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INFLUENCE OF BOUNDARY CONDITIONS ON CMAQ SIMULATIONS OVER METROPOLITAN REGION OF GREAT VITORIA - ES

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1 INTRODUCTION

The Region of Great Vitoria (RGV) is located at Espirito Santo State, Southeast Region of Brazil. The Southeast Region of Brazil is composed by the states of Espírito Santo, Minas Gerais, Rio de Janeiro and São Paulo. It is the richest region of the country, responsible for approximately 60% of the Brazilian Gross domestic product (GDP).

Although the Region of Great Vitoria is an area with unique features and has its own emissions, it suffers also from transported pollutants from another areas and States. For example, there is a cellulose (FIBRIA) and a mineral (SAMARCO) industry located on north and south of RGV, respectively, as showed on Figure 1. Besides the Espirito Santo State emissions, there are transported pollutants which coming from metropolitan areas located in Southeast of Brazil like São Paulo, Rio de Janeiro and Belo Horizonte. Additionally, there are intercontinental pollutants transports that can influence the local concentrations.

Local emissions come from facilities like mineral and metallurgical industries, thermoelectric, ports, airports, vehicles, dust resuspension, etc. Fig. 1 shows the location of RGV and its local monitoring stations called *Rede de Monitoramento da Qualidade do Ar* (RAMQAr).

Previous studies used CMAQ model over RGV in order to have an air quality tool to support local government with questions about air pollution. Loriato (2015) and Santiago (2015) simulated CMAQ over RGV using the local inventory, without any evaluation about boundary conditions (BC). According Jiménez et al. (2007), it is necessary to consider this issue when applying air quality models and the importance of BC over simulations are essential for good results, particularly for O_3. Borge et al. (2010) on his study over Iberian Peninsula, said that in some cases, BC affects only the vicinity of model boundaries, but depending on how the BC is provided to run the simulations, significant differences may be found

There are three practical ways to implement BC for CMAQ: fixed concentration profiles; concentrations predicted in a CMAQ greater domain; and, using chemical-transport global models (Borge et al., 2010). GEOS-Chem (Henderson et al., 2014) and Mozart (Tong and Mauzerall, 2006) can be cited as global chemical-transport models.

According Henderson et al. (2014) current available observations are too sparse vertically to provide boundary information, particularly for ozone precursors, but global simulations can be used to generate spatially and temporally BC. For RGV, observed data are sparse vertically and horizontally, causing even more problems to describe how pollutants, which comes from other places, affect the area of interest.

Based on the impact of boundary conditions on regional air quality simulations, this study aims to survey the influence of BC over RGV.

2 METHODOLOGY

Emission, meteorology, and lateral boundary conditions will be integrated by CMAQ 5.0.2 to predict air pollution over RGV. The Fig. 1 shows the 61x79km domain over RGV, the monitoring stations from Rede Automática de Monitoramento da Qualidade do Ar (RAMQAr) inside (center) of the domain (East and West BC), Fibria's monitoring stations at north of the domain (North BC) and Samarco's monitoring stations at south of the domain (South BC). Fibria is a pulp processing company and Samarco is a mining company, both outside of domain, but their monitoring stations are next of CMAQ domain for RGV. The GEOS-Chem were configured to provide hourly concentrations for a 2010 CMAQ simulation of Brazil using full-chemistry with secondary organic aerosols at 2 degrees latitude by 2.5 degrees longitude. The emissions and transport options were configured following the v9-02 defaults using the regional inventory when it is available (North America, Europe and Southeast Asia).

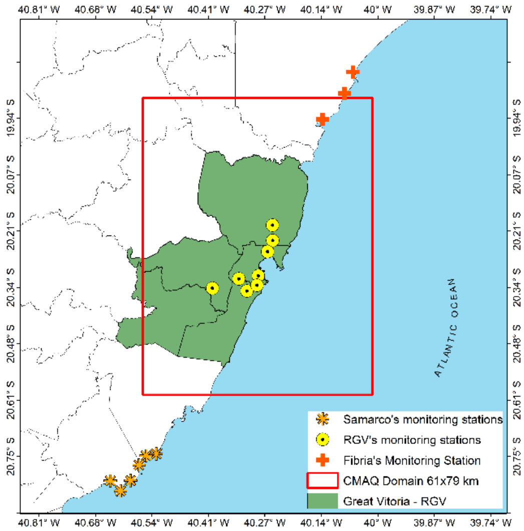


Fig. 1. RGV, CMAQ domain and monitoring stations.

