HIGH-RESOLUTION CMAQ SIMULATION OF AIR POLLUTION OVER THE METROPOLITAN AREA OF VITÓRIA, BRAZIL.

Alexandre M. Santiago[1], Ayres G. Loriato[1], Taciana T. de A. Albuquerque[1], Nadir Salvador[1], Erick G. S. Nascimento[1], Elson S. Galvão[1], Renato S. Marinho[2], Neyval C. Reis Jr[1]

1. Environmental Engineering Department - Federal University of Espírito Santo - UFES - BRAZIL
2. Geography Department - Federal University of Espírito Santo - UFES – BRAZIL

magalhaes.es@gmail.com
fone: 55-27-33352177

Abstract

The main objective of this study is to evaluate the air pollution concentrations over the Region of Grande Vitória (RGV), Espírito Santo, Brazil using The Models-3 Community Multiscale Air Quality Modeling System (CMAQ) version 4.6. An experimental campaign was performed during the winter of 2012, from July 22 to 31, to quantify the aerosols formation and transportation using a LIDAR and SODAR instruments. Meteorological numerical data was obtained using the WRFv3.2.1 (Weather Research and Forecasting) model. Four nested grid was used, 27km (70 x 70 cells), 9km (100 x 100 cells), 3km (100 x 100 cells) and 1km (64 x 82 cells), only the 1-km domain was aligned with the CMAQ domain, which covers the most polluted cities on the State (Cariacica, Serra, Viana, Vila Velha, and Vitória). CMAQ modeling simulations were conducted over 336 hours from 18 to 31 of July, 2012. The SMOKEv3.7 emissions model was applied to build a spatially and temporally resolved the official emission inventory for RGV. The CMAQ and SMOKE domains consist of 64 x 82 grid cells with 1 km horizontal spacing and 20 vertical layers. The air quality simulations use measured concentrations as initial and boundary conditions. Aerosol processes and aqueous chemistry in CMAQ (AERO4) were used, as well as the Carbon Bond V gas phase mechanism. The highest PM10 average concentrations measured at the Local Air Quality Monitoring Stations was observed The highest average concentration of PM10 observed during the study period, the Automatic Network Monitoring of Air Quality (RAMQAr), are the municipalities of Serra (Laranjeiras) (43μg/m^3) and downtown of Vila Velha (31μg/m^3). The best results were presented by CMAQ stations in Vitória (downtown) where the simulate average in period was 24μg/m^3 and observed 24μg/m^3 and Vitória (Jardim Camburi) where both the observed mean and simulated were 28μg/m^3.

Palavras-Chave: modelagem numérica, qualidade do ar, CMAQ, WRF e PM10.

1. Introduction

Several epidemiological studies have shown a direct association between the presence of inhalable particles and health. The same studies report that there is strong correlation between exposure to high levels of PM10 and PM2.5 and increased respiratory disease, lung damage, and mortality among the population (BLANGIARDO *et al*., 2011; SAMOLI *et al*., 2011).
Specifically in Brazil (CONCEIÇÃO *et al*., 2001; MARTINS *et al*., 2002) found statistically significant associations between both child mortality, and among hospital attendances due to cold and pneumonia (MARTINS *et al*., 2002) in cities like Sao Paulo and Rio de Janeiro, with exposure to air pollution. The inhalable particulate matter (PM10), in spite of human body defenses avoids their penetration into the respiratory system, depending on their size, can cause serious health problems. SAMOLI *et al*., (2011) found that an increase of 10μg/m3 increases by 2.54% in the number of admissions for pediatric asthma.

The necessity for a forecast of PM10 air quality becomes more important than the environmental authorities and citizens are demanding information on air quality in advance to take the appropriate actions and measures to protect your health during pollution episodes

(KOO *et al*. 2012). In the Region of the Grande Vitória (RGV) previous studies only performed the quantification and characterization of PM10 and PM2.5 (MAIOLI, 2011), and research related to the nuisance caused by particles sediment (SANTOS and REIS, 2010).

