Evaluating the impact of vehicular fleet in the formation of tropospheric ozone in the Metropolitan Area of São Paulo (MASP): case study, September 2004.

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Abstract

The main objective of the present work is the evaluation of the impact of the vehicular fleet in the formation of the tropospheric ozone in the Metropolitan Area of Sao Paulo (MASP). This evaluation was performed with numerical modeling techniques using the Weather Research and Forecasting with Chemistry (WRF-Chem) air quality model. WRF-Chem was set up to run with four nested domains with grid resolution of 27, 9, 3 and 1km. The emission inventory for the mobile sources was based on the information of number of vehicles, vehicular emission factors and average driving kilometers for vehicle per day. Air quality was simulated for four days, from December 6 to 09, 2004, being this period selected because there were experimental data to determine the vehicular emission factors, better meteorological conditions for ozone formation and there was more ozone observation available. To evaluate the simulation performance, it was used the air pollutant concentrations data from the air quality network of the São Paulo Environmental Agency (CETESB).

Keywords: tropospheric ozone; WRF-Chem model; emission inventory.

Introduction

Over the past several years, ambient ozone concentrations in the MASP have reached levels of more than five times that considered protective of public health by the World Health Organization (WHO). Mage et al., 1996, for example, found that the ozone levels in MASP exceed the WHO air quality standard, with concentration that are greater than two times maximum concentration suggested by the same organization, this can be explained by high emission of ozone precursors CO and NO_2, that also exceed the WHO air quality standard. Currently, even though total emissions of these pollutants have been reduced in the past years, the numbers of Brazilian National Ambient Air-

Quality Standard (one hour maximum value of 160µg/m^3) overtaking have increased. By the other hand, is important enhance that yearly ozone national standard overtaking variability answer to meteorological conditions for its formation, this conditions usually happen in summer and specially during spring time (Carbone, 2008). In the MASP, currently there are approximately 7.2 million passenger and commercial vehicles: 93.5% light-duty and 6.5% heavy-duty diesel vehicles. Of the light-duty vehicles, approximately 76.3% burn a mixture of 78-80% (v/v) gasoline and 22% ethanol (referred to as gasohol), and 17.2% use hydrated ethanol (95% ethanol + 5% water), these data were obtained from CETESB, 2011. Because of vehicular contribution to ozone precursors total emissions in MASP is greater than 95% of total emissions for 2004 (CETESB, 2005), the main objective of this study is evaluate vehicular impact in tropospheric ozone representation in MASP by applying numerical modeling to a high concentration episode that happened in September 2004.

Methodology

The air quality photochemical model WRF-Chem (Grell et al., 2005) was used to represent tropospheric ozone formation and dispersion on the MASP. WRF-Chem was configured to run with four nested grids: 27, 9, 3 and 1 km respectively. All centered in the MASP. The chemistry process module, The Regional Acid Deposition Modell version 2 (RADM2) mechanism (Stockwell, 1986), was activated to run on the finer 3 and 1 km grids. Only the mobile sources were considered as anthropogenic sources. The emissions inventory was built with information of vehicles number, emission factors (FE) and average number of kilometers traveled per day by the considered types of vehicles. In 2004 the vehicular fleet was 5.8 million approximately (Source: DETRAN, State department of Traffic). The emission factor for gaseous and particle compounds was based on measurements inside road tunnels (Sanchez-Ccoyllo et al., 2009 and Martins et al., 2006). The spatial distribution was based on nighttime lights satellite data for 3 km grid and on International Environment Database (IED) CO daily product (Lents et al., 2012) for 1 km grid. The temporal variation is based on measurements of traffic density. NCEP FNL Operational Global Analysis was used as meteorological input, its spatial resolution is 1°x1°, it's also has 26 vertical levels and is available every six hours. The chosen simulation period was from September 06 to 09, 2004.