2.1 Meteorological setup

Meteorological fields were modelled using the Weather Research and Forecasting model WRFv3.6.1 from July 30 to September first. 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°(Fig. 2), 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. The model performance was evaluated according Emery et al. 2001, that suggest benchmark to support decisions about meteorology, additionally we used wind rose and time series to evaluate results with observed data.

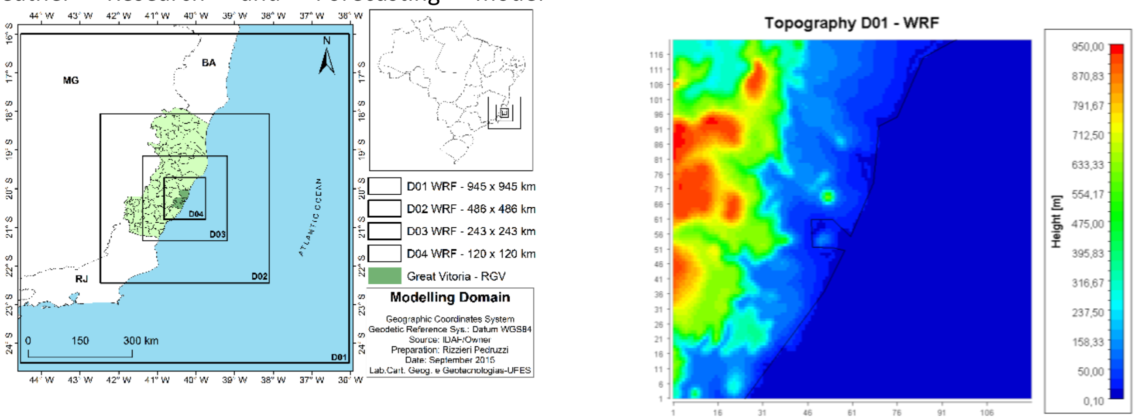


Fig. 2. Nested domains applied in WRF and topography in RGV.

2.2 Emission Inventory

Local emissions were provided for 2010 by the Espírito Santo Local Environmental Protection Agency (Instituto Estadual de Meio Ambiente e Recursos Hídricos - IEMA). The inventory includes industrial emissions, road and vehicles emissions and some specific emissions like residential, transportation and marketing of petroleum liquids, ports and airports. SMOKE v3.5.1 was used spatially and temporally allocated the local inventory. MCIP was used to extract 61x79 1-km grid cells were used from the inner WRF domain (120x120km). Fig. 3 shows the domain over RGV with SMOKE results for PM_{10} and NOx.

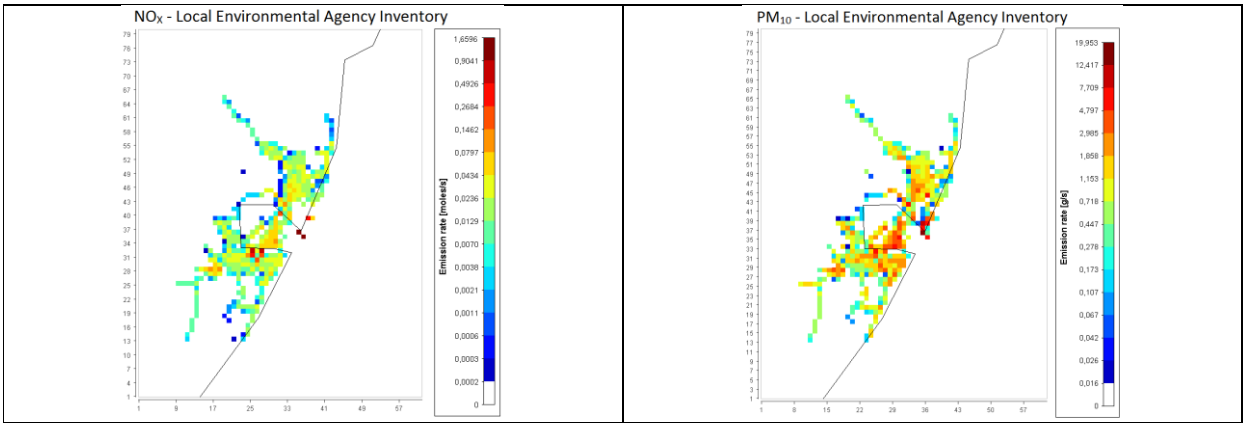


Fig. 3.NO_X and PM10 emissions in RGV.

