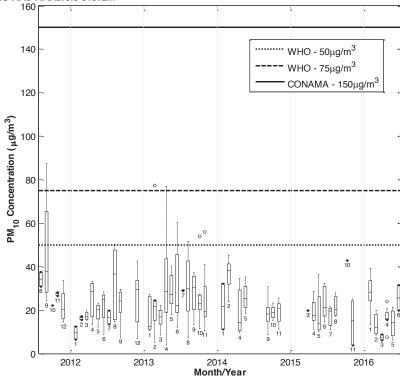


Figure 4. Individual monthly variability of PM10 concentrations between August 2011 and June 2016.

To deliver an individual monthly profile of the mass concentrations over the years, we present Figure 4. For 2012, 2013 and 2015 during the colder months and usually lower precipitation rates, greater  $PM_{10}$  concentrations were observed. This was not verified for 2015 due to sampling failures and for 2016 because this investigation closes in early winter.

#### CONCLUSIONS

During the  $PM_{10}$  monitoring program conducted from 2011 to 2016 in the city of Florianópolis, the current national standards set for Brazil were not exceeded for both daily and annual limits. Therefore, the air quality in Florianópolis complies with the maximum tolerable levels for  $PM_{10}$ . However, WHO annual average guideline is not respected. Accordingly, the concentration levels observed can indicate possible long-term adverse effects of the residents. Further investigations on the influence of meteorological factors can validate the influence of weather conditions in the  $PM_{10}$  concentrations. Finally, the reasonable estimate of historical average of  $PM_{10}$  can be used as a background concentration for modelling studies in Florianópolis and region.

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### Variance analysis applied to ground-level ozone concentrations in São Paulo State, Brazil

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This study applied the variance analysis (ANOVA) technique to ascertain patterns associated with the variability of daily maximum ozone concentrations registered between 1996 and 2013 in 32 sites in São Paulo State, Brazil. The whole dataset was analyzed through a randomized design arranged in a factorial layout (4 x 2 x 32) with four repetitions per treatment where the first factor (a) represented seasons, the second factor (b) distinguished measurements taken on weekdays and weekends, and the third factor (c) distinguished each of the 32 sites. Results presented a three-way interaction between the factors mentioned. It was also possible to identify that maximum ozone concentrations occurred generally during the spring, followed by summer; also, higher values of ground level ozone were registered on weekends in most sites, especially those influenced largely by vehicle emissions.

**Keywords**: Ozone; ANOVA; Weekend Effect

### Session 10 Air Pollution Control



### GAS-SOLID SEPARATION OF A CYCLONE ADAPTED WITH WATER SPRAYERS

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Abstract: Sugarcane bagasse is a lignocellulosic material used as fuel in the energy cogeneration process. Consequently, the burning of the biomass in question generates gaseous pollutants, specifically the Particulate Material, which when emitted to the atmosphere is harmful to the environment and to human health. Therefore, from a cyclone adapted with water sprayers, the objective of the work was to obtain the maximum efficiency of collecting particles derived from the sugar and alcohol industry. For this, the influence of the variables gas velocity, rotation of the feeding dish, temperature and time of collection, were optimized through experimental planning techniques. After fixing the optimal experimental condition, the effect of the addition of water under the collection efficiencies was evaluated by the use of sprayers. The highest collection efficiency of the isokinetic sampling was 81.33%, being increased to 82.43% after the optimization. The fractional efficiency curve for the optimized test showed that there was no collection for the particles with a volumetric diameter of less than 0.3 μm and that for particles with a 10 μm volumetric diameter, the collection efficiency reached 100%. The addition of water to the configuration in which all the sprayers were open, increased the collection efficiency of the isokinetic sampling from 82.43% to 96.64%, representing a 14.21% improvement. In general, it can be concluded that, with the optimization of the separation processes and with the addition of water in the system, the cyclone achieved satisfactory collection efficiency when compared to other gaseous efluent treatment equipment, representing a good use for the sugar and alcohol industry.

Keywords: Air Pollution Control, Gaseous Effluent, Particulate Material, Soot.

#### INTRODUCTION

The Brazilian sugar and alcohol industry has been gaining prominence in the world scenario, not only for its large production scale, but also for the awareness it has been taking from the year 2000 onwards. An example of such awareness is the use of waste from the sugar and ethanol production process for energy cogeneration, which is intended to meet the needs of the industry and in case of surplus, to provide energy for the public electricity grid.

The importance of energy cogeneration using bagasse lies in the fact that it coincides with the dry season of hydroelectric plant reservoirs and, therefore, has an important complementary character (UNICA, 2011). On the other hand, the burning of bagasse for energy cogeneration associated with the interaction between local meteorological conditions promotes air pollution, generating considerable environmental and public health problems.

In this way, it is necessary to control the air pollution, which can be carried out by various equipment, such as cyclones, gas scrubbers, gravitational collectors, bag filters and electrostatic precipitators.

The determination of the most appropriate equipment is based on the study of the economic feasibility, technique, efficiency and compliance with the requirements of the current legislation. In this way, cyclones provide a more simplified removal of particulate matter from gaseous streams and present a low cost of installation and maintenance. The spray adapted cyclone is based on a single cyclone in which a water spray system is adapted, aiming at increasing the collection efficiency of the Particulate Material. Thus, solid particles separated from the gas flow towards the bottom of the cyclone, where the collection takes place in the form of sludge, that is, water together with the Particulate Material (MACINTYRE, 1990). The water injected into the system aims to agglomerate the particulate, which results in a better separation of the cyclone and consequently in a high efficiency for particles smaller than 10 um. Therefore, from a cyclone adapted with water sprays in a laboratory scale, the objective of the work was to obtain maximum particle collection efficiency from the sugar and alcohol industry.

#### **METHODS**

The cyclone used was constructed respecting in principle the geometric relations established by



Stairmand (1951) as showed in Figure 1. However, in order to increase the collection efficiency, eight cylindrical cylindrical structures of the cyclone were coupled with eight fan-type water spray nozzles, with an opening diameter equivalent to 1.8 mm, thus modifying the design proposed by Stairmand.

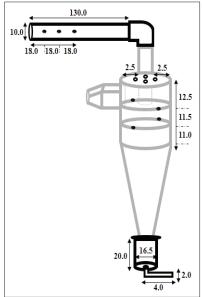


Figure 1. Experimental system (cyclone) used to perform the experiments.

Particulate Material (soot) used to feed the cyclone, was obtained from a sugar-alcohol plant, originating from the exit of the boilers. The determination of the granulometric distribution of soot particles was carried out using the Malvern Mastersize MicroPlus particle analyzer, MAF 5001, with a volume diameter of 9.0 µm and a density of 2.35 g.cm<sup>-3</sup>. For the morphological and elemental chemical characterization of the Particulate Material, the Scanning Electron Microscopy (SEM) technique, coupled to the X-ray Dispersive Energy Detector (EDS), was used by scanning electron microscope model XL-30 FEG - Philips, with the presence of Carbon (31.2%), Oxygen (9.1%), Silicon (51.5%), Potassium (1.1%), Calcium (2%) and Magnesium (2.9%).

For the experiments without the use of water sprays, the variables gas velocity (m.s<sup>-1</sup>), plate rotation (%), temperature (°C) and collection time (min) were considered. With this, a Box-Behnken type factorial design was done, with three replications in the center point and three levels (maximum, medium and minimum). As a result of the planning, 27 different trials were proposed.

As for the experiments with water sprayers because of the difficulty of establishing a single value for the water flow variable in relation to the amount of nozzle, a statistical experimental design can not be developed. Thus, through the technical,

financial and operational feasibility, a simple planning was developed, but covering 24 representative combinations of equipment, through different nozzle arrangements and their respective water flows.

The tests were performed equally for both cyclone entrance and exit using Schleicher & Schuell brand membranes, made of ester mixture, with a pore size of  $0.8~\mu m$  and diameter of 47~mm.

#### FINDINGS AND ARGUMENT

Among the 27 experiments performed with the cyclone operating without the water sprays, the best result was reached for experiment 7, which reached the efficiency of 81.33%. This experiment was carried out using the variable gas velocity of 30 m.s<sup>-1</sup>, the rotation of the plate of 90%, the temperature of 75.5 °C and the time of collection of 40 min. On the other hand, the worst result was obtained for experiment 12, which reached 50.38% efficiency. The same was done with the gas velocity of 10 m.s<sup>-1</sup>, the rotation of the dish of 60%, the temperature of 75.5 °C and the collection time of 20 min. It can also be observed that most of the experiments reached a percentage of efficiency in the range of 70 to 80%, being carried out under different conditions.

With the results of collection efficiency of the isokinetic sampling ( $\eta$ ) on hand, all values obtained for the 27 experimental configurations were fed to the Statgraphics XVII® database in order to allow the statistical treatment. Thus, a more robust analysis was performed and it was verified that only the variables gas velocity and collection time were significant (Figure 2).

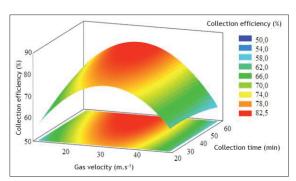


Figure 2. Response surface methodology.

As can be seen, the color scale increases from blue to red as the optimal point is reached. It can be seen from Figure 2 that the collection efficiency of the isokinetic sampling is higher in the range of 25 to 35 m.s<sup>-1</sup> gas velocity for a collection time of 50 to 60 min.

In a more simplified way, it is possible to observe in the contour surface, that the velocity of gas less than 20 and greater than 40 m.s<sup>-1</sup> causes a decrease in the collection efficiency of isokinetic sampling, which is also aggravated by the decrease



of the collection time, confirming the optimum mentioned above.

In addition, analyzing the determination of the significant and insignificant variables, it was observed that Koch and Licht (1977) and Massarani (2001) arrived at the same result presented by the present work, since they affirm that there is efficiency gain when there is increase of gas velocity and that ideally, it is a velocity of up to 30 m.s<sup>-1</sup>. The rotation of the plate was insignificant, since regardless of the percentage of rotation, there is the feeding of Particulate Material in the system. On the other hand, the variable time of collection was considered as significant, since the provides increase οf the same, representative, the collection of particles in the system, in relation to shorter times. Finally, the temperature was determined as insignificant, because the elevation of the same entails proportional increase of the viscosity of the gas, causing the fall in the collection efficiency of the isokinetic sampling. This fact can also be verified by Koch and Licht (1977).

