STUDY OF BOUNDARY CONDITIONS INFLUENCE ON CMAQ SIMULATIONS OVER THE IBERIAN PENINSULA

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Abstract: Air pollution continues to be a major concern in many regions of the world, including Europe, and effective abatement measures are required to meet air quality standards in future years. The Integrated Air Quality Modelling System for the Iberian Peninsula (SIMCA) is a project that it is being implemented in Spain to support the design and evaluation of air quality strategies and abatement plans. The system relies on the WRF+SMOKE+CMAQ models. An important step in the development and implementation of SIMCA consists of understanding the uncertainties involved in modelling process. In this paper, a sensitivity analysis of the CMAQ model to the boundary conditions (BC) needed to simulate air pollution levels in the Iberian Peninsula is presented. The main objective of the study is to assess the model response to different alternatives to supply boundary conditions in the context of the Integrated Assessment Modelling (IAM) activities needed to provide an effective support to the policy-making process. Three ways to provide BC are tested:

- fixed, time-independent, concentration profiles
- concentrations predicted in a CMAQ mother domain (48 km, 1h resolution)
- concentration values from the Geos-CHEM chemical-transport global model (2x2.5º, 3h resolution)

The CMAQ model has been run in two episodes using identical configuration and input data, except for the BC. Model outputs for the main pollutants (SO_2, NO_2, NO, O_3, PM_{10} and $PM_{2.5}$) are then compared with observed concentration values from 165 monitoring stations. The stations selected are distributed across the Iberian Peninsula and include a balanced number of rural, industrial, urban background and traffic locations. The comparison is based on the analysis of a number of statistics commonly used for model evaluation and considers several aggregation levels so the influence of the BC can be assessed in a very detailed way. According to this study, there is no single valid method of providing boundary conditions since the performance of the alternatives tested depend on the pollutant, episode and type of location. Besides the statistical evaluation some other relevant issues in the context of IAM are discussed to gain a better insight into the suitability of the methods analysed.

Keywords: Air quality modelling, boundary conditions, sensitivity analysis, CMAQ,, Iberian Peninsula.

INTRODUCTION

Despite significant emission abatements since 1990, ambient air measurements in urban and rural areas of Europe do not show clear downward trends in some pollutants generally recognised as the most significant in terms of health impacts (EEA 2009). This lack of progress stresses the need for reliable modelling tools, useful to support the design and assessment of abatement strategies to comply with both future air quality standards and emission reduction commitments. The Integrated Assessment Modelling System for the Iberian Peninsula (SIMCA) is intended to provide Spain with such an analysis. The modelling subsystem is composed by three models. Meteorology has been simulated with the Weather Research and Forecasting (WRF) modelling system (Skamarock and Klemp, 2008). Emission processing is based on the Sparse Matrix Operator Kernel Emissions (SMOKE) modelling system (UNC Carolina Environmental Program, 2005, Borge et al., 2008). The Community Multiscale Air Quality (CMAQ) model (Byun and Ching, 1999; Byun and Schere, 2006) is the chemical-transport model used to simulate air quality and deposition levels. Air quality models (AQMs) determine the concentration levels of the species of interest in the atmosphere through a set of coupled differential equations describing the main transport and transformation processes. These equations require initial conditions (IC) and boundary conditions (BC) in order to be solved, that constitutes an important source of uncertainty (Russell and Dennis, 2000). Many authors have agreed on the importance of BC, both for urban and regional scale AQM applications. The analysis of the influence of the options available to supply BC for annual simulations aimed at the assessment of AQ control strategies is particularly important (Samaali et al., 2009, Moussiopoulos et al., 2000, Winner et al., 1995). In this context a sensitivity analysis of the CMAQ model to the boundary conditions needed to simulate air pollution levels in the Iberian Peninsula is presented.

METHODOLOGY

Model Configuration

The CMAQ_SIMCA domain used for this study covers the Iberian Peninsula and consists of 400 columns and 320 rows of 3 x 3 km^2 grid cells (Figure 1). Vertical structure is composed by 30 layers that cover completely troposphere corresponding to sigma levels of 1.000, 0.999, 0.997, 0.995 0.992, 0.987, 0.980, 0.970, 0.950, 0.910, 0.860, 0.800, 0.750, 0.700, 0.650, 0.600, 0.550, 0.500, 0.450, 0.400, 0.350, 0.300, 0.250, 0.200, 0.150, 0.100, 0.075, 0.050, 0.025, 0.010 and 0.000. The configuration of the WRF model corresponds to the optimal setup described in Borge et al., (2008b). Emission datasets for SMOKE model are taken from the National Emission Inventories of Spain (SNEI) and Portugal (PNEI) and processed with SMOKE (Borge et al., 2008a). The inventory was adapted chemically to the Carbon Bond CB05 mechanism (Yarwood et al., 2005). Options chosen for chemical transport model were: Yamartino global mass-conserving scheme to advection, Asymmetric Convective Model version 2 (ACM2) to vertical diffusion, CB-05 gas-phase mechanism to chemical mechanism, Euler Backward Iterative (EBI) solver to numerics and 4th generation modal CMAQ aerosol mechanism with extensions for sea salt emissions and thermodynamics to aerosols.