2.3 Lateral Boundary Conditions

This study evaluates the importance of lateral boundary conditions using 4 alternative databases:

Method 1. Time/space-invariant profiles with zero concentrations;

Method 2. Time/space-invariant profiles with average concentrations from monitoring stations located in RGV or next of the domain's boundary (Fig. 1);

Method 3. Time/space varying concentrations simulated from a larger domain (118x118km, 1km resolution), where the larger domain uses boundary conditions and emissions of test 2;

Method 4. Time/space varying concentrations values from GEOS-Chem (Fig. 4).

The Boundary Conditions was performed according Henderson et al. (2014) for CMAQ Domain 61x79 km over RGV mapping GEOS-Chem Species for CMAQ Carbon Bond' 05 mechanism with aerosol option 6 (cb05tucl_ae6_aq).

Fig. 4 shows an example of boundary conditions simulated by GEOS-Chem for RGV's CMAQ domain.

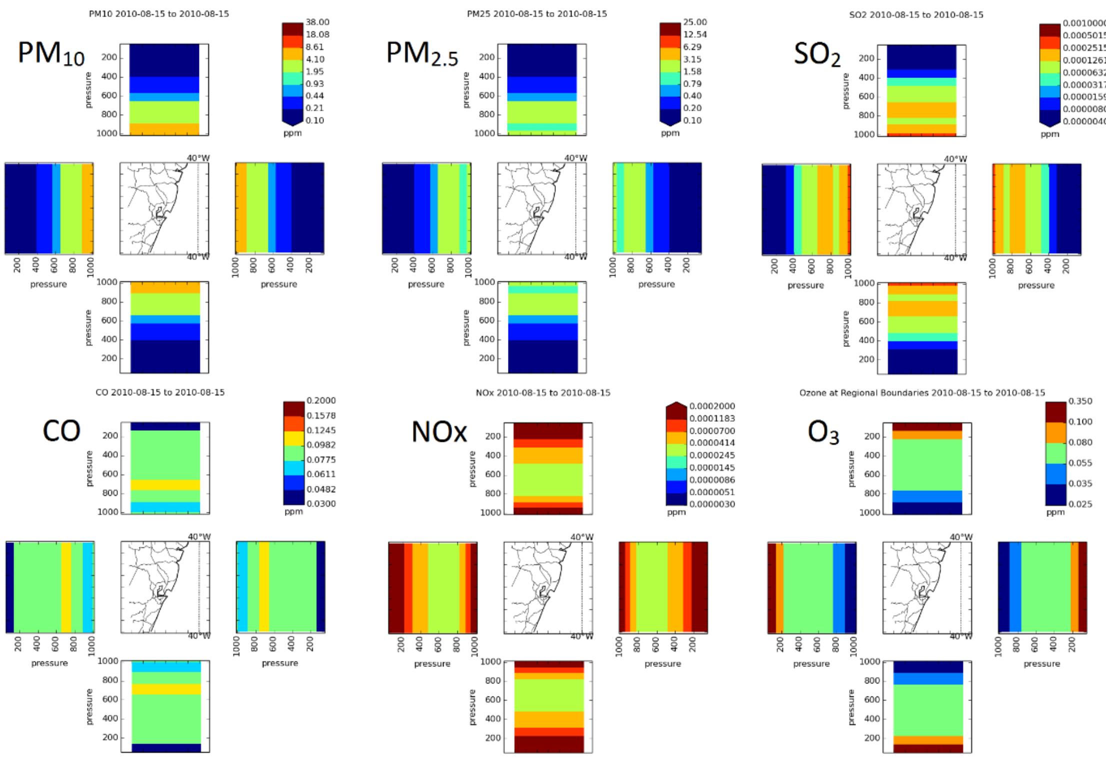


Fig. 4. Example of Boundary conditions from GEOS-Chem for some gases and particles. .

3 RESULTS AND DISCUSSIONS

The model performance were made based on Emery et al. (2001) and the results indicates that WRF simulations perform well in both monitoring stations, according Fig. 5. However we have found some discrepancies between observed and simulated data for some days on august, especially the first 15 days for wind speed and direction, based on time series and wind rose (**Erro! Fonte de referência não encontrada.**, Fig. 6).

WRF Model Evaluation				
Variable	Statistic	Benchmark	Airport Station	Ibes Station
Temperature	MB (K)	≤ ± 0.50	-0.28	-
	MAGE (K)	≤ 2.00	1.38	-
	IOA	≥ 0.80	0.91	-
Wind speed	MB (m.s-1)	≤ ± 0.50	0.13	1.49
	RMSE (m.s-1)	≤ 2.00	2.05	2.05
Wind direction	MB (°)	≤ ± 10.00	-10.17	3.19
	MAGE (°)	≤ 30.00	29.06	26.84

Fig. 5. WRF model evaluation benchmarks and results.

