EVALUATION OF THE CHEMICAL TRANSPORT OF AIR POLLUTANTS IN THE METROPOLITAN REGION OF SALVADOR, BRAZIL

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ABSTRACT

Considering the fact that the exposure to polluted air has been associated with adverse health effects, 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 (MRS) in the Northeast region of Brazil, simulations using the Weather Research and Forecasting (WRF) and the Community Multiscale Air Quality (CMAQ) models were applied. The region's choice was due to the fact that, although Salvador is the 3rd most populated city in Brazil and its metropolitan area is the 7th most populated one, there is a lack of scientific studies about regional air quality and air pollution dispersion, especially in terms of photochemical regional impact assessment of pollutants in this urban area. The aim of this work was to assess the impact of atmospheric pollutants (NO_x and SO_2) over the MRS from stacks held in a petrochemical complex that lies within this metropolitan site. The emissions rates were based on another study since there is no official emissions inventory available for the region. Moreover, as there were no pollutant measurement data to be compared, a qualitative analysis was conducted. The results showed the importance of the application of the state of the art in the computational atmospheric modeling field in order to assess the air quality of the MRS.

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

1 INTRODUCTION

The development and application of appropriate air quality management strategies requires the proper diagnosis of pollution levels in a region. To this end, air quality monitoring stations are implemented with sophisticated instruments for measuring concentrations. However, pollutant concentration levels must be related to specific time and space scales and cannot be correctly represented based on monitoring data exclusively. Additionally, air monitoring is expensive and limited by analytical methods that may not provide detailed chemical composition information to support policy making [1]. Thus, in order to promote a fully evaluation of air quality over a region, 3-D chemical transport models (CTMs) are applied since they can fill these gaps about the information of population exposure to air pollutants. Among the many CTMs available, the Community Multiscale Air Quality (CMAQ) [2] is one of the most widely used air quality modeling system, and it is recommended by USEPA for regional and photochemical air quality modeling, therefore it is the one selected to be used in this work.

CMAQ is able to model multiple atmospheric contaminants, including tropospheric ozone, particulate matter, and a variety of toxic gases. It is used to assist both regulatory agencies and polluting companies in the assessment of air quality to determine the best air quality management scenarios for impacted communities and governments. Moreover, it represents the state of the art in air quality modelling, it has been extensively distributed

WIT Transactions on Ecology and the Environment, Vol 230,
www.witpress.com, ISSN 1743-3541 (on-line)
doi:10.2495/AIR180481

around the world and is maintained by an active scientific community that also develops constant evolutions to reduce the uncertainties in the simulations [3].

In addition to air quality monitoring, the modeling of meteorological fields is also needed to the air quality modeling. Meteorological parameters such as temperature, water vapor content, planetary boundary layer height, wind speed and direction also have effects on the forecasting of air pollutant concentrations and needs to be carefully evaluated [1]. The meteorological data used as input to CMAQ model in this work was generated by the Weather Research and Forecasting (WRF) model [4]. Both modeling systems are open-source powerful programs widely used in the world.

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 Metropolitan Region of Salvador (MRS), in order to provide some scientific background about the impact of local anthropogenic emissions.

2 METHODOLOGY

2.1 Study area description

The study area is the MRS, which is an urban-industrial area with a peninsular configuration, where the Bay of All Saints (*Baía de Todos os Santos*) (BTS) is located in the south-west of the region and, the Atlantic Ocean in the east (Fig. 1). The MRS is located in Bahia state, between the latitudes 12°20’S and 13°10’S, and longitudes 37°50’W and 38°50’W, formed by thirteen cities and it is occupied approximately by 3.6 million habitants distributed over an area of 4375 km^2 (Brazilian Institute of Geography and Statistics, 2010), being Salvador the major city and also the capital of the state of Bahia. The BTS is an inland bay of the Brazilian coast where the sea penetrates into the continent from a narrowing between the city of Salvador and the island of Itaparica. Its presence adds local humidity due to evaporation of the waterbody, modifying and creating a microclimate in the region.