2. Materials and Methods

2.1. Description of the modeling systems

For the simulations in this study, was used the meteorological model WRF_ARW version 3.2.1. The main features of the WRF_ARW can be found in Technical Description ARW available in http://www.mmm.ucar.edu/wrf/users/docs/arw_v3.pdf. WRF require lateral boundary conditions that represent the actual state of the atmosphere over time integration of dynamic equations. The initial and boundary conditions to WRF model were provide by NCEP's Global Forecast System (GFS) with 6-h intervals and spatial resolution 1°×1° (UCAR, 2007).

The WRF was applied for the days 18–31 July 2012, but the first four days of model output were discarded from the data analysis (4-day spin up) and the analyses with CMAQ were performed from July 22 to 31, 2012. In which an experimental campaign was conducted to obtain data for model validation WRFv3.2.1. This study used a configuration of four domains of which domain d01 covers much of the Southeast, covering all its states and especially the Espírito Santo, Rio de Janeiro, northern São Paulo, southern Bahia, much of the state of Minas general and part of the Atlantic Ocean. The study domain (d04) has a small area (64 x 82 cells, 1 km), however with high horizontal resolution, its scope is local and includes the city of Vitória and part of like Cariacica, Serra and Vila Velha (Figure 1).

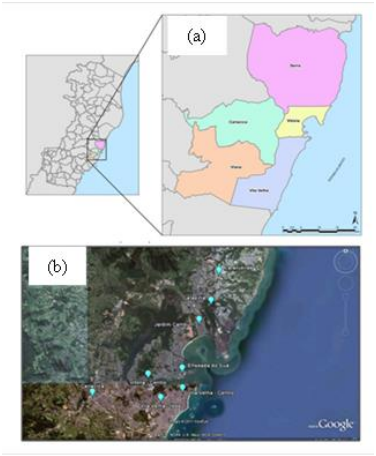

Figure 1: (a) Grande Vitória region, d04 domain. (b) RAMQAr locations.

In order to simulate the concentrations of PM10 the model chosen was the United States Environmental Protection Agency (EPA) CMAQ (BYUM *et al*, 1999) version 4.6. CMAQ needs meteorological parameters provided by WRF the emission rates of sources inside and outside the study area provide by SMOKE, using the IEMA's Inventory (2009-2010) beyond initial and boundary conditions (ICON and BCON) that were the averages of the last five years the concentrations of pollutants measured in the stations of RAMQAr.

2.2. Model performance

The analysis of models performance, even for models widely used by the scientific community should in fact be verified, one configuration of the model can be considered valid for a given region, but to another their results may not be consistent (BORGE *et al*. 2008). In

this sense, in this study some statistical metrics widely used in the literature to assess the performance of mathematical models APPEL *et al*., 2012, SIMON *et al*., 2012, KOO *et al*., 2012, BORJE *et al*., 2008), such as normalized mean bias (NMB) e normalized mean error (NME), ratio, mean error (ERR) e correlation coefficient (r) were applied. These statistics show NMB and NME values around 5-15% e 30-35%, respectively, for urban scale photochemical models (SEINFELD and PANDIS, 1998).

3. Results and discussions

This study was conducted from 07/22/2012 to 08/01/2012 during a measurement campaign of atmospheric aerosol in the Federal University of Espírito Santo. The performance of simulations using the CMAQ model was assessed using the statistical parameters compared to observed data obtained from automatic stations of monitoring of air quality present in the study area. Table 1 shows the statistical comparison between observed and simulated data, where (a) is a station located in the Laranjeiras, (b) in Carapina, both in Serra, (c) in Jardim Camburi, (d) in the Enseada do Suá and (e) in the downtown, all in Vitória, (f) the downtown and (g) in Ibes, both in the municipality of Vila Velha and finally (h) is a station located at Vila Capixaba, county of Cariacica.