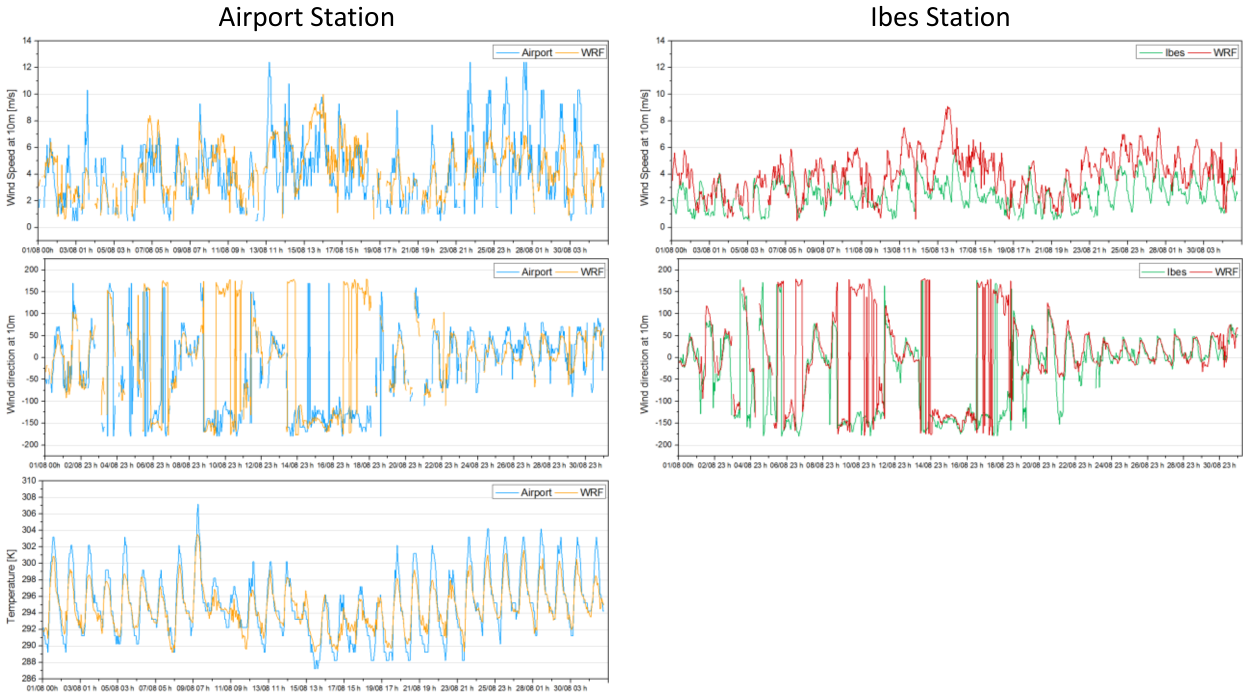


Fig. 6. Time series for wind speed, wind direction and temperature for Airport station (left) and time series for wind speed and wind direction for RAMQAr Ibes station (right).

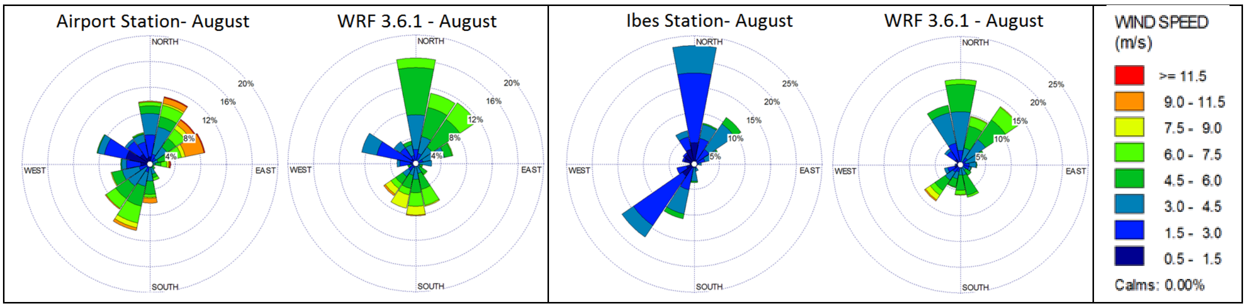


Fig. 7. Wind rose for observed and modeled data for Airport station (left). for observed and modeled data for RAMQAr Ibes station.