According to the Köppen climate classification, Bahia’s coastline is located within the tropical humid climate that constitutes the so-called “Af zone”, with occurrences of precipitation monthly and the lack of a defined dry season. Even so in [5]–[7] analyzed the rainfall index of Salvador city and identified the wet period as April-May-June-July whereas the less rainy period is September-October-November-December. The mean annual temperature in Salvador is 26°C, and monthly averages vary between 24°C in August and 27°C in February and March. Relative humidity is high throughout the year, with an annual average of about 80%, where February is less humid (79%) and May is the most humid (84%), reaching a maximum humidity of 95%. [8] showed that the predominance of wind direction in the MRS during the year is from the east, followed by the east-southeast direction. The east (E) wind remains predominant between the months of October to March. The south (S) and east-southeast (ESE) wind are predominant in June and July while the south (S) and southeast (SE) wind are predominant in May and August. In terms of the hourly average wind speed, the highest values occur in the afternoon and, the lowest ones during the dawn and the early hours of the morning.

Beyond the activities related to tourism and commerce, the area also accounts with several industrial activities, which the main activities were enumerate at Fig. 1. The Cristal Pigmentos do Brasil S.A. (1) manufactures chemical products, including titanium dioxide and sulfuric acid, used in the manufacture of paint, paper, plastic bottles, vinyl siding and packaging materials, among others. The Camaçari Petrochemical Complex (PIC) (2) consists with the automobile plant of Ford Motors and its suppliers (among others Bridgestone

Firestone, Continental), and the petrochemical complex of Braskem that includes producers of petrochemical products used to make thermoplastic resins, fertilizers and copper metallurgy, as well as other applications. The Aratu Industrial Center (CIA) (3-4) has several enterprises of chemical segments, footwear, food, metallurgy, furniture, plastics, fertilizers, electronics, beverages, textiles. And lastly the Landulpho Alves Refinery (RLAM) (5) which belongs the Petrobrás S.A. and works with several petroleum products such as LPG, gasoline, diesel fuel, lubricants, paraffin, among others.

As one can see there are different industrial sources contributing to the total emissions over the region without counting motor vehicles. According to the National Traffic Agency, the MRS has a vehicle fleet which represent 30% of total amount of the state of Bahia, being around 75% of the total classed to Salvador city.

Notwithstanding the presence of various emissions sources, the present work focus on the atmospheric pollutants NO_x and SO_2 from stacks held in PIC due to the lack of information about the other industrial sources. In any way petrochemical sector represent a significant quantity of all industrial activities in the region and, according to [9], the petroleum industry produces more than 2500 refined products, employing a wide variety of processes which emit lots of atmospheric contaminants. Namely the most common air contaminants from oil–gas sector are volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs), nitrogen oxides (NO_x), sulfur dioxide (SO_2), methane (CH_4), and particulate matter (PM) [10]. The choice of this region was due to its growing industrialization, population and urbanization, besides the fact that there is no previous work performing any assessment in this area using photochemical and regional air quality modeling.

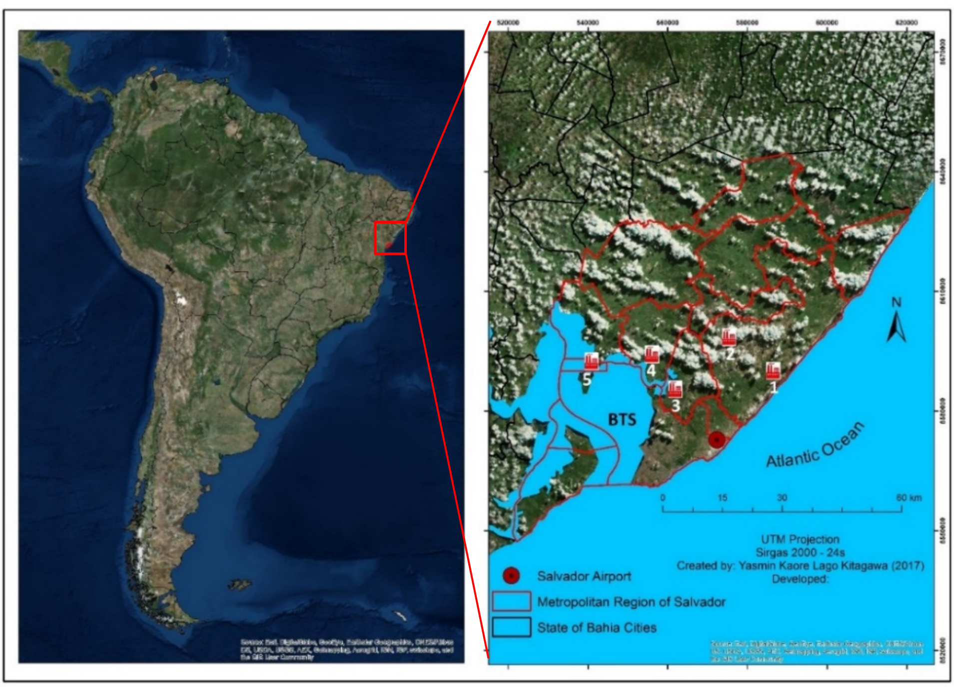


Figure 1: The location of the MRS in Brazil (left) and in Bahia State (right). It is also presented the All Saints bay (BTS) and the major industrial complexes.