The comparison of diameters is not a correct practice, since each one is about different relations. However, the conversion of the volumetric diameter (Dv) into aerodynamic diameter (Da) was shown to be close as reported in Figure 3.

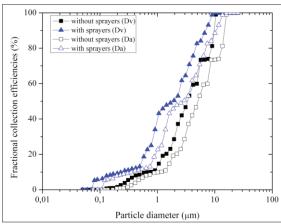


Figure 3. Results for the experimental fractional collection efficiencies, given in volumetric diameter (Dv) and aerodynamic diameter (Da).

One of the major disadvantages of dry cyclone will be its low fractional collection efficiency of approximately 60% for the range of respirable particles, those with Da less than 10  $\mu$ m. However, as can be observed in Figure 3 and for the same range of particles, with the addition of water in the system, efficiency of up to 93% was achieved. In contrast, when thinking about public health and the environment, even with the addition of water in the system, the cyclone studied presented fractional collection efficiency results of concern.

Since, for the range of inhalable particles, those with Da less than 2,5  $\mu m,$  the maximum efficiency obtained was 32%.

Thus, considering some of the elements found in the chemical characterization of soot and if we were dealing with an industrial plant, this percentage of efficiency for the collection of inhalable particles, associated with the exposure time, could cause several damages to human health and the environment environment. As for example, the development of silicosis, disease triggered by the inhalation of silicon powder; Pulmonary siderosis, disease caused by the inhalation of Iron powder; As well as burned, caused by the reaction of Magnesium, which is highly flammable.

#### **CONCLUSIONS**

Through the experimental planning and all operational settings established for the variables gas velocity, plate rotation, temperature and collection time, the maximum collection efficiency achieved for the experiments performed without water sprayers was 81.33%.

The water spray in the system was more expressive in the experiment in which all spray nozzles were open, allowing the collection efficiency of the isokinetic sampling to increase from 82.43 to 96.64% of the optimized experiment without water sprays in relation to the experiment carried out with water sprayers. However, for the range of inhalable particles, those with Da less than 2.5  $\mu m$ , the maximum efficiency obtained was 32%.

Finally, it can be concluded that with the optimization of the processes and with the addition of water, the cyclone achieved significant collection efficiencies when compared to other gaseous effluent treatment equipment, representing a good alternative of use for the sugar and alcohol industry. However, in the case of public health, post-filtration of inhalable particles is recommended.

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#### PULSE JET BAG FILTERS: WHY INVEST IN SCIENTIFIC RESEARCH?

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Abstract: The industrial air filtration by bag filters, although being a traditional method of gas cleaning, was not a priority in research for a long time in function of the limitations of the fibers manufacturing technology. The development of new synthetic fibers and the growing worldwide concern about breathable air quality have renewed attention to this technique. The bag filter is known to have high particle collection efficiency, reaching values greater than 99.9% for a wide particle size range including submicron particles and has some advantages over other industrial air filtration systems. Despite being a consolidated equipment in the market, there is still a lot to be developed and improved, especially regarding the filtration of fine (PM2.5) and ultrafine (PM0.1) particles by industrial bag filters. So this article presents the challenges industry faces in relation to bag filters and how scientific research can help improve them.

Keywords: Air filtration, bag filter, fabric filter, baghouse, pulse jet cleaning.

#### **INTRODUCTION**

The bag filter is known to have a collection efficiency greater than 99.9% for a wide particle size range including submicron particles, and is an equipment whose construction and operation are simple (Sparks and Chase, 2016). However, it offers an appreciable resistance to gas flow, which implies the need to work at low air-to-cloth ratio (0.5 to 10 cm/s) to maintain the pressure drop at operational levels and, consequently, large filtration areas are required, reaching thousands of square meters and so a large amount of bags are needed. Therefore, improvements like small reductions in pressure drop, optimizing filter cake removal and increase bag life results in significant reduction of construction or/and maintenance costs (Leith and Allen, 1986).

Although bag filters have been used for many years in the removal of particulate matter and are consolidated in the industrial processes of air filtration, there is still a great demand by the industries in improving its performance, especially concerning bag life span which has a great impact on maintenance costs. However, for this to happen, it is necessary to invest in scientific research to generate more knowledge about this equipment, especially about innovative filter medium that are resistant to high temperature and humidity and that are more efficient in the capture of ultrafine particulate (nanoparticles), with lower energy expenditure (Leith and Allen, 1986).

Much of the scientific research on filter bags to date has been focused on filtration theory rather than solutions to real problems faced daily by an industry. Thus, there is still a need to better understand the challenges faced by the bag filter users and how scientific research can collaborate with them. Strengthening the relationship between university research and industry is important to meeting the real needs of companies and help reduce their operational costs, as well to generate more knowledge and improve this filtration process.

#### **ARGUMENT**

In 2015, the bag filter market amounted to 9.13 billion US dollars, and it is estimated that in 2020 12.12 billion US dollars will reach (Marketandmarkets, 2016). One factor contributing to such growth is the reduction of emission limits by environmental agencies around the world, which requires more efficient filter medium. Generally, environmental standards are based on PM10 to indicate emission limits, such as the Brazilian resolution of CONAMA n 382. As fine particles (PM2.5) was classified as a first-degree carcinogen by the World Health Organization (WHO), these standards in Brazil are still being revised to include them in legislation. In Brazil, for example, in 2013 some states have issued decrees setting tougher emission limits for particulate matter, as Espírito Santo (state decree no. 3463), São Paulo (state decree no. 59113) and Rio de Janeiro (state decree no. 44072). They were based on a WHO guideline (WHO, 2006) that proposes emission limits for PM2.5 and PM10, as reported in Table 1. As stated in WHO (2006), by reducing the PM10 limit from 70 to 20  $\mu g/m^3$ , air pollutionrelated deaths are reduced by around 15%. So it's necessary to use more efficient filter medium for both PM10 and PM2.5, combining high life span and



low cost, which is possible through scientific research.

Table 1. Air quality guidelines for particulate matter

Particulate	Annual mean	24-hour mean
matter PM2.5	(µg/m³) 10	(µg/m³) 25
PM10	20	50

Reference: Adapted from WHO (2006)

In addition to complying with the emission limits determined by the authorities, the industries also seek to minimize their operating costs. In order to achieve this, they must use a filter medium which material stands for the gas characteristics (temperature, humidity corrosivity) and the particulate characteristics (hygroscopy, abrasiveness and size). It is also necessary that the filter has extended span life and operate with low pressure drop, high collection efficiency and low emission.

However, industries have been premature failure of the filter bags due to holes and tears. They reduce its life span and consequently the frequency increase replacement of the bags, which generates a high cost of maintenance. A possible reason for these problems is the inadequate selection of filter medium for a certain industrial process. Usually the selection is done by choosing the most appropriated filter medium from the tables provided by suppliers and/or by analogy with other processes. A third form of selection - more technical and less subjective - is through scientific research, by running tests that simulate the process operating conditions, evaluate the performance of different filter medium, and analyze variables such as collection efficiency, residual pressure drop, cleaning frequency and particle penetration through filter media. In this way, the material selection would be underpinned by experimental data, so that it would minimize premature failures of the bags and avoid unnecessary costs.

However, this type of study is rare in the literature and one of the reasons is poor collaboration between universities and industry. As a result, much of the scientific research is focused on filtration theory rather than solutions to real problems faced daily by industry. In addition, there are few research groups in Brazil, such as the Department of Chemical Engineering of UFSCar and Department of Industrial Technology of UFES, which seek to understand these difficulties.

Thus, it is important for industries to strengthen the relationship with universities by investing in scientific research in order to obtain the most suitable filtering medium for their bag filters, which has a long life span and is in

compliance with emission limits of the environmental regulations.

#### **CONCLUSIONS**

So why should industry invest in scientific research related to it? As previously discussed, the following reasons can be cited:

- Emissions limits are getting more stringent, both as to PM10 and PM 2.5, so that requires a most efficient filter medium;
- Premature bag failure due to tears and holes can be attributed to inadequate selection of filter medium. A possible solution is to underpin this selection by running tests that determine the most suitable filter medium for a specific process;
- Through scientific research it can be obtained a high quality filter medium that guarantees low emission, resulting in a better air quality and contributing to the reduction of air pollutionrelated health issues.

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### EXPERIMENTAL TECHNIQUES FOR THE CARACTERIZATION OF AIRBORNE PARTICULATES EMISSION FROM MINERAL PRODUCTS

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Abstract: Due to the risk associated with inhalation of dust, several control mechanisms have been adopted. The presence of water in the the particles interstices is a viable option to inhibit the dust generation. Another form of control is the use of surfactant solutions. Therefore, this work aims to develop a bench to characterize the dust generated during the handling of the material, using the dust tower technique, which enables material discharge tests, causing dust generation and simultaneously makes the direct measurement of the respirable airborne particles for the evaluation of the suppressing agents efficiency. Another objective is to evaluate the material drying mechanism and emission of dust particles generated during train wagon transportation. To reproduce the airflow over the wagons, a 600mm x 600mm section wind tunnel, capable of reaching speeds up to 30m/s, and a 1:20 scale model are used. The wagon speed infuence on the dust emission is evaluated by means of two air speeds, 40km/h and 70km/h, for different moisture content. For dust tower tests, dry coking coal and at 5% moisture has been evaluated. The results show that the use of water only is able to significantly reduce the emission of dustness. In the wind tunnel tests, iron ore pellet feed at 12% moisture was used. The results show that the increase in the air speed causes a greater dustness emission.

Keywords: Dust generation, Particulate emission, Dust tower, Train wagon, Dust supression.

#### INTRODUCTION

Air pollution caused by the dust generated during handling and rail transportation of ores is a serious problem. Given the risk associated with the inhalation of dust, the air quality regulation has established increasingly stringent standards. In 1987, the EPA (Environmental Protection Agency) adopted standards to regulate the concentration of particles with 10µm of diameter or smaller (PM10), since the greatest health risks come from the particles which can become imbedded into the lung tissues and not only from those easily inhaled. In 1997 the EPA adopted the first standards for particulate matter with 2.5µm diameter (PM<sub>2.5</sub>) or finer, claiming that these particles are retained in lung tissue, causing irritation or necrosis (EPA, Thus, several mechanisms of dust suppression have been studied, especially those regarding to the use of surfactant solutions. Most of these studies state that the best dust suppressant are those which wets the fine particles with ease, because it decreases its contact angle. However, it characterizes just how the suppressor wets a given material, which does not correlate directly with the ability to suppress dust (Cristovici, 1991). In order to address this gap, some studies have been carrying out aiming to develop techniques to evaluate the efficiency of suppressors, such as the use of a dust tower which simulates the material behavior during its handling (Copeland and Kawatra, 2011). Another issue is related to the emission of particulates during

transportation of ores. Leal Filho et al. (2011) studied iron ore dustiness generation during rail transportation using an experimental unit composed of a wind tunnel 6m long and 0.5m in diameter capable of reproducing air velocities up to 28m/s on a 1:50 scale train wagon prototype. Ferreira and Vaz (2004) also used a 2m x 2m section wind tunnel with 13.4 m/s speed and 1:25 scale wagon models to evaluate the emission of dust during the coal transportation.