The Fig. 8 shows time series and Fig. 9 average concentration of PM_{10} for August 2010 changing boundary conditions. Some problem with some days of August in Laranjeiras, Carapina and Jardim Camburi occurred for PM_{10}, the model overestimated the concentrations, and some higher concentrations on observed was not predicted by CMAQ, because the raw local inventory does not has hourly emissions to represent this hourly peaks, associated with hourly discrepancies in meteorology. For others stations, the model had a better agreement, but some peaks were not predicted. Station of Cariacica was the only one in which the model underestimated the concentration, probably due to local interferences as road constructions and influences of internal traffic at CEASA, a local central food supplies, where the stations is located.

The influence of BCs over simulations was quite similar, especially for PM_{10} time series, comparing with monitoring values. A small difference was observed among average concentrations of august.

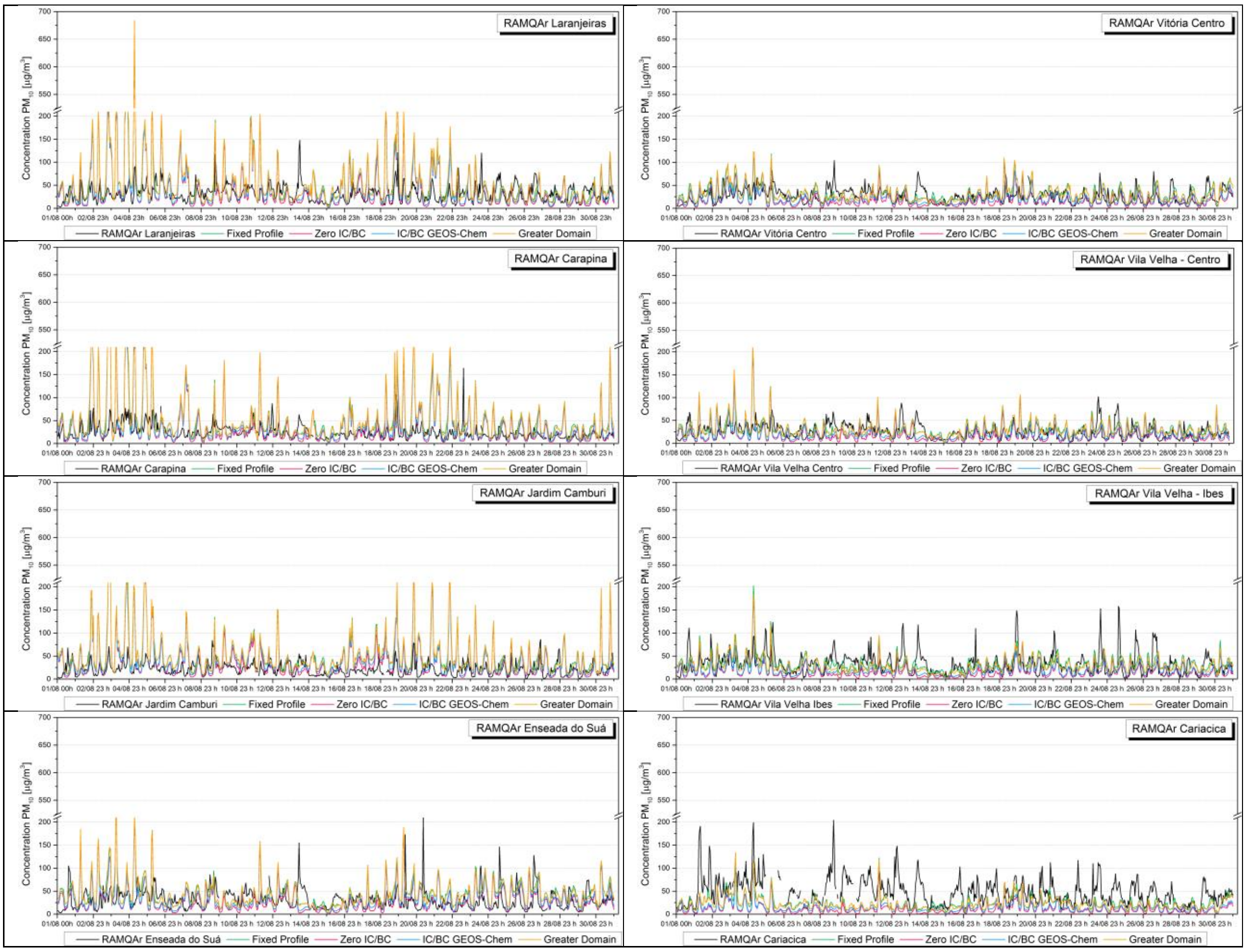


Fig. 8. Time series for PM_{10} comparing modeled and observed data (left) scenario for average concentration for august (right).