Table 1: Statistics applied to the results simulated by CMAQ forward to the observed data at stations of RAMQAr.

Station/Statistics	**a**	**b**	**c**	**d**	**e**	**f**	**g**	**h**
mean – station (µg/m^3)	43	20	28	28	24	31	22	54
mean – CMAQ (µg/m^3)	19	23	28	40	24	25	27	23
ratio	0.5	1.2	1.4	1.9	1.1	1.3	1.6	0.4
NMB (%)	-55.9	16.0	2.0	44.6	0.8	-20.1	22.1	-58.1
ERR (µg/m^3)	26.7	12.6	16.0	25.2	15.5	18.9	19.4	38.9
NME (%)	61.5	64.5	59.0	91.0	65.5	66.9	87.0	71.5
r	0.3	0.4	0.4	0.1	0.4	0.1	0.0	0.3

According to Figure e.1 and h.1, Laranjeiras and Vila Capixaba stations data showed the highest values, 156 and 170 µg/m^3, respectively, however CMAQ simulations showed the highest values in Vitória downtown 194 µg/m^3 (e) and 214 µg/m^3 in Vila Capixaba (h), showing that CMAQ was able to predict the concentrations peak in station (h). However, for this station, the statistic show the highest ERR (38.9) and greater tendency to underestimate the concentration of PM10 as NMB values (-58.1). At stations (c) and (e) the averages simulated by CMAQ were equal the averages observed in the same period, showing no significant trend as NMB values, nonetheless, the values of NME showed up out of range as Seinfeld and Pandis (1998).

It is observed in Figures (a.2 to h.2) a strong degree of dispersion of the data resulting in a low value of r, indicating that the model was unable to predict with accuracy the hourly variations of the concentration of PM10 in the region.

The period between the days 23-24 and 30-31 showed peaks of concentration higher than compared to the observed data. However, it is not possible to justify these episodes due to requirement of deeper analysis and other simulations to verify if the problem may be coming from the emissions inventory data, simulations of the time, or the initial and boundary conditions.