#### **DUST TOWER AND TEST PROCEDURES**

In order to measure the emission of dust from materials, a bench has been developed based on the dust tower designed by Copeland and Kawatra (2011), capable of reproducing the handling of various materials and measuring the dust generated during the process. However, some modifications were made in relation to the original project to fit the needs of the current project, such as the inclusion of a lifting system consisting of an electric hoist, a hopper and a rotary valve, to facilitate the lifting of the material to be tested to the top of the dust tower (preventing the operator from climbing stairs to manually dump the material), increasing the test autonomy and controlling the mass flow of through the tower. The facility has a total height of 5m, in which the height of falling (dust tower part) of the material is 2.4m. This height has been chosen since it is generally found in the handling of iron and coal ores. A suction system was coupled to the side



pipe of the dust tower for aspiration of the finer particles of the material, simulating the airborne dust particles. To measure the PM10 and finer particles released on falling material through the tower, an isokinetic nozzle is used inside the piping coupled to a Particles Plus 8306 particle counter. Figure 1 illustrates the dust tower developed by the Federal University of Pará.

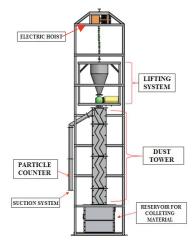


Figure 1. Dust tower facility.

The dust tower test procedure is done by preparing 3kg of sample material at a desired moisture, with the aid of an automatic mixer, for a better homogenization of the solid and water. The sample is then taken to the hopper and, with the aid of the lifting system, is suspended until the test height. The dust tower components are then assembled and fastened with screws and rubber between the components flanges for system sealing. After the dust tower is completely assembled, the vacuum system is switched on until the operating mode is reached. The suction airflow is regulated by a frequency inverter that controls the fan rotation and, consequently, the suction speed. The particle analyzer is then switched on for 15s with a sampling rate of 2s to measure the particle concentration in the environment and establish a reference line. The rotary valve is then activated, releasing 1kg material to flow through the dust tower. The particle analyzer stays on for another 30 seconds after the material has completely run through the dust tower. With the remaining 2kg of material in the hopper, two other tests are performed (1 kg per test). For this paper, only three test are performed for each material at a specific moisture.

#### TRAIN WAGON MODEL IN WIND TUNNEL

To evaluate the emission of particulates during the transport of material in train wagons, an open test section (600mm x 600mm) blower wind tunnel has been used, with a maximum velocity of 30 m/s, to simulate the train wagon speed during material

transporting. A 1:20 scale model of a wagon used in the transportation of iron ore by the company Vale in the Vitória-Minas Gerais railroad (EFVM), was constructed of sheet metal with dimensions of 430mm x 120mm x 72.4mm.

The layout of the wagon model inside the test section of the wind tunnel is shown in Figure 2. The model is placed on a metal support, which is part of the weighing system, using a load cell with a resolution of 5g. A 6mm diameter L-type pitot tube and a KIMO MDP-2500 handheld micromanometer are used to measure the air flow velocity in the test section. Relative humidity and ambient temperature are measured by means of a TESTO 622 thermo-hygrometer.



Figure 2. Train wagon model test in wind tunnel.

The test procedure begins with the preparation of the sample material to be tested for a given moisture. Then the wagon model is filled completely with the material and its initial mass is measured. The wagon model is then positioned inside the test section of the wind tunnel on the weighing system and the wind tunnel is turned on at the desired speed. Due to the aerodynamic forces acting on the model, every 15min the air flow is interrupted to weigh the mass of material in the wagon, for further calculations of the mass loss. In this work, two air flow velocities are evaluated: 40km/h and 70km/h, which are minimum and maximum values, respectively, usually found for the speed of a wagon used in the EFVM. Each test has a total duration of 90 min. At the end of the test, the wagon model with the material is taken to an electric muffle, at 100°C for 24h, for drying and determination of the material moisture. Only three tests are performed for the same moisture and velocity, to try to ensure a better reliability of the results.

#### **RESULTS**

The Vale Institute of Technology (ITV) provided 2 different ores (Pellet Feed and Coal) to be evaluated for dust emission in both the dust tower and wind tunnel. Figure 3 and Figure 4,



respectively, present the Particle Matter (PM) results obtained for the sample of dry and at 5% moisture coking coal.

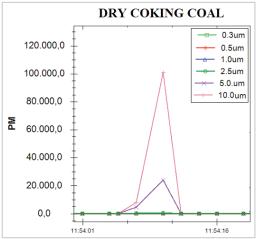


Figure 3. Particle concentration (PM) as a function of time for dry coking coal.

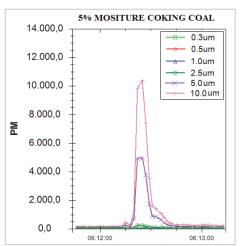


Figure 4. Particle concentration (PM) versus time for coking coal at 5% moisture.

The dry and the 5% mositure sample have been initially used to verify the influence that the amount of water present in the material has on the dust suppression during handling. The results show that the dry material presents a peak in the amount of particles of  $10\mu$ m and  $5\mu$ m, with a maximum value of 100,000, while in the wet material, this value is reduced to 11,000.

The Pellet Feed was tested in a wind tunnel to evaluate the influence of the speed of the wagon on the emission of dust, through two air velocities, 40km/h and 70km/h, at 12% mositure. Figure 5 shows the comparison between the loss of mass of material during 90min of test, for each speed. The results show that the greater the speed of the wagon, the greater the loss of mass of material

and, consequently, the greater the dust generation.

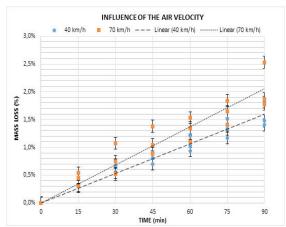


Figure 5. Pellet Feed mass loss for different air velocities.

#### **CONCLUSIONS**

The emission of ore particulates has been extensively studied due to the health problems caused by the finer particles. Thus, several mechanisms of suppression of dust emission have been used. This work presents the development of a bench using the dust tower technique, which characterizes the handling of ores. The results found for tests with dry coking coal and at 5% moisture show that the use of only water already plays a significant role in reducing the emission of the finer particles. It was also evaluated the emission of dust in model of wagon to simulate the loss of mass and emission of dust during the rail transport. The results showed that for the same moisture content, there is a greater loss of mass and, consequently, higher emission of dust to the speed of 70km/h, when compared with 40km/h.

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### STUDY OF THE IMAGE ANALYSIS TECHNIQUE AS A MEASURING METHOD FOR FUGITIVE EMISSION VELOCITY FIELD

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Abstract: The air pollution emissions which are released to the atmosphere without being preliminary collected by capture system are called fugitive emissions. Currently, there is a lack of measuring instruments available to study and quantify them. The objective of the present work is to study the use of image analysis technique as a measuring method for fugitive emission velocity. To simulate a fugitive emission an experimental apparatus was built using an air humidifier with a special designed nozzle to better control the vapor emission. To capture the images, the camera was positioned in front of the apparatus, and the background was covered by a black sheet in order to ensure the contrast. The Lucas-Kanade algorithm was used to evaluate the vapor movement. It is possible to state that the velocity was captured by the analysis, once the vectors appear where and when the plume arises. Furthermore, vectors module, given by their size, increase with time along with the plume evolution, which shows qualitatively that the method captures velocity changes over time. The next step for validating the method is the comparison of the results with measures from PIV or sensible anemometer, given the very low velocities found. The present work highlighted the potential use of the image analysis technique for fugitive emission velocity field measurement.

Keywords: fugitive emission, image analysis, Lucas-Kanade algorithm.

#### **INTRODUCTION**

According to ERBES (1996), there are different potential air pollution emission points, which are: point source emissions, fugitive emissions, mobile source emissions and secondary emissions.

Fugitive emissions are those which are released to the atmosphere without being preliminary collected by capture system. This classification includes emissions that (1) escape of an existing capturing system whit exhaust hoods, (2) are emitted during material transfer, (3) are emitted from building housing material processing or handling equipment, or (4) are emitted directly from process equipment. (U.S. Environmental Protection Agency, 1993)

Currently, there is a lack of measuring instruments available to study and quantify fugitive emissions. EPA has developed methods to determine visually the opacity of air emissions (Method 9) and frequency of fugitive emissions (Method 22), which are related to dust concentration information.

One of the most popular instruments for local flow measurements in numerous applications is the Particle Image Velocimetry (PIV). This technique is a non-intrusive method based on a pair of timecorrelated particle images having a short time lag of several to hundreds of microseconds. The PIV measurement includes illuminating a cross section of the seeded flow field where multiple images are recorded using a camera located perpendicular to the light sheet ant then analysed to evaluate the displacement information (Jensen, 2004; Tu et al., 2017). However, such equipment is considered quite expensive (Prasad, 2010; Sayeed-Bin-Asad et al., 2016).

Previous work had been developed using PIV technique to estimate flow field of air pollution emissions (fugitive or not) for industrial applications such as Ansart et al. (2009), Furieri et al. (2012) and Els et al. (2013).

Hongwei et al. (2015) developed a study to compare velocity field obtained by using optical flow algorithm and PIV measurement. The authors concluded that the optical flow algorithm could obtain a smoother velocity field than PIV in the conditions of pixel scale and is more suitable for velocity field measurement of complex flow.

The objective of the present work is to investigate the use of image analysis technique as a measuring method for fugitive emission velocity field. By studying the air flow of the fugitive emission is possible to optimize the design of new and existing



air pollution control equipment, contributing to air quality improvement.

#### **METHODS**

To simulate a fugitive emission an experimental apparatus was built using an air humidifier with a special designed nozzle to better control the vapor emission (Figure 1).

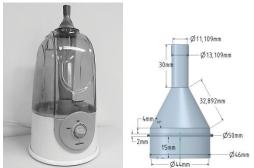


Figure 1. Air humidifier (left) and special designed nozzle (right).