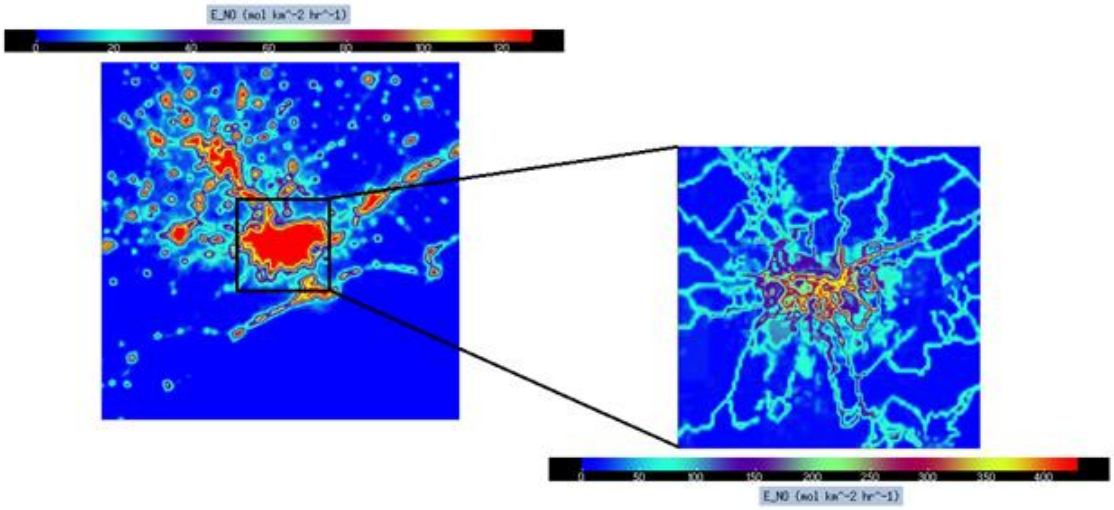

Fig. 1. NOx emission rate for 3 km (left) and 1 km (right) grids at 18h, local hour.

Results

The results of the comparison between measured and simulated pollutants show that the physical and chemical configurations represent well the ozone formation diurnal cycles; nevertheless, there are discrepancies in the representation of the occurrence of the maximum concentration. This can be explained as a result of the same emission profile used for all the grids point and vehicles types. Ozone concentration in 3 km grid presented better statistical parameters; however, simulated minimum concentrations were overestimated in both grids, probably as result of underestimated NOx emission at minimum ozone concentration time, this behavior was observed by Tie et al., 2007 in some simulated regions. Figure 2 shows the comparison of observed with 3 km and 1 km simulated ozone in eleven stations of CETESB air quality network in MASP. In general, correlation and concordance indexes were bigger than 0.8. Mean RMSE for 3 km and 1 km cells were 31.9 and 32.2 $\mu g/m^3$ respectively. The paired peak prediction accuracy was -8.2 and -17.1 $\mu g/m^3$ for 3 km and 1 km grid cells respectively. Figure 3 shows a Taylor Diagram (Taylor, 2001) for ozone concentrations in the eleven evaluated stations of CETESB air quality network, where graphically is shown that 3 km grid resolution presented better performance. This situation is associated to the emissions scheme used in both grids and the transportation of ozone and its precursors among metropolitans regions in the Sao Paulo State, that it's not considered in 1 km grid.

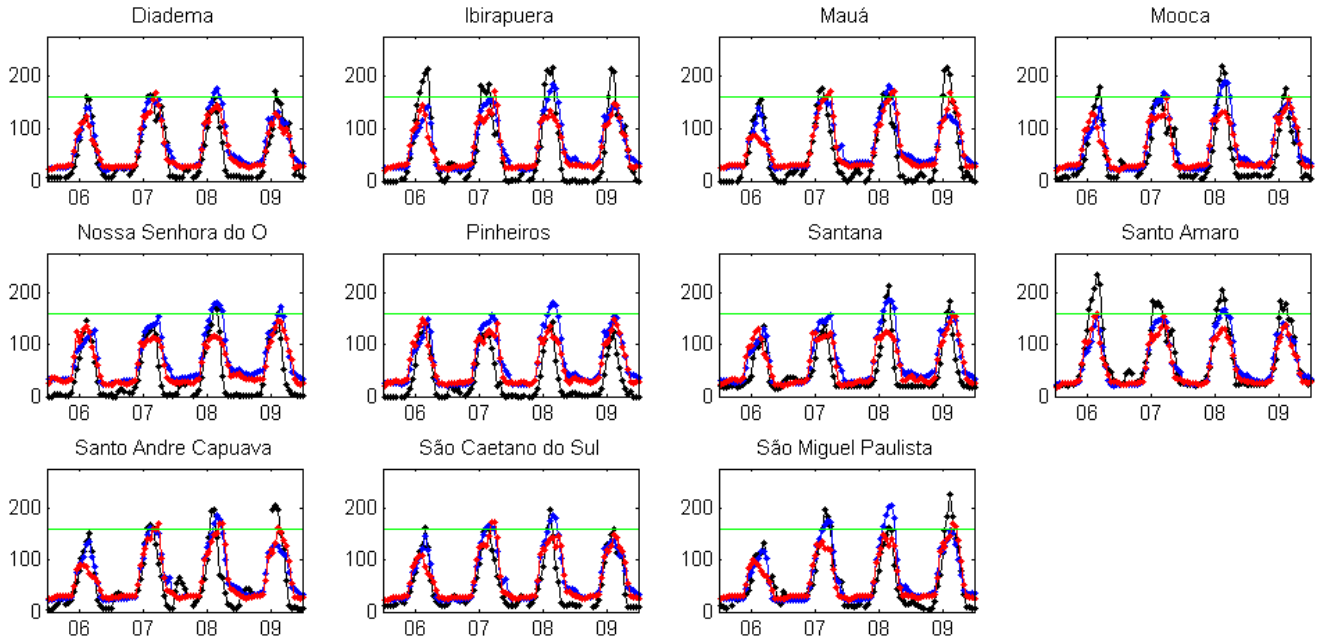

Fig. 2. Observed (black) and simulated for 3 km (blue) and 1 km (red) grid cells ozone concentration (in µg/m^3) for eleven stations of CETESB monitoring network air quality stations in MASP for September 06-09, 2004. The green line represented the air quality standard for this pollutant (one hour maximum value of 160 µg/m^3).