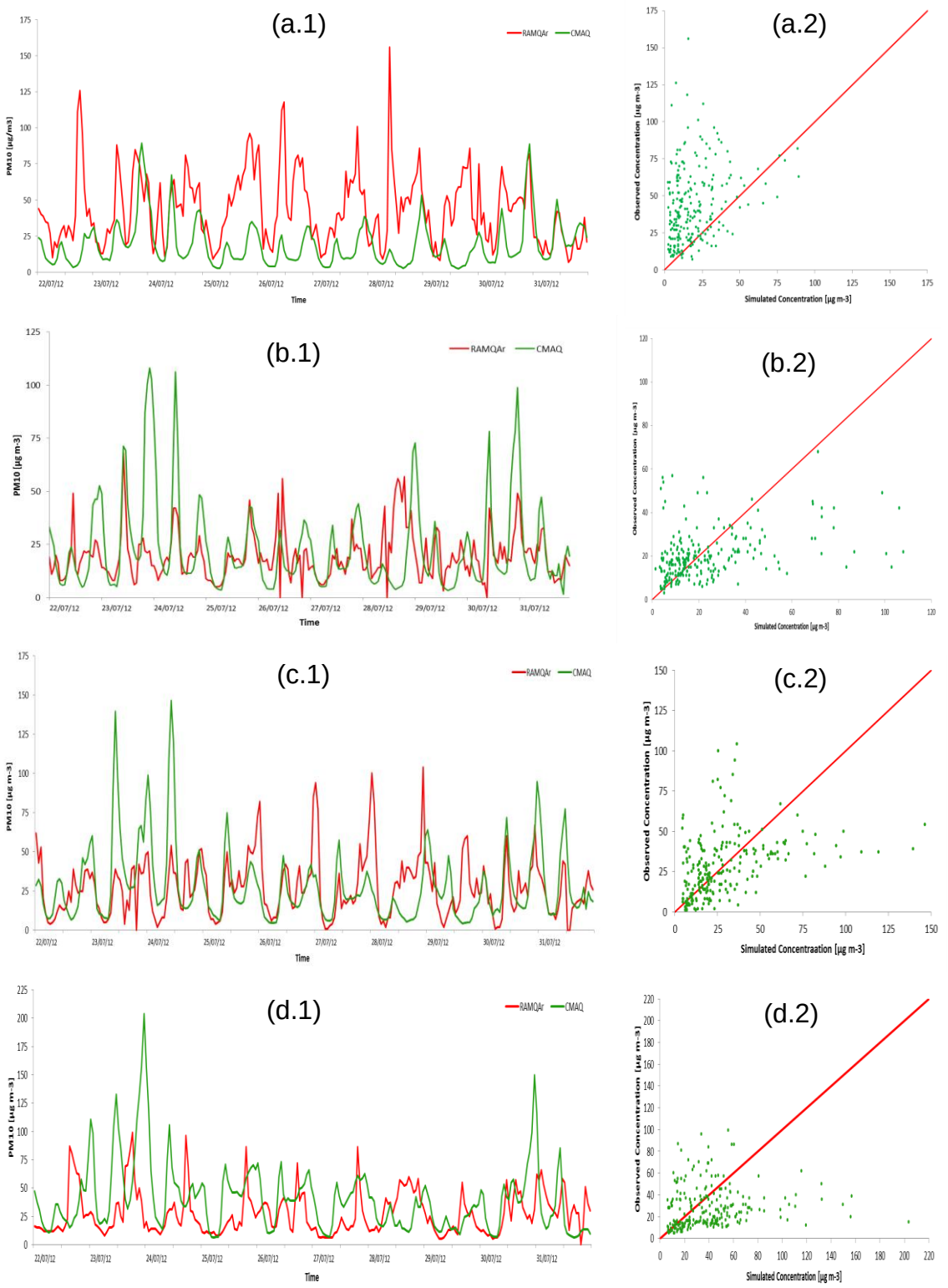

Figure 2: Time series of PM10 concentration at RAMQAr stations, where (a.1) is the Serra – Laranjeiras station, (b.1) Serra – Carapina station, (c.1) Vitória – Jardim Camburi station, (d.1) Vitória – Enseada do Suá station, (e.1) Vitória – Centro station, (f.1) Vila Velha – Centro station, (g.1) Vila Velha – Ibes station, (h.1) Cariacica – Vila Capixaba station and (a.2, b.2, c.2 d.2, e.2, f.2, g.2 and h.2) the dispersion between simulation and observations in the same stations for july 22 to 31, 2012.