To capture the images of the emission a Nikon camera D5500 was used. The camera was positioned in front of the apparatus, and the background was covered by a black sheet in order to ensure the contrast (Figure 2). A know dimension reference was fixed on the sheet to enable the conversion of the velocity from pixels/s and mm/s.

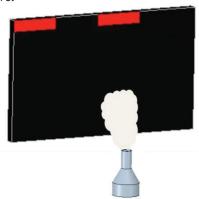


Figure 2. Scheme of the experimental apparatus.

The technique used to evaluate the captured images was the optical flow, and the algorithm was Lucas-Kanade, which estimates objects movements by looking at changes in pixel intensity. As a result, the algorithm gives a set of optical flow vectors distributed over the image (ROJAS, n.d.). The software used to run the algorithm was MATLAB®.

An anemometer was used to measure the outlet velocity.

#### FINDINGS AND ARGUMENT

For the analysis, there were captured 3230 images during the experiment.

Figure 3 shows the velocity field (vectors) evolution over time. It is possible to state that the velocity was captured by the analysis, once the vectors appear where and when the plume arises. Furthermore, vectors module, given by their size, increase with time along with the plume evolution, which shows qualitatively that the method captures velocity changes over time.

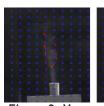






Figure 3. Vapor plume velocity field over time.

The calculated average velocity in the outlet region was 26.4 mm/s (0.0264 m/s), excluding outliers and considering time range which comprised the most stable flow, without external interferences such as wind and changes in lighting, which could compromise the analysis.

From the pictures it is also possible to observe that there is only one point in the region of the nozzle. This fact compromises the quality of the data obtained, and further trials with a larger nozzle or a reduced mesh are recommended.

The next step for validating the method is the comparison of the results with measures from PIV or sensitive anemometer, given the very low velocities found.

Also, further trials in industrial scale could contribute to the consolidation of this application. This evolution will be important in order to make cost effective field measurements for fugitive emission, enabling improvements in the design of existing and new equipment for air pollution control. In addition, this technique can be coupled with others, such as Computational Fluid Dynamics (CFD), in order to define optimized dedusting flow rates.

#### **CONCLUSIONS**

The present work highlighted the potential use of the image analysis technique for fugitive emission velocity field measurement. It was possible to observe that the method captures the movement of the vapor plume, calculating its velocity field. This technique could be a great resource in air pollution control within industry. In the trials, there was only one point in the region of the nozzle outlet, which could have compromised the quality of the data obtained. Further trials with a larger nozzle or a reduced mesh are recommended. In addition, industrial scale trials and coupling with other techniques such as CFD are suggested.



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### CFD analysis of the inlet duct influence on a Fabric Filter flow distribution

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Abstract: In order to minimize the particulate matter emission by the industry, air pollution control equipment are often used. The fabric filter, widely used equipment for dust control and material recovery, has high efficiencies when properly designed. Previous works have shown the benefits of using CFD simulation in fabric filters, especially to assess the impact of the layout on the flow distribution. This work aims to evaluate the influence of two inlet duct layouts on the flow distribution in an existing fabric filter. They are: (I) a base case, and (II) an alternative design, which considers a divided entrance duct in order to conduct a proportional flow rate to the hopper inlets. The results show that the flow rate distribution in each inlet is more uniform in the alternative design. However, the alternative layout does not have a positive impact on the flow distribution throughout the bags. Both cases show an uneven filtration velocity distribution, and areas which greatly diverge from the value set on project. The alternative case shows a worse pressure distribution on the outer surface of the bags, in such a way that this design modification is not recommended.

Keywords: CFD, fabric filter, gas filtration, air pollution control

#### INTRODUCTION

Industry is an important source of air emissions and, in order to reduce its impact on air quality, measures to prevent and control air pollution must be taken. To minimize the emission of particulate matter (PM), complying with air emission standards, fabric filters are widely used (Cooper and Alley, 2011). In this equipment, dusty gas flows through a number of fabric bags, in such way that the particulate is retained and the clean gas is released.

There are several important design variables to be considered such as: filtration velocity, cleaning method, can velocity, fabric used in the bag and filter configuration. The last one was usually defined by the designer's know-how and experience. However, due to the exponential computational development in the last decades, the use of Computational Fluid Dynamics (CFD) to evaluate equipment design is gaining popularity. Previous works have shown the impact of the filter configuration on fabric filter's efficiency applying CFD simulation to compare different designs (Pereira et al., 2015; Nielsen, Skriver and Castaño, 2011; Feldkamp, Dickamp and Moser, 2008; Damian et al., 2004).

In this context, this work aims to evaluate the flow distribution in a fabric filter installed on a steelmaking company, comparing current inlet duct and an alternative inlet duct configuration, using CFD simulation. In order to assess the effect of the design on the fluid flow, the pressure distribution and the mass flux throughout the bags in each design will be compared.

#### **METHODS**

The filter evaluated in the present work is part of the dedusting system of the raw materials handling of a Blast Furnace of a steelmaking company in Serra, Espírito Santo. The main features of the filter are the following:

- Flow Rate: 119,982 m<sup>3</sup>/h
- 570 bags
- Filtration velocity: 1.71 m/min
- 175 mm of bags diameter
- Inlet velocity: 19.18 m/s

Alternatively to the current design, a proposal made when the filter was conceived is evaluated, in which a divided inlet duct would aim to achieve a better distribution of the flow throughout the hopper inlets.



A geometry construction was performed using ANSYS SpaceClaim software for both base case and the alternative, which are shown in Figure 1. Note that the only modification in alternative design is the inlet duct, all other features are maintained. Geometry mesh was performed using Meshing module. To ensure that the results were not influenced by the mesh, a mesh independence test was performed considering the velocity profile on the filter outlet. The final mesh had 26.7 million nodes.

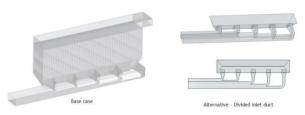


Figure 1. Base case and alternative design

The modelling was based on the governing equations of mass and momentum conservation and the simulation used the Finite Volume Method in the CFX 16.0 software. The flow was considered steady state, the fluid incompressible, the conditions isothermal and no particles were considered. Boundary conditions prescribed were inlet mass flow, outlet pressure and no slip wall. In the alternative design, 40% of total mass flow rate was prescribed in the fraction directed to the first two inlets and 60% to the last three inlets. The turbulent model was k- $\epsilon$  and the porosity model was based on Darcy's law. The values of the porosity, 81.5%, and permeability, 5.0178x10<sup>-11</sup> m², of the bags were obtained from a supplier.

The simulation was performed in parallel processing in 16 cores in a computer with 128 GB of RAM.

#### FINDINGS AND ARGUMENT

Assessing the results of the base case, a pressure drop of 1017 Pa (105 mmwc) was found. Once the simulation did not considered the dust particles, it is important to highlight that the pressure drop due to the dust cake formed on the surface of the bag was not taken into account. The dust cake is an important contributor for the total pressure drop in a fabric filter. For comparison purposes, the pressure drop of a typical operating fabric filter in the same application in this industry is around 1470 and 1765 Pa. In the start-up of similar fabric filters, with clean bags and no dust cake, a pressure drop of 780 to 1080 Pa have been found in the same plant.

Evaluating the mass flow in each hopper inlet (Figure 2) it is possible to see that the distribution is more uniform in the alternative design, which was expected as the inlet flow rate was divided

proportionally to the first two and the last three inlets.

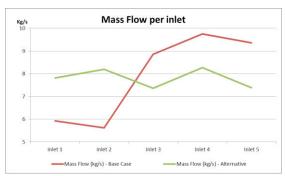


Figure 2. Mass flow per inlet in base case and alternative

The filtration velocity distribution is shown in Figure 3 (left). It is possible to see that, in general, the division in the inlet duct does not have a strong impact on this variable. In both cases, the filtration velocity distribution is very uneven. It is important to highlight that the filtration velocity stablished on the project is equivalent to 0.029 m/s. In general, both cases show areas reaching values very different from the project. It is important to highlight that, with the cake formation, these results may change. However, the air flow distribution is satisfactory for comparison purposes.

Looking closer to the posterior side of the filter, evaluating the pressure distribution on the outer surface of the bags (Figure 3, right), it is possible to see that the alternative case negatively impact its uniformity. It is possible to identify pressure peaks close to the inlets 1 and 2. This indicates an uneven flow distribution and, therefore, uneven cake formation. This can reduce filtration efficiency as a few areas will receive a higher dust load, whilst others are underused.

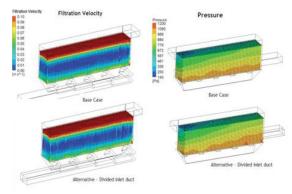


Figure 3. Filtration velocity distribution and pressure distribution throughout the bags

The total pressure drop in the alternative case was 1045 Pa, slightly higher than the base case (1017



Pa) explained by the increased turbulence on the hopper region.

The filtration velocity distribution is inadequate in both cases and should be improved. The division of the inlet duct as proposed did not enhanced the flow distribution as expected previously, which indicated the advantages of using CFD simulation previously to equipment modifications.

Further design modifications, especially in the inlet duct, can be evaluated using CFD and are recommended. Additionally, a reduction of the filtration velocity should be evaluated, as the project value (0.029 m/s or 1.71 m/min) is rather high compared to values used currently for this application.

#### **CONCLUSIONS**

The work reinforces the advantages of using CFD simulation as a practice in the industrial sector to evaluate the design of dedusting system equipment. For the particular case, CFD was used to assess two different inlet duct designs, with or without division of the flow, in terms of mass flow rate in each inlet, filtration velocity distribution and distribution of the pressure on the outer surface of the bag. The results show that, although the flow rate distribution in each inlet is more uniform in the alternative design, the divided inlet duct does not have a positive impact on the flow distribution throughout the bags. recommended the evaluation of different inlet duct layouts and alterations in the filtration velocity by reducing total inlet flow rate.