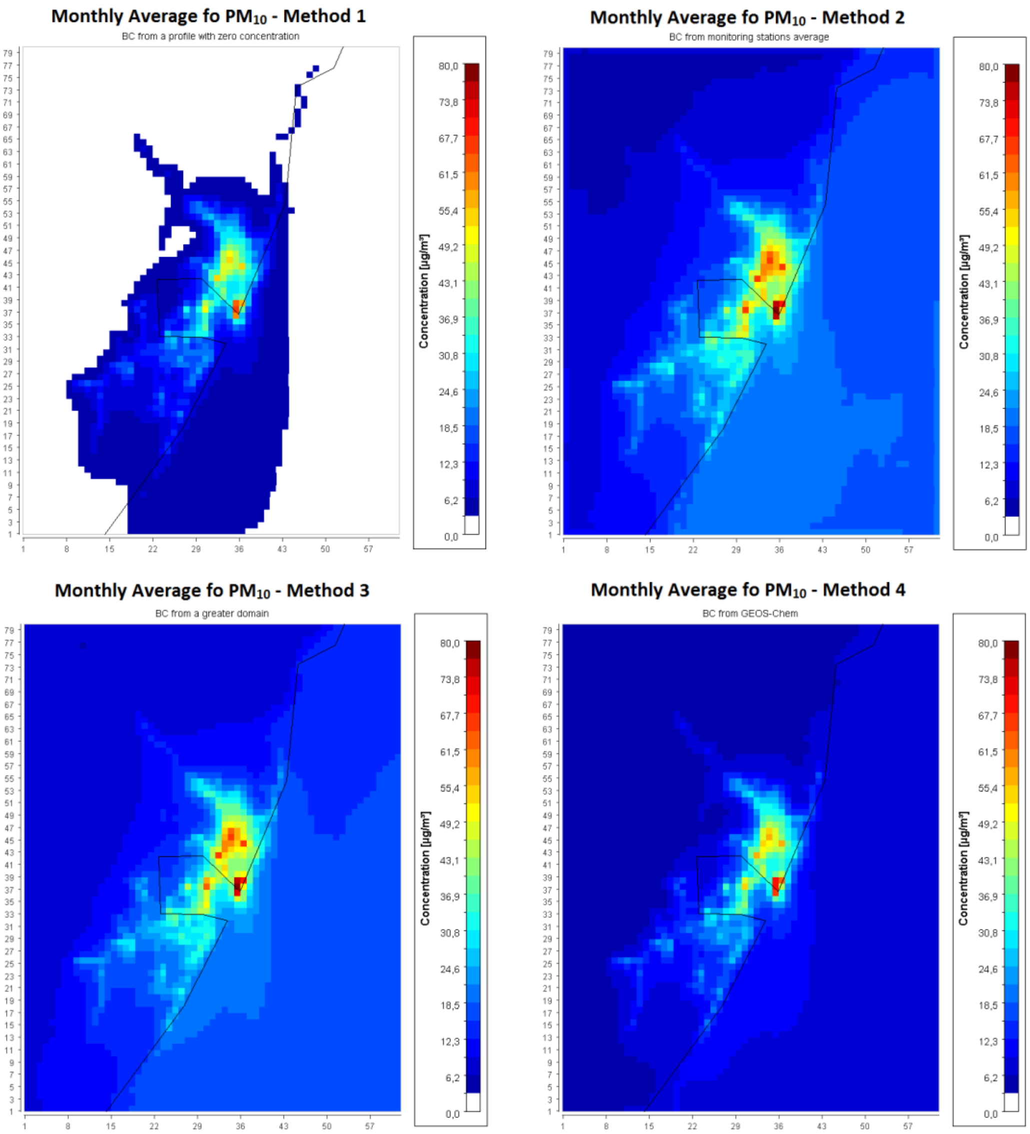
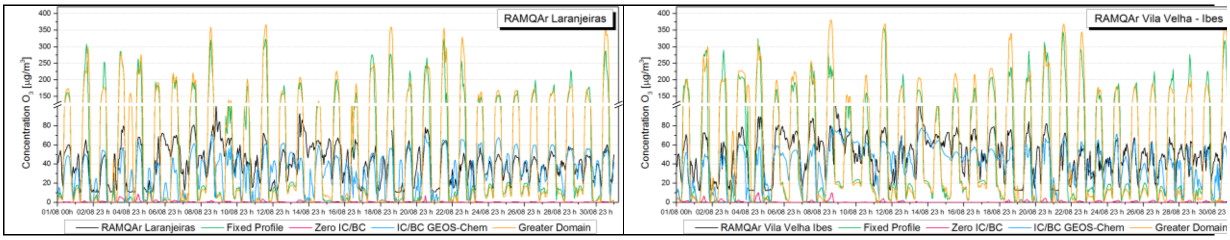


Fig. 9. Monthly average concentration of PM_{10} for August 2010 for each method of BC.