The episode selection simulations were conducted in two periods of the year 2005; from 19 February 00h UTC to 28 February 00h UTC (winter episode) and from 18 June 00h UTC to 27 June 00h UTC (summer episode). Winter episode was chosen due to high values of sulphur dioxide (SO_2) while summer episode was selected by high concentration values of ozone and particulate matter (PM_{10} and $PM_{2,5}$). Details regarding the two episodes can be found in Borge et al., (2008b).

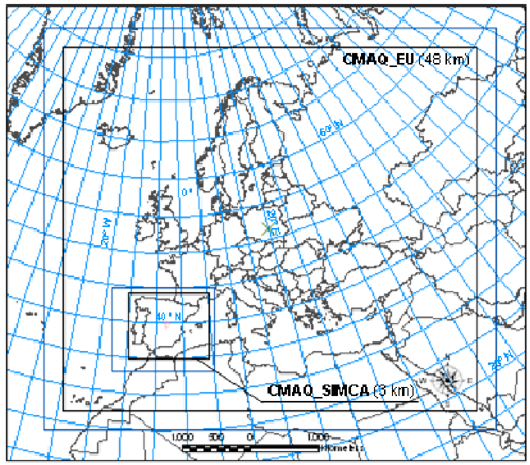

Figure 1: CMAQ modelling domains (Lambert Conformal projection). In blue, WRF domains.

Options to provide boundary conditions

According to Samaali et al., (2009), three basic strategies exist to provide information in order to build boundary conditions for chemical transport model. The first option consists of including all emissions sources that have influences in the region of interest. Other method supposes to assume fixed concentrations in the boundaries. The third method involves the application of a nesting approach, so that dynamic BC are obtained from larger-scale simulations. The last two methods are studied in three alternative paths:

- Concentration profiles (profile method)
- Concentrations predicted in a CMAQ European mother domain (CMAQ-EU method)
- Concentration values from the GEOS-Chem chemical-transport global model (GEOS-Chem method)

The profile method relies on fixed concentration profiles (clean air) suggested by US EPA. For CMAQ-EU simulation, dynamic BC (1 h temporal resolution) are taken from a CMAQ simulation in the CMAQ-EU domain (48 km. resolution) through a 1-way nesting strategy. Emissions are taken from EMEP inventory with 50 km spatial resolution while Biogenic are taken from 1ºx1º Global Emission Inventory Activity (GEIA) proposed by Guenther (1996). Ancillary data are taken from EuroDelta experiment (Van Loon et al., 2007). Further details about this method and additional consideration to achieve a consistent approach the scales are discussed in Borge et al., (2009). The Geos-Chem BC are based on the application of the GEOS-Chem global chemical transport model (Bey et al., 2001) with 30 layers, a spatial resolution of 2ºx2.5º and 3h temporal resolution. This model has been used for similar studies around the world (i.e., Tombrou et al., 2009, Appel et al., 2007). Geos2cmaq tools (Moon and Byun, 2004) were used to adapt the outputs of the GEOS-CHEM to the CMAQ model.

Air quality monitoring data

Outputs from CMAQ model were compared with air quality data records which have been measured for each episode in different locations across the main domain (Figure 2) in order to understand model behaviour and find out the influence of the BC provided.

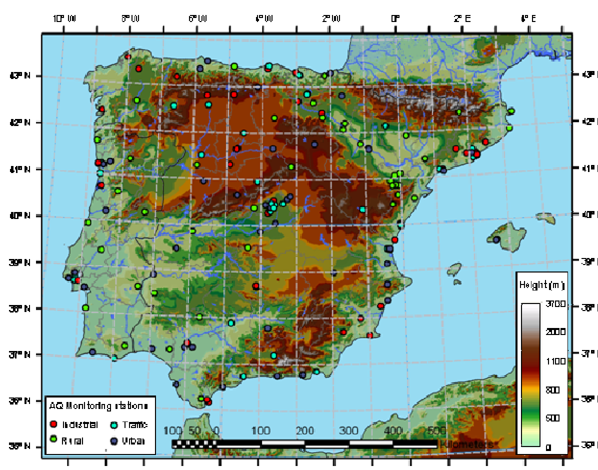

Figure 2: Air quality monitoring stations selected to perform the BC study

Monitoring stations were selected by geophysical conditions, availability data and representativeness data of whole domain. Hourly records form 165 monitoring stations (SO_2, NO_2, NO, O_3, PM_{10} and $PM_{2.5}$) were used in the analysis. The selection includes a balanced number of rural (26%), industrial (23%), urban background (27%) and traffic (24%) locations.