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### Comparison between EN 779 and the literature efficiency for collection efficiency of nanoparticles

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Abstract: The intense heat waves induces people to become increasingly dependent upon air conditioners on. The energy comsumption and the air quality can be damaged if an unapropriate filter is used. The balance between filter efficiency and pressure drop should be take into account when looking for the suitable filter. However, it is complicate to choose which them is the best when there are many options at the market filter with distincts applications. The differences between Standardization of filters tests also difficultes the understanding of their real performances. The brazilian standard is ABNT NBR 16101:2012, which is completely based on EN779 (European). Considering this purpose, the goal here is to make a comparison of efficiency values obtained between EN779 methodology and literature review. Then, the aim of this work is to evaluate the efficiency of micro glass filter by european and literature pathways. The filter media area was 17.42 cm² and it was used 0.1% of DEHS in Isopropyl alcohol as aerosol. The methodology used was the technique of eletric mobile, where was possible to count the number of particles upstream and downstream the filter media. The results for 0.4 μm were similar, close to 100% using both options (European and literature). However, the results showed lower efficiency (94%) for other particle sizes. Maybe, the European Standardization should include other particle sizes (0.17μm) to the efficiency estimation as American (ASHRAE 52.2) does.

Keywords: filter media, nanoparticles, EN 779, efficiency.

#### **INTRODUCTION**

Nowadays, people spend great part of their time with air conditioners on. In order to achieve better levels of air quality, there are some filters inside air conditioners to collect unwanted particles. They are cheap, easy handling and sometimes even renewable.

Although their great convenience, the market offers a variety of filters for air conditioners. They can be pleated, bag, panel or even HEPA (High Efficiency Particulate Air Filter), between other models.

In addition to these models, their filter media can also be different. Cellulose, polyester, micro glass, quartz and activated carbon are some options.

Despite this wide range of filters, it is difficult to find the best one when there are many options at the filters market with different performances. Their performances as efficiency and drop pressure are certified based on Standardization of filtration tests.

There are two main International Standardization of filtration tests that are followed in Brazil: European (EN 779) and American (ASHRAE 52.2).

According to these standardizations, there are two main proprieties of filter that should be analyze in order to define its performance. The first on is efficiency. It describes the filter capacity to retain particles when the flow is passing through it. Permeability is the second propriety. It measures the resistance (drop pressure) to the air flow through the filter media. As time went on, filters efficiency and pressure drop get higher. This last factor contributes to increase the energy comsumption. Now, it is possible to understand why it is important to find the suitable filter for each situation. The equilibrium between efficiency and pressure drop should be considered before making a choice.

The American Standardization (ASHRAE 52.2) has developed its own way to measure efficiency. It is based on MERV (Minimum Efficiency Reporting Values). Three efficiency is computated for a range of polydispersed particle size: E1 (0.3-1.0 $\mu$ m), E2 (1.0-3.0  $\mu$ m) and E3 (3.0-10.0  $\mu$ m). Together, the three values of efficiency will define the filters performance. Here, all the tests are executed using KCl as aerossol. Together, E1-E2 and E3 defines the filter MERV classification.

MERV classification goes from 1 to 20 number. Coarse filters have lower efficiency (less than 40%) and are represented with lower MERV numbers (1 to



8). The middle filters (less than 80%) are classified as 9 to 12 MERV numbers. The fine filters (less than 95%) are 13 to 16 MERV numbers. Finally, absolute filters (above 95% of efficiency) are 17 to 20 MERV numbers.

On the other hand, European (EN 779) defines efficiency only based a monodispersed particle size of 0.4 µm. The aerossol used here is Di-Ethyl-Hexyl-Sebacat (DEHS). Here filters are divided into three categories: course, middle and fine filters. Course filters as denominated as G1-G4 own efficiency less than 40%. Middle filters (M5-M6) own 40-80% of efficiency. Finally fine filters (F7-F9), efficiency above 80% and below 95%. Above 95%, filters are classified as HEPA (High Efficiency Particulate Air Filter).

In addition to these two standardizations, there is a brazilian standards(ABNT NBR 16101:2012). It is completely based on the European.

Despite these standards, there are some studies using a conventional way to calculate efficiency. It is simply based on the difference between up and downstream number of particles of the filter media. Bortolassi (2017), Barros (2016) and Donovan (1985) found values of efficiency using this pathway.

The difference on tests execution and the way of results are showed may cause difficults to understand the real performance for each filter.

Considering this concern, it is necessary to better understanding the difference of two main Standardization: European (EN 1822/779) and America (ASHRAE 52.2).

Since brazilian standards are based on european, the study here, first will executate tests on this standardization. Then, the results shown here refers to EN 779. America Standardization tests will be executed afterwards.

The main objective of this work is to make a comparison between efficiency values estimated by EN 779 and literature review way to estimate efficiency.

#### **METHODS**

Firstly, the filter media characterization was made. The fiber diameter, porosity, thickness and permeability coefficient can be found in the Table 1. All of them, except permeability, were obtained through Inspect S50 SEM (Scanning Electron Microscope) photographs. The photos were analyzed using the software Image Pro plus 7.

All the measures were taken at room temperature around (26-28°C) and humidity between (35-55%). The filter media area was 17.42 cm². It was used 0.1% of DEHS in Isopropyl alcohol as aerosol. Before the experiment gets started, every leaking was checked and contained. For each measurement of permeability and efficiency was executed three times. In other words, there are three points for each measurement.

The filter media used was HEPA (High Efficiency Particulate Air Filter) of glass. They were provided by Energy Industry and Trade LTDA.

The results of efficiency and permeability were obtained using air stream provided by an air compressor (Shulz). Before passing through the filter apparatus, the air flow passed to some air purification filters (Model A917A-8104N-000 and 0A0-000) and a Kriptônio and Americium neutralizing source (TSI Model 3054). It was possible to control the flow rate (valve) and check the flow rate value (Gilmont Instruments Inc flowmeter). The number of particles up and downstream was computated by SMPS device (electrostatic classifier-TSI 3080 and ultrafine particles counter-TSI 3776).

#### FINDINGS AND ARGUMENT

The collection efficiency obtained by EN 779 Standardization is determined by a specific particle size  $(0.4\mu m)$ . According to the EN 779 it is necessary to collect 13 points, 7 upstream and 6 downstream and use Equation (1) and (2).

$$E_{1,i} = \left(1 - \frac{n_{i,1}}{\frac{N_{i,1} + N_{i,2}}{2}}\right) \cdot 100 \tag{1}$$

$$E_i = (E_{1,i} + E_{2,i} + E_{3,i} + E_{4,i} + E_{5,i} + E_{6,i})/6$$
 (2)

Where  $E_i$  is the average efficiency for a particle size I;  $n_{1,i}$  is the number of particles downstream and  $N_{1,i}$  upstream.

In addition to these equations, the literature brings other possible pathway to estimate efficiency using a third Equation (3).

$$E_{1,i} = \left(\frac{N_{i,1} - n_{i,1}}{N_{i,1}}\right) \cdot 100 \tag{3}$$

In this work, both equations were used and the results for  $0.4~\mu m$  were similar, close to 100%. The European, using Equation (1) and (2) gave an efficiency of 100 %. Now, the literature pathway, using Equation (3) brought 99.788 % of efficiency.



It is possible to see the comparison of efficiency between the two methods in Table 2. Although the values of efficiency were similar, using the Equation (3) results were more precisely.

It is interesting to notice that efficiency depends on the particle size. The Figure 1 brings collection efficiency in function on particle size. The results varies from 0.94 to 1.00. The lower particle size the higher the efficiency value variation.

This last observation leads us to question if European standardization efficiency approximates more to reality than American does. Since American computes a wide range of particle size in its efficiency values.

Table 1. Fiber media characterization

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Fiber diameter (μm)	1.01±0.57	
Porosity	0.92± 3.46E <sup>-2</sup>	
Thickness $(\bar{L})$ ( $\mu$ m)	409.9 ±28.44	
Permeability coeff (cm²) (K1)	1.02E <sup>-8</sup> ±4.16E <sup>-10</sup>	

Reference: Lista,2017.

Table 2. Collection Efficiency for 0.4 µm

European EN 779	100.000%
Literature Efficiency	99.788%

Reference: Lista, 2017

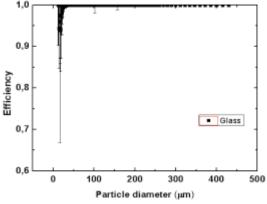


Figure 1. Collection Efficiency for different particle size

#### **CONCLUSIONS**

Evaluating the collection efficiency using Standardization Equation from EN779, glass filter HEPA obtained 100%. Measuring efficiency using a different equation also for  $0.4\mu m$  particle size obtained 99.788%.

The particle size influences on the efficiency results. It was noted a value of 94%. Therefore, as suggestions, it should be analyse the efficiency for more particle size beyond  $0.4\mu m$ .

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### DESIGN OF A LOCAL EXHAUST VENTILATION SYSTEM FOR LABORATORIES: A CASE STUDY OF COAL AND COKE LAB

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Abstract: In Coke plants, one issue is the analysis of the coke characteristics. Those analyses are performed in Coal and Coke Laboratories and the activities generates high contaminants emission in the work place. In order to guarantee that the contaminant concentration is low so that the workers will not have an exposure in excess of the stablished standards typically a local exhaust ventilation system is one of the best practice solution. Based on this context, the objective of the present study is to develop a design of a Local exhaust ventilation system for the coal and coke laboratories. The main emissions sources in those laboratories are: crushers, industrial sieve, drum index and sprayers. To establish the system it was designed the essential components such as hoods, ductwork, air pollution control equipment and fan selection. The hood will capture pollutants at their place of origin; the ductwork will conduct the airflow to the control equipment, which will filter the air before it is released into the atmosphere; and the fan is what supplys the energy to perform the suction of the exhaust system. The design was based on the recommendations of ACGIH Industrial Ventilation Manual and USEPA. The final project has a flow rate of 9.53 m³/s, and a system fan with static pressure of 199.55 mmca and power requirement of 28 hp. The use of a Local Exhaust Ventilation system is shown as a valid and effective method, however, it highlights that the association of this system with other reduction proposals of those risks is essential.

Keywords: local exhaust ventilation, particulate matter, dedusting system, coal and coke laboratory, occupational health.