2.2 WRF simulation details

The study was carried out using the WRF model, version 3.6.1, which was responsible to simulate the meteorological fields. As mentioned before, many studies have been developed using the WRF given the fact that the model allows to perform numerical modeling for a better understanding of the atmospheric dynamics, physics and phenomena associated with precipitation, heat and cold events, pollution, renewable energy, wind cycles, severe storms, etc. Detailed information about the physics, equations and dynamics can be found on [5].

The dynamical solver used was the WRF-ARW core that integrates the fully compressible nonhydrostatic Euler equations, with terrain-following hydrostatic pressure vertical coordinates. The grid format is Arakawa-C in the horizontal plane and time integration is performed with a 2nd and 3rd-order Runge-Kutta scheme with a smaller time step for acoustic and gravity-wave modes. The spatial discretization, in both horizontal and vertical directions, uses 2nd to 6th-order advection schemes.

The model was run with three nested domains with grid resolutions of 9 km, 3 km and 1 km, respectively (Fig. 2). An overview of the physics options adopted is listed in Table 1, and the spatial configuration is shown in Table 2. The domain of interest has horizontal resolution of 1 km and twenty-one vertical levels with the model top set at 50 hPa. The WRF meteorological input data came from National Centers for Environmental Prediction (NCEP) Final Analysis (FNL) on 0.25° x 0.25° grid resolution at every six hours. The land use data were provided by United States Geological Survey (USGS) at 5 min, 2 min and 30 s resolutions. The time period analyzed was March 20th to 25th 2016, with 24h spin-up in order to obtain realistic initial conditions. In the second and third domain which was run at 3 km and 1 km spatial resolution, respectively, simulations were carried out using explicit convection.

Table 1: Simulation details specifying physics options.

Physics parameterization	Schemes selected
Microphysics	Kessler [11]
Cumulus	Kain–Fritsch [12]
Shortwave radiation	Dudhia [13]
Longwave radiation	Rapid Radiative Transfer Model (RRTM) [14]
Surface layer	MM5 similarity [15]
Planetary boundary layer	Mellor-Yamada, Nakanishi and Niino 2.5 [16]
Land surface model	Noah land surface scheme

Table 2: Details of the model configuration.

Domain	D01	D02	D03
Horizontal resolution	9 km	3 km	1 km
Domains of interest	11.18°-14.33° S 36.68°-39.92° W	11.99°-13.61° S 37.59°-39.25° W	12.18°-13.37° S 37.78°-39.00° W
Cell numbers	39x39	60x60	132x132
Domain size	351x351 km	180x180 km	132x132 km

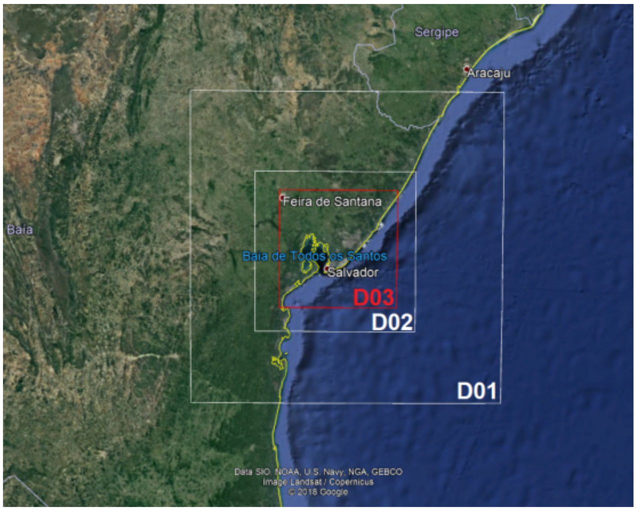


Figure 2: Location of the three nested domains with grid resolutions of 9 km (D01), 3 km (D02) and 1 km (D03).