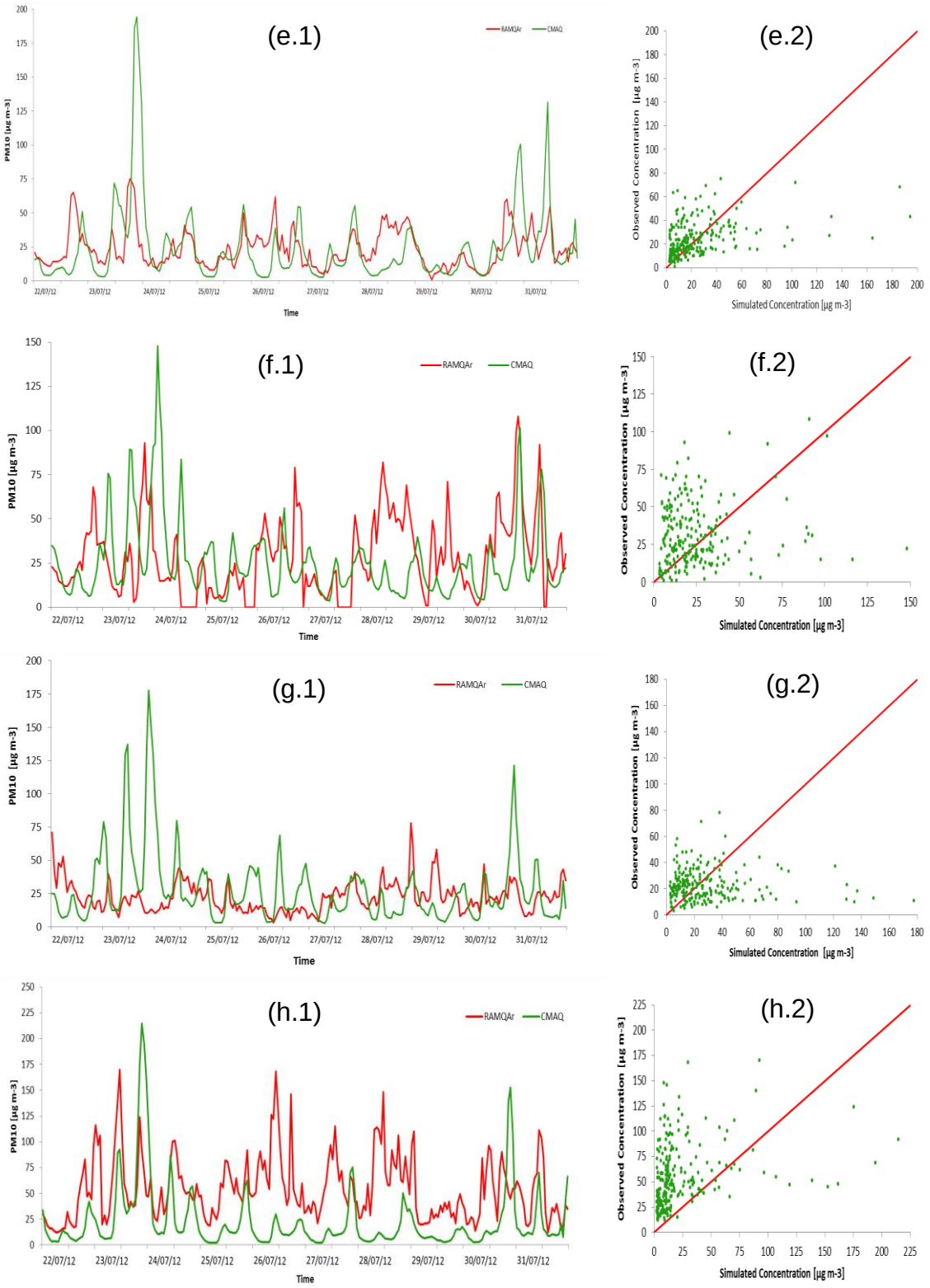

Figure 2 – continuation: Time series of PM10 concentration at RAMQAr stations, where (a.1) is the Serra – Laranjeiras station, (b.1) Serra – Carapina station, (c.1) Vitória – Jardim Camburi station, (d.1) Vitória – Enseada do Suá station, (e.1) Vitória – Centro station, (f.1) Vila Velha – Centro station, (g.1) Vila Velha – Ibes station, (h.1) Cariacica – Vila Capixaba station and (a.2, b.2, c.2 d.2, e.2, f.2, g.2 and h.2) the dispersion between simulation and observations in the same stations for july 22 to 31, 2012.

4. Conclusions

This study is mainly intended study the concentration of particulate matter over a region of Grande Vitória using Models-3/CMAQ from 22 to 31, July, 2012. The results showed a good representation of the mean concentration of PM10 in the period, nonetheless the temporal variation was not well characterized by CMAQ. Further analyzes are needed to adjust the accuracy of the model such as checking the inventory of emissions and meteorological simulations with adjustments in the WRF parameterizations. Despite the limitations, the model CMAQ presented as a useful tool for the evaluation of air quality.

5. Acknowledgment

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