#### INTRODUCTION

In the process of coal and coke characterization in laboratories, workers are vulnerable due to the large emission of dust. It is necessary to control these emissions in a way that does not harm the health of the worker. Often more than one strategy is used at the same time to protect workers health. The levels of recommended strategies, in their order of consideration and importance are (ACGIH, 2010): Elimination /substitution of the dangerous substance; Modification of the process; Engineering controls; Administrative control procedures; protective equipment (PPE). In coal and coke laboratories, the effective strategy adopted is engineering controls, through the installation of dedusting systems (ACGIH, 2010). A Local Exhaust Ventilation system consists of hoods, ductwork, air pollution control equipment and fan. The hoods will capture pollutants at their place of origin; the ductwork will direct the airflow to the control equipment; and the fan is who will supply the energy to perform the suction of the system flow. The measure is the best among the others, once the system captures the emission at its place of origin, thus preventing it from spreading into the environment. In this context, it is important an exhaust ventilation system in order to guarantee the air quality at the work place. Therefore, the objective of the present work is to design a Local Exhaust Ventilation system capable of controlling air pollution in coal and coke laboratories. To do this, the airflow required for the system will be determined through the evaluation of individual

emissions. Hoods will be designed for each point of emission. The ductwork for the transportation of contaminated in the air is also designed. The selection of a fan a the basic design for the air pollution control equipment will be performed based on the total gas flow.

#### **METHODS**

#### Case study description and associated emissions

Typically, coal and coke laboratories are located indoors and with little natural ventilation, thus contributing to the emitted particulate material remaining inside the laboratory. In order to control the emissions, a Local Exhaust Ventilation System will be designed for all emission points. It is important to mention that the methodology is valid for any laboratory of coal and coke with similar activities to those studied in the present work. Among the equipment that most contribute for a high emission, it can consider the crushers, sprayer, industrial sieve, drawer sifter and Drum Index. The crushers are used in the fragmentation of the material in suitable sizes. The sprayer is used to make the material even finer in the powder form. The industrial and drawer sieve performs, through mechanical vibration, the separation of the material by its granulometry. The Drum Index simulates the reaction of the coke inside the blast furnace, subjecting it to successive falls within a chamber. In this way, these 5 (five) equipment will be the focus for the design of the emission control system.



#### Design of the ventilation system

### <u>Hood design and determination of the total flow</u> rate

The first step of the project is to identify all the emission sources where the hoods will be installed. In addition, for the evaluation of the airflow required for the system, it will be necessary to obtain the position for each hood and to define the hood type. In the crusher (points 1, 2, 3, 4, 9 and 10), the emissions occurs at the top and bottom. In the drawer and industrial sieve (points 5 and 6) it occurs in the removal and tipping of the coke, respectively. In the Drum Index (point 7), the emission occurs in the removal of the coke from the equipment and in the sprayer (points 8, 11, 12 and 13), occurs in the cleaning and pulverization of the coal and manual sifting of the coke. The hood will be designed in accordance to the following requirements: hood type and shape, location in relation to the source, suction flow rate and pressure drop. The sum of the input flows for each of the hood, it was possible to estimate the total flow rate.

#### **Ductwork Design**

The velocity of airflow in the ducts will be defined based on the variation of velocities suggested by the Manual Industrial Ventilation (ACGIH, 2010). The speed can not be high to the point of causing deterioration of the duct walls, nor low, causing the deposition of the material driven. The diameter of the ducts is calculated from equation 1, where Q is the flow rate in the duct, V is the average velocity in the ducts and D is the duct diameter. The distributed pressure drop is calculated from Darcy-Weisbach's equation 2 (FOX et al, 2010), where f is the friction factor; L is the length of the stretch; D is the duct diameter; V is the average velocity in the ducts. According to Fox et al (2010), the localized pressure drop is calculated from equation 3, where K is the loss coefficient and can be obtained by using tables available in the bibliography. For the study, only the existence of 90° curves, 45° curves and drawer registration, calculated by means of the equivalent length, and branches, calculated from the coefficient  $\mathsf{K},$  were considered, obtaining the localized loss of load at the end. The sum of the two equals the total loss of charge in each section.

$$D = \sqrt{\frac{4 \times Q}{\pi \times V}} \tag{1}$$

$$h_{dist} = f \frac{L}{D} \frac{V^2}{2a} \tag{2}$$

$$h_{loc} = K \frac{V^2}{2} \tag{3}$$

#### Dimensioning of air pollution control equipment

Fabric filters are considered easy to install, operate and maintain. Dimensioning begins by defining the air-to-cloth ratio for the calculation of the total area, based on EPA (1995) and Cooper

and Alley (2011). Then the material of the sleeve is selected, its dimensions and quantities required, the number of compartments for the filter and the dimensions of the mirror, based on the number of sleeves. Finally, the cleaning system of the sleeves and the hopper is dimensioned. The input data for the dimensioning were obtained both from the bibliography, as well as from the experience of professionals in the area and suppliers of control equipment.

#### Dimensioning the chimney

For the dimensioning of the chimney for the exhausting of the gas without pollutants to the atmosphere, reference is made to Technical Standard L9.221 of CETESB (1990), which describe the Minimum sampling area dimensions. However, there are no minimum standards specified for the height of the chimney. Thus, the sizing will be based on data from the professionals' experience, so that it guarantees the minimum area required by the organ, considering a speed range between 16 and 20 m/s, since high speeds can generate noise. The load loss in the chimney is calculated according to equation 2.

#### Fan selection

For the selection of the ideal fan for the system, some operational information of the case under study is necessary: Processed fluid and gas density, altitude and temperature of operation, flow and static pressure at the input, static pressure at the output and static pressure of the fan. The static pressure of the fan (equation 4) is defined as suggested by ACGIH (2010), where SP<sub>1</sub> is the static pressure at the fan input; SP<sub>2</sub> is the static pressure at the fan output; VP1 is the dynamic pressure at the fan input and FSP is the static pressure of the fan. Taking the values of total system load loss, total design flow, and fan efficiency, the fan is selected from the driving power, which is calculated by equation 5, where N is the driving power,  $Q_T$  is The total design flow,  $\Delta p_T$  is the total system loss, and  $\eta$  is the fan efficiency.

$$FSP = SP_2 - SP_1 - VP_1 \tag{4}$$

$$N = \frac{Q_T \, x \, \Delta p_T}{3600 \, x \, 75 \, x \, n} \tag{5}$$

#### FINDINGS AND ARGUMENT

In all, there are 13 points of capture of particulate material. The equations for the calculation of flow rates and capture velocity were defined based on ACGIH recommendations (2010). With this information, we obtain the flow rates for the points, as well as the pressure drop in the capture, as shown in Table 1.

The Table 2 present the summary of the ductwork design, which was considered the airflow and velocity inside the ducts, diameter and pressure



drop. In the velocity choice, it was decided to use 17 to 25 m/s. Static energy balancing was also chosen in order to guarantee the desired airflow in each captor while maintaining the desired velocity in each branch and in the main duct.

Table 1: Summary of the dimensioning of the captors for each

ennission point.					
Captor	Position	V (m/s)	Q (m³/s)	Pressure drop (mmca)	Section
1	Point 1	10.00	0.50	44.14	1-K
2	Point 2	1.00	0.36	41.03	2-K
3	Point 3	10.00	0.50	44.14	3-J
4	Point 4	1.00	0.36	43.27	4-J
5	Point 5	1.00	0.33	41.91	5-H
6	Point 6	1.00	0.35	39.86	6-G
7	Point 7	1.00	1.50	44.40	7-F
8	Point 8	1.00	1.80	44.52	8-F
9	Point 9	10.00	0.50	47.32	9-E
10	Point 10	1.00	0.36	49.56	10-E
11	Point 11	1.00	0.90	45.74	11-D
12	Point 12	1.00	1.17	45.61	12-C
13	Point 13	1.00	0.90	45.41	13-B

Table 2: Summary of the ductwork dimensioning for each section.

		secu				
Parameters	1-K	2-K	K-I	3-J	4-J	J-I
Airflow (m³/s)	0.50	0.36	0.86	0.50	0.36	0.86
Velocity (m/s)	21.03	21.28	21.00	21.03	21.85	17.89
Diameter (mm)	174.6	146.8	228.8	174.6	144.8	247.9
Pressure drop	44.64	44.64	1.85	45.23	45.23	1.27
Parameters	I-H	5-H	H-G	6-G	G-F	7-F
Airflow (m³/s)	1.73	0.33	2.05	0.35	2.40	1.50
Velocity (m/s)	21.47	21.51	21.32	20.97	23.46	22.14
Diameter (mm)	320.0	138.7	350.0	144.9	360.7	293.7
Pressure drop	0.41	46.91	0.60	47.56	0.83	48.39
Parameters	8-F	F-A	9-F	10-E	E-D	11-D
Airflow (m³/s)	1.80	5.70	0.50	0.36	0.86	0.90
Velocity (m/s)	22.17	17.88	22.01	23.39	17.17	22.47
Diameter (mm)	321.6	637.0	170.6	140.0	253.0	225.8
Pressure drop	48.39	0.86	F0 F0			10.01
	40.39	0.86	50.52	50.52	1.69	49.26
Parameters	D-C	12-C	50.52 CB	50.52 13-B	1.69 B-A	49.26 A-VC
Parameters	D-C	12-C	СВ	13-B	B-A	A-VC
Parameters  Airflow (m³/s)	D-C 1.76	12-C 0.90	<b>CB</b> 1.76	13-B 0.90	B-A 3.83	A-VC 9.53

The flow registered in section A-VC is the total airflow system and to be treated in the fabric filter, in this case  $9.53~\text{m}^3/\text{s}$ . Table 3 presents the summary of the dimensioning of the fabric filter in question. According to the methodology of dimensioning of the chimney, the project airflow and velocity in the chimney (adopted 16~m/s), we have the section area of  $0.60~\text{m}^2$  and diameter of 840 mm. Since the distance from the soil to the fabric filter is 9.34~m, a 14.34~m chimney is used. The pressure drop obtained in the chimney was 5.28~mmca.

The total system pressure drop was 199.55 mm, so it will be necessary to install a 28 hp fan to supply the entire system.

Table 3. Summary of the dimensioning for the fabric filter structure.

Fabric filter structure			
Description	Parameter	Value	Unit
Total airflow	Q	571.83	m³/min
Air-to-cloth ratio	$V_f$	1.12	m/min
Total filtration area	$A_f$	508.75	m²
Diameter of sleeves	D <sub>m</sub>	160	mm
Sleeves length	Lm	4	m
Sleeves area	Asleeves	2.01	m²
Number of sleeves	N <sub>sleeves</sub>	253	-
Number of sleeves per row	$N_{sleeves,row}$	11	-
Number rows	N <sub>row</sub>	23	-
Number of compartments	N <sub>c</sub>	1	-
Total Mirror Area	Ae	15.81	m²
Spacing between sleeves	е	0.25	m
Duct velocity input	$V_{di}$	17.00	m/s
Duct velocity output	V <sub>do</sub>	20.00	m/s
Output area	A <sub>output</sub>	0.48	m²
Duct diameter output	$D_{do}$	779	mm

#### **CONCLUSIONS**

The use of a Local Exhaust Ventilation system is a valid and effective method for controlling emissions in coal and coke laboratories, since they are captured at source. The evaluation of the individual emissions of each source, resulted in 13 main points. A total flow rate was then determined of 9.53 m<sup>3</sup>/s. The duct transport velocity was defined in a rage of 17 to 25 m/s that wear could be avoided as well as dust settling. The ductwork was designed based on balance-by-design method. Based on the experience of professionals in the area and from the methods used, it was possible to size an air pollution control equipment with the dust collecting efficiency in accordance with the regulatory limites. Finally, the total static pressure due to the system loss is 199.55 mmca, requiring a fan with a power of 28 hp adequate of exhausting all airflow.