It was used hourly observations from the surface meteorological station of Salvador Airport (12.91°S, 38.33°W – Fig. 1) for validating WRF simulation. Then the simulated data was extracted from the grid point nearest to the latitude and longitude of the Salvador meteorological station in order to compare with the observed data. The WRF output was compared with observed data through statistical measures of mean bias (MB), root mean square error (RMSE), mean absolute gross error (MAGE), and index of agreement (IOA). To analyze wind, comparisons of wind speed (WS10) and direction (WD10) at 10 meters were also made through joint frequency distribution plots, referred to as wind roses that were generated by VSQA software [17].

2.3 CMAQ simulation details

In order to simulate the chemical transport of the NO_x and SO_2, the CMAQ model, version 5.0.2 was used. The emissions inventory is the critical point in the air quality context [18], and it was also for this work since it has not yet been developed for MRS. Thus to build it, a literature review was done in such a way that it was used Lyra's work [19] who estimated the emission rates of SO_2 and NO_x based on the amount of fuel consumed in the industrial complex of Camaçari and the USEPA emission factors, considering some emissions sources located in the region.

Again, because of the absence of full information about the other source types, it was decided to work exclusively with the point source category, for which information about latitude-longitude coordinates and stack parameters (e.g. stack height and diameter, exit gas velocity, exit gas temperature) were provided. According to [19] most of point sources are derived from furnaces and boilers, very common in refineries and petrochemical complexes. Another proceeding to be done to set up the inventory is the chemical speciation which converts inventory pollutant data to species needed by CMAQ model. [20] carried out NO_x in-stack measurements for various combustion sources and showed that the NO_2 average was 0.05 (5%). AP-42 [21] 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 used in this work was of 95% for NO and 5% for NO_2.

The applied chemical mechanism was CB05. The CMAQ plots were made using R software packages [22].

3 RESULTS AND DISCUSSION

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) and the Monin-Obukhov length were checked in order to observe the hourly variation generated by the atmospheric turbulence, which is responsible for the pollutants diffusion.

The data to assess simulated PBLH variation were extracted from the grid where Airport station is situated since it is where there are meteorological data available to the region. It is worth to point out that there is another station in the region which is monitored by the Brazilian National Institute of Meteorology (INMET), however the INMET station is located very close to the ocean, and when the WRF model does the discretization of land use and soil categories, the model considers water bodies as the dominant category of the cell grid where the INMET station is situated. Thus, due to the high thermal capacity of ocean waters, variations in the air temperature are smaller over their surfaces than over land surfaces, making the outlook of PBLH variation difficult to be noticed.

Fig. 3 depicts the mean hourly variation of simulated PBLH for the analysed period which was the end of summer and the beginning of autumn, characterized by high temperatures that ranged between 25°C and 33°C, and dry weather conditions; except for day 23 when it was registered an accumulated precipitation of 11.4 mm. Nevertheless, by analysing the PBLH, it could be inferred that WRF model underestimated this variable, since [23] presented an average PBLH for the region of approximately 1349 m.

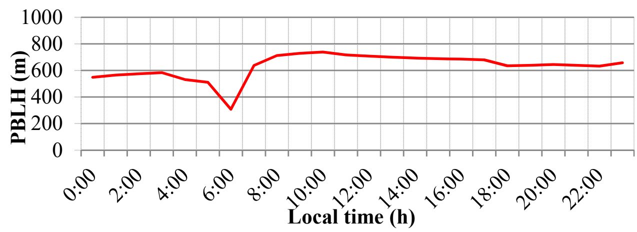


Figure 3: Mean hourly variation of simulated PBLH at Airport station grid.

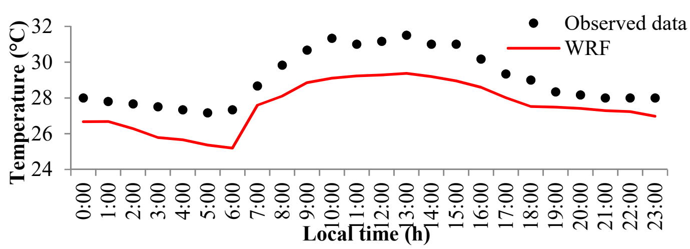


Figure 4: Mean hourly temperature at 2 m above surface at Airport station.