Evaluation Methodology

The analysis of an ample variety of statistics (Table 1) performed in this study may mitigate the limitations of the evaluation method used (observed Vs predicted values). A description of statistics, properties and interpretation are shown in other studies (Borrego et al. 2008; Eder and Yu, 2006; Boylan and Russell, 2006). Different aggregation levels have been studied depending on station, episode and station type. At last, a global representation of data is shown to compare all different alternatives to provide BC.

Table 1: Summary of statistics used for model evaluation and experiment comparison. P-predicted, O-observed

Statistic	Values (range)	Definition
Mean Bias (MB)	Each unit (ppb or µg/m^3	$MB = \frac{1}{IJ}\sum_{\substack{i=1\\j=1}}^{IJ}\left(P_j^i - O_j^i\right)$
Normalized Mean Bias (NMB)	% (-100 - ∞)	$NMB = \frac{\sum_{\substack{i=1\\j=1}}^{IJ}\left(P_j^i - O_j^i\right)}{\sum_{\substack{i=1\\j=1}}^{IJ} O_j^i}\times 100$
Mean Error (ME)	Each unit	$ME = \frac{1}{IJ}\sum_{\substack{i=1\\j=1}}^{IJ}\left|P_j^i - O_j^i\right|$
Normalized Mean Error (NME)	% (0 - ∞)	$NME = \frac{\sum_{\substack{i=1\\j=1}}^{IJ}\left|P_j^i - O_j^i\right|}{\sum_{\substack{i=1\\j=1}}^{IJ} O_j^i}\times 100$
Root Mean Squared Error (RMSE)	cu	$RMSE = \sqrt{\frac{1}{IJ}\sum_{\substack{i=1\\j=1}}^{IJ}\left(P_j^i - O_j^i\right)^2}$
Unpaired Peak Accuracy (UPA)	% (-100 – 100)	$UPA = \frac{P_{max} - O_{max}}{O_{max}}\times 100$

RESULTS

Surface level as well as vertical distribution of concentration values in the BC obtained were scrutinized and significant differences were found. Taking O_3 as an example, it was found that the CMAQ-EU method systematically provided higher estimates at ground level than GEOS-Chem in winter (around 60%), being time-independent concentration values prescribed by the profile method in between. In summer, however, GEOS-Chem predicts slightly larger average and maximum values than CMAQ-EU, except for the northern boundary. Top level O_3 concentration is set to 70 ppb in the fixed-profile BC (approximately twice as much as at surface level), quite similarly to the resulting top-level concentration BC provided by the CMAQ-EU method. Topmost concentration values in the BC obtained for the GEOS-Chem model are far larger (300-500 ppb).

CMAQ simulations

The impact of BC in model response was studied for the main pollutants. Following with the example of O_3, the differences of the three methods tested are illustrated in Figure 3. The summary of the statistical comparison for O_3 results is shown in Table 2.

Table 2: Aggregated statistics for O_3

Statistic	Winter			Summer			Total		
	Profile	CMAQ-EU	GEOS-Chem	Profile	CMAQ-EU	GEOS-Chem	Profile	CMAQ-EU	GEOS-Chem
MB (ppb)	14.1	17.0	9.1	6.2	7.8	10.5	10.1	12.4	9.8
NMB (%)	54.8	66.2	35.5	15.9	20.2	27.1	31.5	38.6	30.5
ME (ppb)	16.2	18.4	12.9	14.8	15.9	17.0	15.5	17.1	14.9
NME (%)	63.1	71.5	50.2	38.1	41.0	43.9	48.1	53.2	46.4
MFB (%)	50.0	56.8	37.2	21.8	25.8	31.4	36.0	41.4	34.3
MFE (%)	60.1	63.9	53.9	42.0	44.2	45.9	51.1	54.1	49.9
RMSE (ppb)	19.8	21.7	16.4	18.7	19.7	20.9	19.2	20.7	18.8
UPA (%)	-4.6	37.6	-10.9	-43.8	-45.6	-43.6	-43.8	-45.6	-43.6
r	0.398	0.412	0.412	0.457	0.421	0.423	0.469	0.447	0.521