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## COMPARING MEASURED EMISSIONS FROM CONVEYORS WITH COMPUTATIONAL FLUID DYNAMICS SOLUTIONS

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**Abstract:** This work was developed to provide an analysis of actual emissions from conveyors in a huge industrial installation and help to improve its control. The results obtained are believed to better describe the behavior of a complex flow inside a covered region with side inlets submitted to wind cross flows. Although the orders of magnitude of results from the CFD calculations differ from experimental evaluation it is important to realize that both are models, approximated physical and mathematical assemblies trying to reproduce the reality. Inferences from the results variations inside each of these two models are fundamental to feed and sustain the engineering decisions.

Keywords: Conveyors belt, CFD, emissions, models.

#### **INTRODUCTION**

Emissions from conveyors can be of some importance in total particulate material emitted from an industrial plant when large amounts of raw materials are handled. Impacts on the neighboring areas can be significant under some weather conditions. Emissions control methods based on water spray or addition of water to the handled material must be evaluated under the restrictions imposed by local rainfall regime and the seasonal behavior of water reservoirs levels.

Transportation of raw material with low water content can be considered along with improved design of conveyors covertures. The use of CFD (Computing Fluid Dynamics) to minimize emissions yields good results when the actual emissions scenarios are used as input. The more exact the knowledge of the input parameters the better the significance of the simulation results.

In fact even CFD modeling must be calibrated to achieve results with enough accuracy when compared with laboratory or in situ measurements to avoid errors in extrapolation of generated parameters for future designs.

When dealing with engineering solutions to avoid particulate emissions it is a good practice to test existent controls and compare effectiveness obtained under experimental tests with those generated by computational calculations validating and justifying the simulations of future solutions.

Experimental studies on conveyor emissions are sparse and the work by Kessler and Prenner1 is a good source of how to choose the influential parameters and how to introduce them in computational calculations.

Chen2 has studied experimental and CFD simulation of dust emissions from conveyor transfer chutes establishing a guide on how to select meaningful parameters for comparison between the two approaches.

In previous works by Bono and Awruch3, Anderson et al4 and Czétány and Láng5 is discussed the use of structured and unstructured mesh generation for use in CFD applications.

In this work, experiments were designed to measure particulate emissions from conveyors to compare its values with the results from CFD simulations aiming the establishment of more realistic emissions factors and the enhancement of design parameters to improve effectiveness of control systems by the so called engineered devices. Measurements were done to quantify the generated levels of potential emissions to be achieved under new engineered solutions to be proposed. The experimental setup was built at ArcelorMittal steel plant in Vitória, Brazil as part of a program to establish the importance of emissions from conveyors and chutes and to minimize their contribution to ambient particulate matter concentrations. The production in the steel



mill integrated unit is  $7.5\ \text{million}$  metric tons a year.

Coke and return material from sinter process charges were tested under 2 meters per second mean wind velocity calculated without the decimal places. The wind direction changes observed during the experiments tend to compensate the background influence when the sample results were filtered by average calculation.

#### **EXERIMENTAL PROCEDURES**

The experiments were conducted using high-volume (HiVols) samplers to collect suspended material and is expected that at under a 2 cubic meters per minute (m3/min) flow rate these samples are representative of particles up to 120 µm in aerodynamic diameter.

In the measurements of side emissions from conveyors exposed to transversal wind fields, four HiVols samplers were used forming a rectangle with 5 meters (m)  $\times$  3.6 m with the greater dimension along the conveyor longitudinal axis.

The air flow induced by HiVols did not influence the velocity field at the conveyors side output. The distance between the conveyors side and HiVols inlet was 0.8 m and the calculated radius of HiVols sphere of influence was 0.27 m, under 0.01 meter per second (m/s) capture velocity. A conveyor transporting coke, coded 332, and a conveyor transporting recirculation material from sintering process, coded SE01, were tested.

Samples of coke and recirculation material below 2 millimeters (mm) in diameter were submitted to particle size distribution analysis. The analysis results indicated that 80% of coke and 100% of recirculation material were below 100  $\mu m$ . The mean particle geometric diameters were determined to be 90  $\mu m$  for coke and 40  $\mu m$  for recirculation material. During the measurements water spray controls were turned off.

Both conveyors are covered with semi cylindrical shells but the side areas used to access the rolls and the return conveyor are kept open, as shown in the geometry defined for CFD calculations.

#### **COMPUTATIONAL MODELLING**

The conveyors geometry was approximated by a trapezoidal form, containing the solid material as a homogeneous phase of particles with geometric diameters 90  $\mu$ m for coke and 40  $\mu$ m for recirculation material. The air was treated as the second phase at 300 degrees Kelvin (K) and 0.1 megapascal (MPa).

The domain discretization was based on unstructured mesh, octree technique, covering three meters of longitudinal extension to make possible the evaluation of recirculation flows in that direction due to the combination of transversal wind field and the velocity field generated by conveyor movement. In the final configuration 800000 elements were used.

The discretization approach in the transversal planes of analysis generated a denser mesh at solid-air interface to better describe the erosion of material.

The mesh used in the cross section of the conveyor is shown in Figure 1.



Figure 1. Discretization mesh in the cross section of the conveyor.

#### RESULTS AND DISCUSSION

The results from HiVols sampling, as shown in Table 1, represent the material collected as milligrams (mg) for each metric ton of materials transported by the conveyors during the tests.

Table 1. Measurements of side emissions from conveyors.

MEAN LATERAL EMISSIONS FROM CONVEYORS				
	(mg/t)			
Stations	SE01 (return from	332 (coke)		
	sintering process)			
1	12.7	2.5		
2	12.3	0.6		
3	9.1	7.9		
4	12.3	3.9		

Reference: Rogério Queiroz jan/2017

If compensation for background concentrations due to the variation of wind directions are made, then the measured values can be taken as representative of the emissions orders of magnitude.

Under these assumptions the emissions from transportation of recirculation material from sintering process are three times the emissions caused by coke transportation.



Figure 2 depicts the volume fractions of solids generated by CFD simulations integrated along 3 m, when the charge on the conveyor is coke, case 1, and recirculation material from sintering process, case 2, considering semi cylindrical shells covers.





Figure 2. Coke charge (left) and recirculation from sinter process (right).

It is possible to infer from the two results that the coarse material recirculation under the shell is less intense than the recirculation calculated when finer material is used. This enhanced mix of finer material is caused by efficient transfer of momentum from the turbulent kinetic energy from air flow to the particles, causing the emissions.

Using image processing to identify the portions of the different materials that are leaving the conveyors is possible to quantify that ratio as 52, one order of magnitude greater than the experimental results. Probably this difference is due to the use of only one particle diameter to represent the entire charge on the conveyors instead of density probability functions to describe the particles diameters distribution. A solution for minimizing the emissions was tested and its results are shown in Figure 3

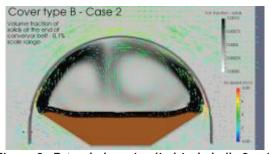


Figure 3. Extended semi cylindrical shell, 2 m/s transversal wind speed and charge of recirculation material from sinter process.

Extending the semi cylindrical shell causes the air flow to create quasi stagnation points that lead to momentum reduction inside the covered zone generating less intense turbulence and inducing less mixture of finer material.

As no decrease in the order of magnitude of CFD results is expected in this last approach when compared to experimental values it is possible to

state that the solution tested will cause less emissions, even if the solid charge is taken as a homogeneous phase composed by 40  $\mu$ m particles.

Used in this way, CFD simulations and experiments can be helpful to technicians and decision makers in establishing the necessary changes and enhancements in design of particulate emissions controls to use in conveyors.

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### PERFORMANCE EVALUATION OF AN ELECTROSTATIC PRECIPITATOR FROM THE SINTERING AREA OF A STEEL PLANT

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Abstract: This article presents the analysis of an Electrostatic Precipitator (ESP) that had a performance reduction in particulate matter collection. Isokinetic measurements and particulate matter characterization analysis were conducted, as well as sizing calculations based on the data of the existing precipitator. It was verified that the operating values differed from the design ones and, comparing them with usually recommended values by ENFIL S.A. Controle Ambiental, it was concluded that the current internal velocity was high and could be harmful for the equipment. Therefore, various process and construction recommendations were made for this particular ESP.

Keywords: Electrostatic precipitator, performance, particulate matter, CFD.

#### INTRODUCTION

The electrostatic precipitator (ESP) is an equipment used to remove particulate matter (PM) from a gas flow. Its working principle comprises the use of electrostatic forces to collect the suspended particles in the gas, with the aim of retaining the bulk of those particles inside the precipitator, which results in a clean gas flow exiting the equipment. The schematics of this equipment are presented in Figure 1.

The interior of the ESP consists of emission electrodes positioned between two collecting plates. When energized, the emission electrodes ionize the gas close to them, which allows the ions to couple to the solid particles in the gas, assigning them a positive or negative charge.

The particles are drawn to the collecting plates by Coulomb forces, being collected in a hopper after rapping of those plates.

ENFIL S.A. Controle Ambiental was hired by a Steel Company to evaluate the possible causes of the collecting performance reduction of the Electrostatic Precipitator installed in the primary sintering area of their steel plant.

The aim of this article is to analyse (1) the design of the ESP and compare it to the current design conditions, (2) the isokinetic measurements and (3) the ohmic resistivity, particle size distribution and chemical composition of the particulate matter, in order to recommend technical improvements for the performance of the equipment.



Figure 1. Schematics of a Dry Type Electrostatic Precipitator (ESP)

Reference: ENFIL S.A.

#### **METHODOLOGY**

The analysis of the ESP design was made through calculations based on the information given by the Steel Company. Hence, it was possible to compare current parameters with its corresponding design values.