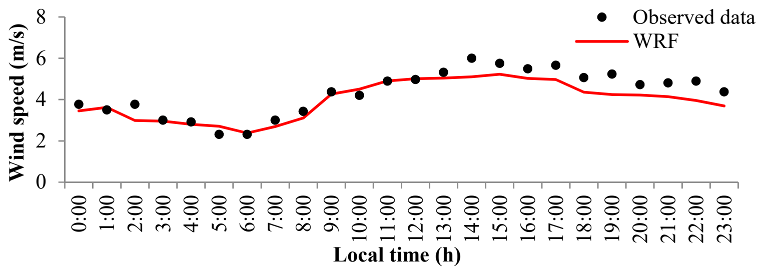
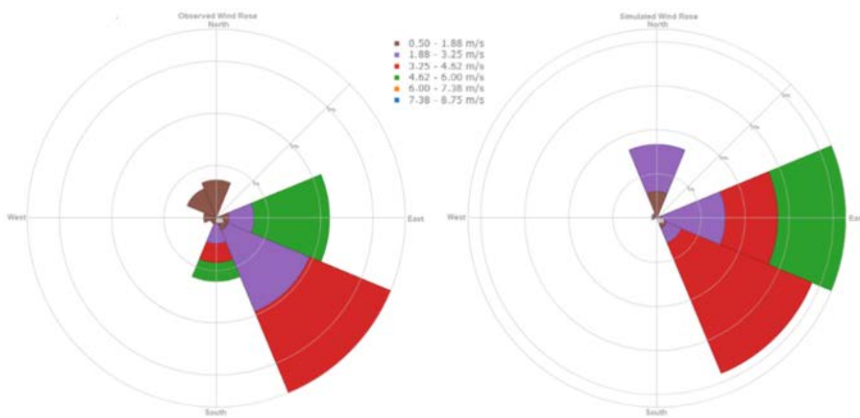


Figure 5: Mean hourly wind speed at 10 m above surface at Airport station.



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(a) (b)

Figure 6: Wind roses of the observed (a) and simulated (b) data at Airport station.

Figs 4 and 5 show the mean hourly variation of temperature at 2 m (T2) and WS10 observed and simulated data, respectively. One can note that the simulation was underestimated for T2, nevertheless the WRF model was able to capture the hourly variation. On the other hand, simulated WS10 presented to be very close to observed data and also depicts very well the diurnal cycle. Regarding WD10, the observed wind direction came chiefly from the southeast (Fig. 6(a)), while the simulated data had some variations coming from east (Fig. 6(b)).

Table 3 presents the statistical metrics of T2, WS10 and WD10, comparing the simulated values with the observed data at Airport station. One can see that the deviations between simulated and observed data were relatively small for T2 and WS10, they also indicated that the model underestimated these parameters. Since IOA values are closer to 1 than 0, it means the model performed reasonably well. For WD10 the negative value implies that the modeled wind direction was rotated counterclockwise when compared to observed values, also shown it through Fig. 6. MAGE expresses the mean magnitude of the errors of the simulations, signifying the model has rotated around 35° counterclockwise.

Table 3: Statistical comparison between observed and simulated T2, WS10 and WD10 data for Airport station.

Variable	T2 (°C)	WS10 (m/s)	WD10 (°)
Observed mean	28.93	4.19	133
Simulated mean	27.62	3.99	109
MB	-1.31	-0.20	-25.59
RMSE	1.60	1.15	43.22
MAGE	1.42	0.91	34.72
IOA	0.76	0.82	0.85

Fig. 7 shows NO, NO_2 and SO_2 concentrations at first level (approximately 10 m), on March 22nd and 23rd, at 10 UTC (7 a.m. local time). The time selection was made by examining the PBLH (shown in Fig. 3) and Monin-Obukhov length, which revealed when the changing occurred in the atmospheric stability, from stable to unstable condition between 6 and 7 a.m. local time. The choice of these both dates is related to the fact that for the other simulated days the behavior of the plume was quite similar to day 22nd, changing only the concentration values, except on 23rd when there was a change in the wind direction that may be related to be a rainy day. Thus, it could be noticed by Fig. 7 that the change in the wind direction impacted different regions of the State of Bahia. Most of the days (20–22 and 24–25), the plume reached Dias d'Ávila and São Sebastião do Passé cities. However, on March 23rd, the wind direction changed and got cities like Camaçari, Simões Filho, Lauro de Freitas, Salvador, Vera Cruz and Itaparica. Fig. 7 also indicated that the highest concentrations occurred near the sources and, regardless of the pollutant, the plume presented the same behavior.