For O_3 time series GEOS-Chem BC provided the best agreement comparing with observed data for all monitoring stations, achieved a good agreement even on hourly variations. For simulations using boundary conditions from a greater domain and average concentration from monitoring stations overestimated the concentrations and zero BC did not allow the ozone formation.

From average scenarios of period, it is possible to see differences among the simulations, but a huge difference was observed over simulation using profiles with zero concentrations (the scale of figure that uses Method 1 is different from the others).



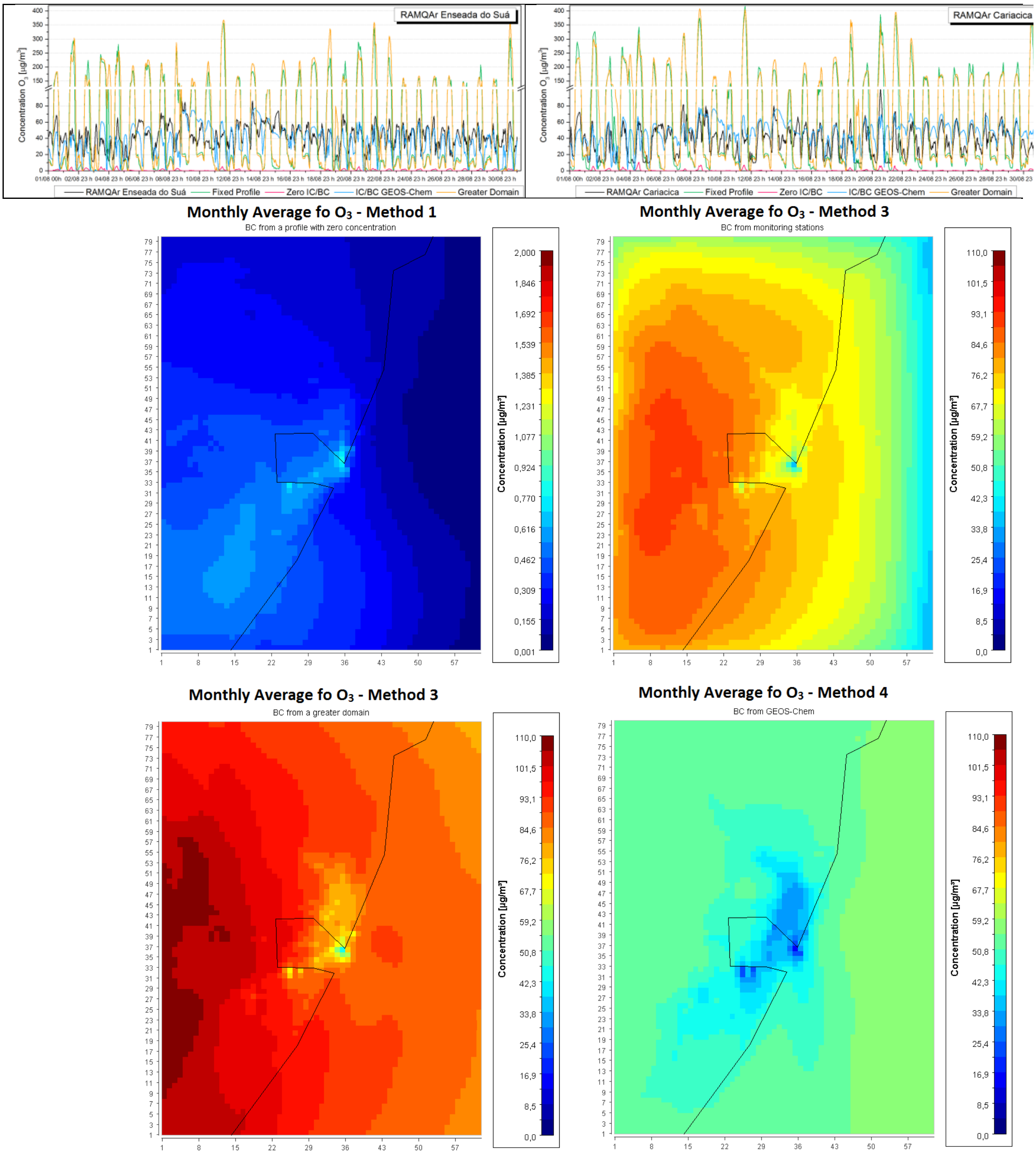


Fig. 10. Time series for O_3 comparing modeled and observed data (left) scenario for average concentration for august (right).