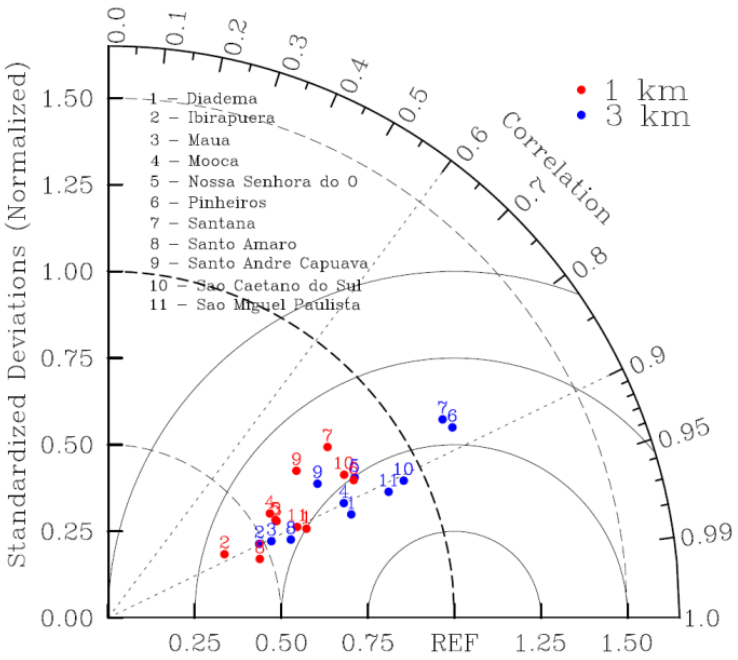

Fig. 3. Taylor Diagram for ozone concentrations.

By applying the criteria suggested by Sillman, 1995, where a value of 0.28 for CH_2O/NO_y ratio during afternoon, considering $NO_y=NO+NO_2+HNO_3+PAN+NO_3+2N_2O_5$, could define a NO_x and VOCs limited regime transition; we can concluded that MASP is under a strong VOCs-limited regime. This result is consistent with results obtained by Martins, 2006; Sánchez-Ccoyllo et al., 2006 and Orlando et al., 2010.

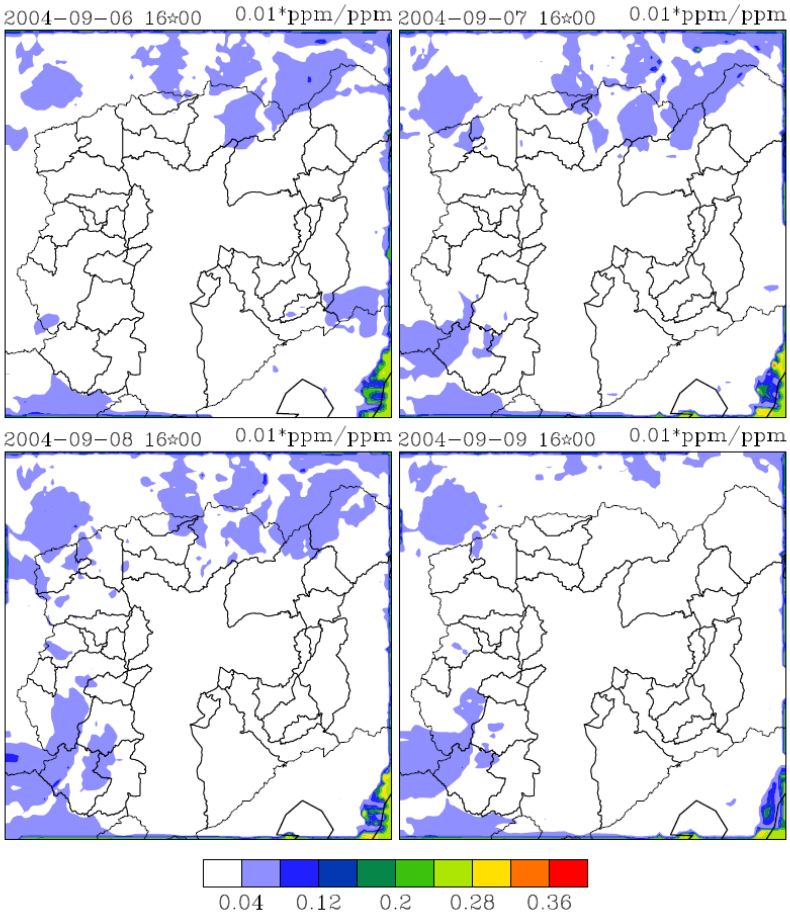

Fig. 4. Surface representation of CH_2O/NO_y modeled ratio at 14h, local time in MASP.

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