Air pollution studies require space-time distribution knowledge of pollutant concentrations. In order to evaluate the air quality in the main cities of MRS as well as in the settlements located next to PIC, the concentration values of NO, NO_2 and SO_2 were analyzed using the four virtual air quality monitoring stations. The stations were placed in the cities center of Camaçari and Salvador, as also in the Airport, and Lamarão which is a district of São Sebastião do Passé. Then using the data extracted from these points, concentration time series (Fig. 8) were made for March 22 to Lamarão (d) and 23 to Salvador (a), Camaçari (b) and Airport (c).

One can see that, regardless of the values, the concentration peaks occurred in the early hours of the morning, mainly between 6h – 7h o'clock in all locations to all target pollutants. The area that presented the highest values was Lamarão, meaning it is the region most affected by PIC air emissions. Lamarão was also the only area which did not display no-zero concentration values throughout the day, implying that the population which lives in this area can be in constantly touch with these air pollutants. Regarding the hourly concentrations, one can also note that Camaçari and Lamarão areas showed concentration values higher than, for instance, the primary air quality standards established by USEPA for NO_2 (0.1 ppmV) and SO_2 (0.075 ppmV) during the peak times (see Fig. 8, in which the values were highlighted). To exceed these limits can be harmful for the population health, especially "sensitive" populations such as asthmatics, children, and the elderly, according to USEPA. In this way, it can be concluded that wind direction has a fundamental importance during the peak times