The true migration velocity  $(W_d)$  was obtained from the data available in the isokinetic measurements' report, conducted by an Analytical Service Company. The methods used by this company are correct and, considering that all the procedures were strictly followed, the results are reliable. The dust collected from the ESP of the Steel Plant was submitted to CLEAN AIR in the U.S.A. for resistivity characterization (according to IEE 548-1984 Standard), chemical composition (according to ASTM D4326 methods) and particle size distribution (Bahco Centrifugal Classified,



procedures from ASME Power Test Code 28, Section 5).

Besides that, a computational fluid dynamics (CFD) study was conducted with the purpose of verifying the internal flow behaviour of the ESP based on design and operating values. The software STAR-CCM+ 11.02.010 was used for this, with the Reynolds Averaged Navier-Stokes, Realizable K-Epsilon turbulent model.

#### RESULTS AND DISCUSSION

Table 1 shows the design and current values according to the analysis performed.

Table 1. Summary of the process parameters analysis

anatysis			
Description	Design value	Current operating value	
Migration velocity (cm/s)	6.08	7.7	
Internal velocity (m/s)	1.5	1.93	
Collecting area (m²)	32,400	-	
Retention time (s)	10	7.7	
Ohmic resistivity (ohm.cm)	-	1.5 ×10 <sup>9</sup> to 3.0×10 <sup>9</sup>	
Chemical Composition	-	K <sub>2</sub> O and Na <sub>2</sub> O 0.39 %	
Particle size distribution (Fines < 1 µm)	-	2.18 %	

From the calculations based on the isokinetic measurements, a conservative value of migration velocity  $(W_d)$  was found, within the recommended range of 6 - 10 cm/s. Greater values of  $\,W_d$  result in smaller collecting areas, whereas lower values of  $W_d$  cause a larger performance margin in the precipitator.

The internal design velocity calculated is at the upper limit of the suggested value for this type of process (between 0.8 and 1.2 m/s). However, the current operating velocity is high, which might reduce the performance, especially considering that the flowrate tends to increase throughout the years, since the pressure and flowrate are both adjusted with the operation of the equipment.

The collecting area obtained by the design calculations shows that there's a reasonable design margin compared to the minimum area required; nevertheless, the operation occurs at a 20% margin. The retention time is below the minimum 10 s recommended. The high internal velocity plus the low retention time results in an unsuitable operating flowrate for the ESP.

The efficiency of the ESP was calculated based on the isokinetic measurements and was then related to the migration velocity  $W_d$ , as shown in Figure 2.

From Figure 2, it can be noted that the true efficiency of the precipitator is above the design condition, showing that, in a preliminary analysis, even with internal velocities above the design ones, the equipment reaches the necessary and sufficient efficiency to meet its design requirements.

Nonetheless, the particle concentration assumed at the entrance is optimistic and not proven by sampling. According to the ohmic resistivity, the value of  $W_d$  is 9.3 cm/s and, in keeping with ENFIL's criteria, the calculations should be done with a  $W_d$  within 9 and 10 cm/s.

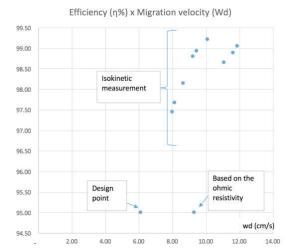


Figure 2. ESP efficiency versus migration velocity

Two resistivity measurements were made, at different moisture levels (7.9% and 10.1%), in ascending and descending temperature modes. The resistivity curves for both modes are similar for the different moisture values. From the graphs obtained (e.g. Figure 3, at 7.9% moisture), the maximum value of this parameter at the reference temperature of 150 °C was  $1.5 \times 10^9$  ohm.cm at 10.1% moisture and  $3.0 \times 10^9$  ohm.cm at 7.9% moisture, both below  $1.0 \times 10^{12}$  ohm.cm (high resistivity).

The resistivity value found can be considered intermediate, i.e. the dust is not critical for the electrical energization, hence it should be expected a good operating performance, which does not occur. Therefore, the resistivity is not limiting for the proper collection of the particulate matter.



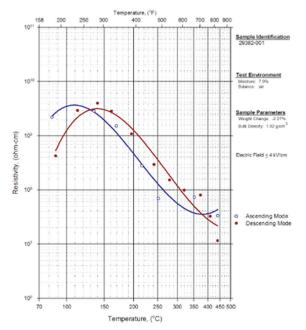


Figure 3. Ohmic resistivity graph, ascending and descending mode, at 7.9% moisture

According to the analysis of the chemical composition of the PM, the quantity of alkali ( $K_2O$  e  $Na_2O$ ) is a low and desirable value, which is interesting for the efficiency of the ESP. High alkali levels do not favour the particulate matter collection and allows for corrosion in the equipment and blast furnace refractory, for example.

The particle size distribution showed that there are more than 1% of fine particles (< 1  $\mu$ m), which are hard to be collected by the precipitator and increase the possibility of re-entrainment of dust in the gas flow.

In the CFD study, a high turbulence region was found in the connection duct with the entrance plenum, which results in an uneven distribution of flow that is harmful for the ESP (Figure 4a). Uneven velocities were also spotted inside the ESP, as well as diagonal flow streamlines.

Consequently, there was a need for a new flow distribution in order to correct the effects perceived. Thus, the positioning of guides inside the duct and the inlet nozzle, as well as a baffle plate in the first electrical field was studied. With the addition of these components, an improvement of the flow behaviour was detected, i.e. a better distribution of the flow and less occurrence of turbulent regions.

Figure 4b illustrates the computational simulation for the current operating mode and also for the improvement expected with the insertion of guides at the entrance duct of the electrostatic precipitator. The high turbulence region is highlighted by the dashed circles.

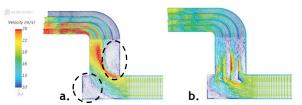


Figure 4. Velocities inside the connecting duct, obtained by CFD. (a) Current operating mode, with turbulence and (b) with recommended guides.

#### **CONCLUSIONS AND RECOMMENDATIONS**

According to the known design criteria, the equipment was correctly sized. Therefore, its performance reduction should be analysed with regards to the mechanical, electrical and operating construction features.

The current internal gas velocity is high and has no margins, which might result in a difficult energization of the dust and, hence, the collection of the particulate matter. Besides that, as the operating time increases, there is a tendency for the gas flowrate to become larger and, therefore, raise the internal velocity and re-entrainment of the particles in the gas flow, leading to the intensification of the dust emissions at the stack.

Following up the turbulent areas identified in the CFD study, a need for the correct directing of the gas flow was acknowledged as a way to avoid turbulence and improve the flow distribution inside the precipitator.

Based on the stated above, it is recommended to (1) operate at the design flowrate, i.e. reduce the entrance of fake air, improving the permeability of the sinter layer; (2) operate outside the temperature range where the resistivity is high, i.e. below 110 °C or above 140 °C; (3) reduce the alkali sources when possible, restricting them to 1% maximum and (4) install guides inside the duct and entrance nozzle, as well as one baffle in the first electrical field.

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# Assessment on the causes for Sinter Plant Stack Plume Visibility at ArcelorMittal Tubarao and ongoing investments in additional controls for visibility reduction

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Assessment on the causes for Sinter Plant Stack Plume Visibility at ArcelorMittal Tubarão and ongoing investments in additional controls for visibility reduction; The Sinter Plant Stack is one of the major atmospheric emissions sources of an integrated Siderurgic Plant. In order to controls its emissions, the Sinter Plant has air controls, in most of the cases equipped with Electrostatic Precipitators to comply with local standards. Despite de compliance with legislation, the visibility of emission is an issue that can generate complaints from the community due to the visual impact of the stack plume. Air emissions from a Sinter Plant stack were broadly characterized to evaluate potential contributors to visible emissions. Gases and aerosols in the stack gases can contribute to visible emissions to various degrees depending on their physical, chemical and optical characteristics. The most problematic of these emissions are those that are visible to the observer despite low mass emissions meeting environmental regulatory standards. Physico-chemical transformations and photochemical reactions among windbox stack gas constituents as the stack gases cool and mix in the atmosphere also influence plume visibility. Tests were conducted to characterize aerosol and aerosol precursors at the stack including: particulate matter (PM) concentration, size and chemical composition; condensable aerosol precursors (e.g., H2SO4, HCI); NOX and SO2 and other compounds. Selected measurements also were made at the electrostatic



precipitator (EP) inlet to assess EP performance. At this sinter plant, submicron aerosols, which are expected to contribute the most to stack plume opacity/visibility, comprise 40 percent of stack particle emissions by mass and more than 99 percent of the particles by number. Potassium and chloride, which are volatile at combustion temperatures, are enriched in the fine particles in the windbox gas, the dust collected in the EP and even further in the stack PM emissions. Potassium and chloride (probably as potassium chloride) are enriched in the fine particles and account for most of the submicron particles. While the overall EP collection efficiency for particulate mass was high, collection efficiency was very low for fine particles smaller than 10 µm. Although potassium and chlorine are found at relatively low levels in practically all of the feed mixture materials and contribute less than 1 percent of the total feed mixture, they comprise 10 percent of the PM at the EP inlet (mass mean diameter of approximately 100 µm) and 63 percent of the PM at the stack (mass mean diameter of approximately 1.9 µm). Sulfuric acid was present at very low concentration in the stack gas (less than 1 ppmv), and so is not expected to contribute significantly to visible emissions. The large fraction of submicron particles in stack emissions suggests they may play a significant role in visible emissions. Compared to other sinter plant studies, potassium and chloride were found at higher levels and mean particle size was considerably smaller in the stack gas. This highlights the unique nature of each sinter plant's emissions, most likely reflecting differences in feed materials, sinter plant design and operation, and emission controls. The results indicate that control of fine, submicron particle emissions is likely to have the greatest impact on predicted plume opacity and downwind visibility. Reducing emissions of fine particles, composed primarily of potassium and chlorine, has the greatest impact on predicted plume opacity for this site (90% of reduction). Sulfuric acid, SO2, HF and HCI were found to have insignificant contributions to predicted opacity.



These findings differ from another study, which emphasizes the unique nature of sinter plant emissions resulting from differences in feed materials and product requirements among different steel mills. In order to reduce considerably the visibility by removing the fine particles (dust emissions below 5 mg/Nm3), ArcelorMittal Tubarão started in 2016 the implementation of a new bag filter after the existing EP. This ongoing investment is foreseen to start up in January of 2018, performing gains with visibility reduction and air quality improvement due to the fine dust removal.