The Fig. 11 and Fig. 12 show the model evaluation proposed by Boylan et al (2006) for simulations over RGV. For PM_{10} the statics are overall similar, with better agreement in some monitoring stations than the others, but the results for method that uses GEOS-Chem boundary conditions are better than the others, for MFB five stations are on the best fit zone and the other methods didn't achieve this results. For O_3, the GEOS-Chem boundary conditions obtained the best results, specially the MFE. This likely means that the emission inventory for the region needs more work

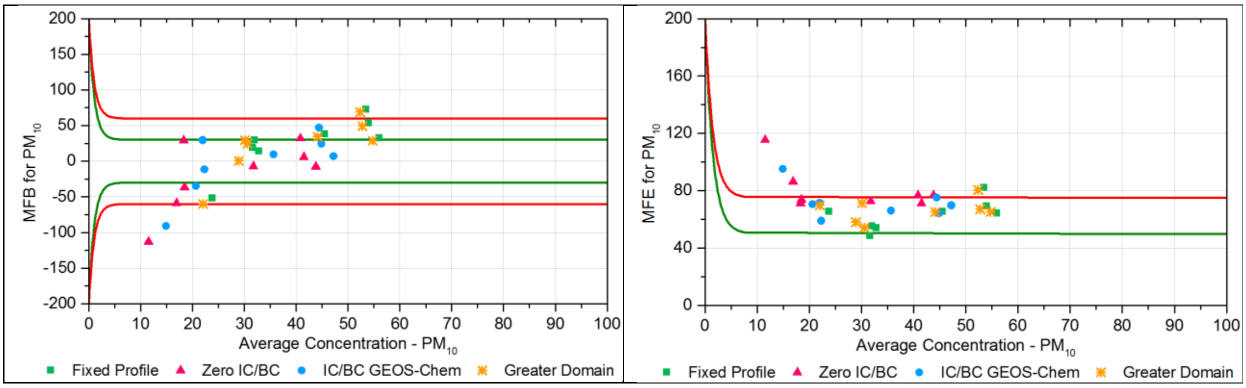


Fig. 11. MFB (left) and MFE (right).for PM_{10} .

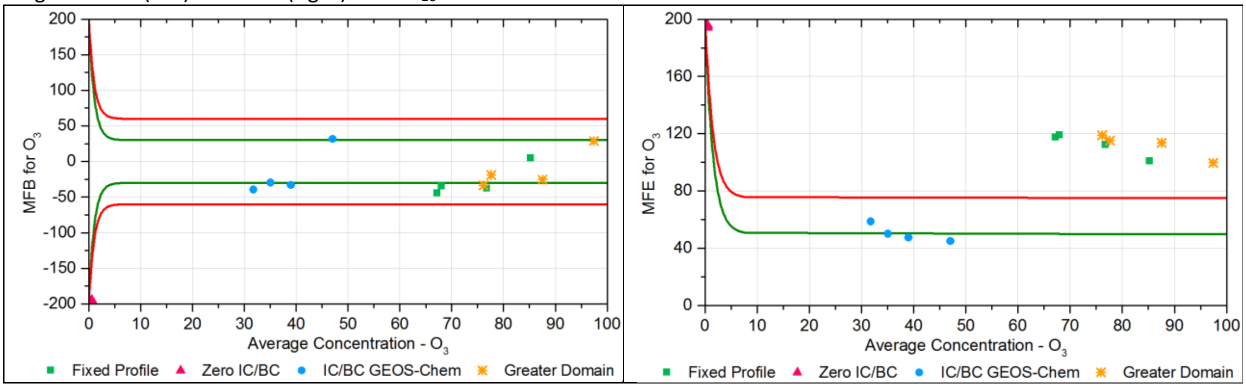


Fig. 12. MFB (left) and MFE (right) for O_3.

4 CONCLUSIONS

The models (WRF and CMAQ) performed a good agreement with observed data, but some improvement are necessary, in special on WRF to get better agreement with wind speed and wind direction.

Results for PM_{10} show that there are singularities that modeling is not predicting, caused maybe for local interferences and meteorology simulations.

The boundary conditions have a huge influence over RGV in special O_3, but for PM_{10} this influence was weaker. Generally, simulations that uses BC from GEOS-Chem obtained better results.

5 ACKOWLEDGEMENTS

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