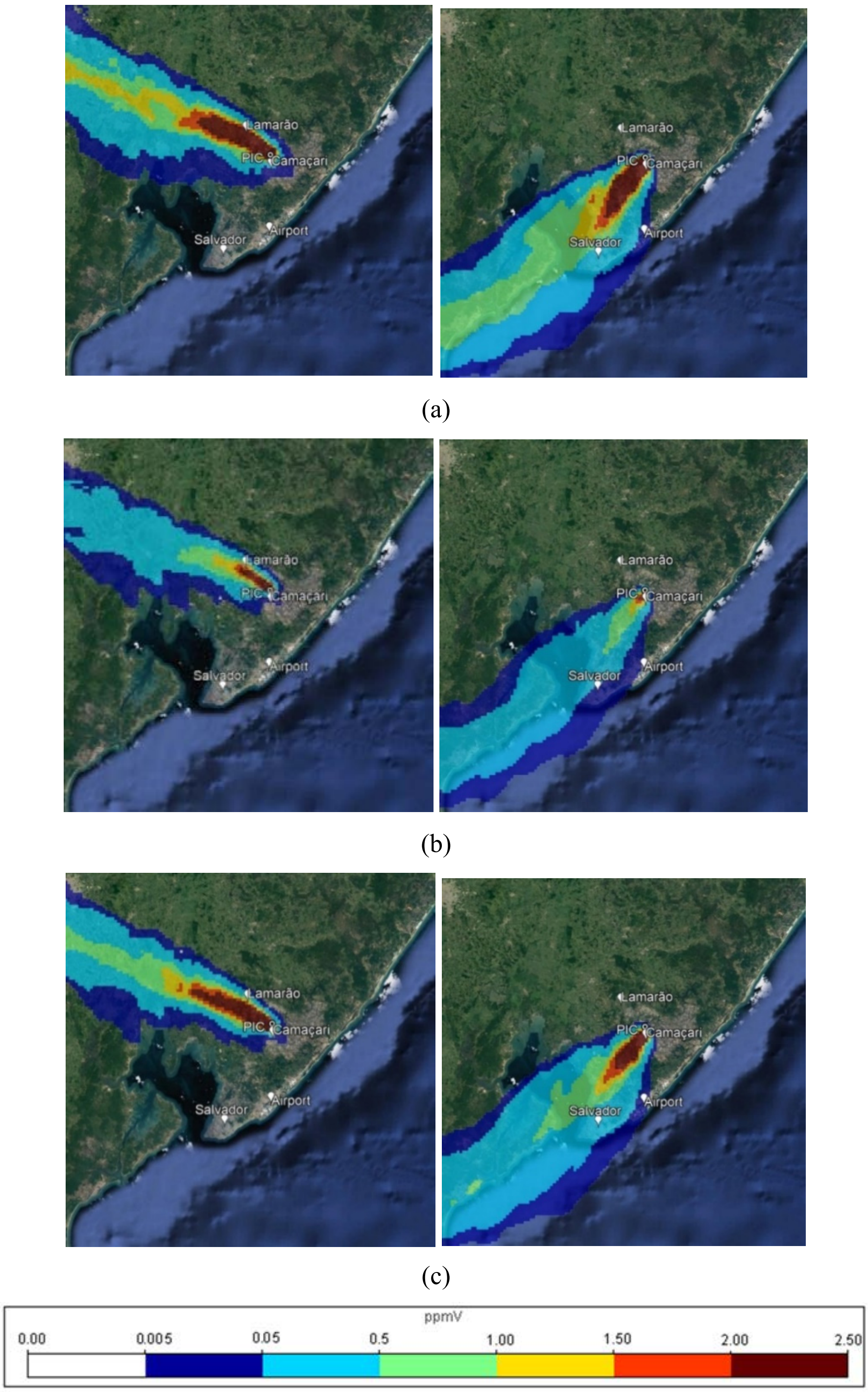

Figure 7: NO (a), NO_2 (b) and SO_2 (c) concentrations on 22nd March (left) and on 23rd March (right) at 10 meters at 10 UTC (7 a.m. local time).

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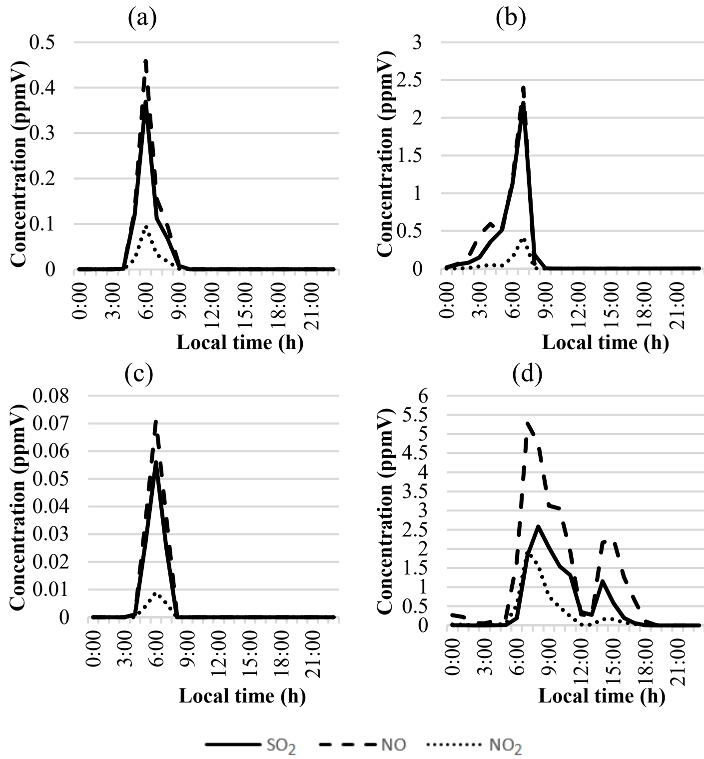

Figure 8: Daily concentration of NO, NO_2 and SO_2 in Salvador. (a) Camaçari; (b) Airport; (c) on March 23rd; and Lamarão (d) on March 22nd.

in the region, indicating the need of a better emissions control, especially when the atmospheric conditions can lead to critical levels.

4 CONCLUSION

The main purpose of this work was to apply WRF and CMAQ atmospheric models to qualitatively assess the dispersion of the atmospheric pollutants (NO_x and SO_2) from stacks located at Camaçari Petrochemical Complex in the Metropolitan Region of Salvador (MRS). Notwithstanding it was a 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 of the MRS. 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. The results also showed that Lamarão and Camaçari are the most affected areas by PIC emissions. For future works it is suggested to perform the validation of the air quality regional photochemical modeling with CMAQ using monitoring data, and 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.

ACKNOWLEDGEMENTS

The authors thank the Supercomputing Center for Industrial Innovation (CIMATEC Yemoja) for providing the computational infrastructure needed to run the models, and the Fundação de Amparo à Pesquisa do Estado da Bahia (FAPESB) and also the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for the financial support.

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