IOA	0.447	0.333	0.554	0.737	0.710	0.717	0.636	0.578	0.671

Positive biases demonstrate that the CMAQ model tends to overestimate O_3 levels in this application. Independently of the method used to provide BCs it was found that the overestimation is concentrated in the low O_3 concentration range (less than 40 ppb). This tendency to overestimate low values is the main responsible for the general poor performance observed for the winter episode, with NMB ranging from 35.5% (GEOS-Chem) to 66.2% (CMAQ-EU). The worst results correspond to the CMAQ-EU method since the overprediction of CMAQ occurs both in the mother and nested domain, conferring this method a particularly low performance in winter. BCs from GEOS-Chem clearly improve the performance of the CMAQ model in winter, which is consistent with the findings of Appel et al., (2007). Although the general performance is much better in summer (IOA above 0.7 for the three methods tested), however, the results from the profile method are slightly better than those of GEOS-Chem. Total aggregated statistics suggest that GEOS-Chem is the best alternative to improve model performance as far as ozone is concerned, maximizing the differences in model response between winter and summer episodes. This contrast is observed also spatially, in particular in the eastern part of the domain. In contrast with the results for other pollutants (e.g. NO_2), it was found that the effect of alternative BCs can have a clear influence domain-wide.

The vertical O3 distribution was examined and it can be concluded that the consideration of very different O_3 BC in the topmost part of the modelling domain does not impact significantly model predictions at surface level with the vertical structure used (top pressure and layer definition) during the particular episodes simulated. This contrast with previous studies were excessive vertical transport of O_3 was observed when downscaling from GEOS-Chem (Emery et al., 2009).

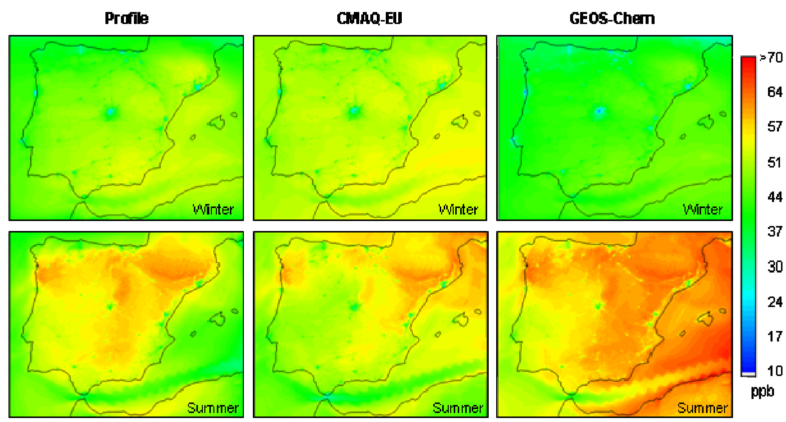

Figure 3: Mean O_3 predicted values for the winter and summer episodes for the three experiments.

CONCLUSIONS

The influence of chemical boundary conditions (BC) on the response of the Community Multiscale Air Quality (CMAQ) model over the Iberian Peninsula was investigated in this study. High resolution (3 km) simulated concentrations of the main pollutants (NO_2, NO, SO_2, O_3, PM_{10} and $PM_{2.5}$) were compared through a comprehensive statistical analysis of observed and predicted values according to three alternative methods to provide BC. The convenience of one method over the others is not clear, since it strongly depends on specific modelling purposes as well as other practical factors. It was found that model sensitivity to BC for nitrogen and sulphur oxides was limited, being restricted to the vicinity of model boundaries. However, significant domain-wide differences were found when modelling ozone and PM depending on the BC provided to run the tests. Although model performance was affected by spatial and seasonal factors, the results indicate that model-derived, dynamic BC improved CMAQ predictions when compared to those based on static concentrations prescribed in the boundaries. Aggregated statistics suggest that the GEOS-Chem produced the best results for O_3 and $PM_{2.5}$ while NO_2 and PM_{10} were slightly better predicted under the CMAQ nesting approach. The adoption of the GEOS-Chem downscaling approach would require a thorough analysis of possible inconsistencies regarding not only emissions but other important issues such as chemistry and chemical species mapping, dynamics, etc. As for the nested approach, the analysis performed suggests that further research on the reasons why the WRF-CMAQ systems tends to overpredict low O_3 values is needed. Regardless of this and other improvements in the context of the integrated assessment modelling system, the influence of BC for mesoscale air quality modelling over the Iberian Peninsula may be further investigated. In particular, the analysis of the results for a complete annual simulation would increase the significance of the analysis.

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