AIR QUALITY STUDY OVER THE ATLANTIC COAST OF IBERIAN PENINSULA

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ABSTRACT

The west coast of Iberian Peninsula, surrounded by the Atlantic Ocean, is characterized by complex topography and some favourable synoptical situations, which imply the appearance of mesoscale circulations strongly influencing the transport of pollutants. In addition, the regions of Galicia (NW Spain), and the North of Portugal, have important air pollutants sources (power plants, chemical industries, traffic and biogenic emissions), all of them contributing to the air quality along the Atlantic coast and even affecting the centre of the Iberian Peninsula. The main purpose of this work is to describe the application of two numerical systems: meteorological model (MM5) (Grell et al., 1995) and the air quality model (MARS) (Moussiopoulos, 1992), to the NW of the Iberian Peninsula.

In order to achieve the proposed objectives the results of a global numerical weather prediction model (GCM), namely the AVN (Aviation model from the National Centres for Environmental Prediction of USA) were used as initial and boundary conditions into the regional meteorological model of the Pennsylvania State University/ National Center for Atmospheric Research Mesoscale Meteorology Model (MM5) over an area that includes a large part of the Iberian Peninsula, using its nesting capabilities. To analyse the photochemical production over the fine grid domains an interface between MM5 and the photochemical model (MARS) was built up, constituting the first attempt to integrate these two models.

The achieved results must be considered as preliminary since the application of this particular prognostic numerical system indicates that more refinement on the boundary layer parameterisations as well on the initial and boundary conditions applied to the

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MARS model is needed, although the system represents reasonably well the ozone measured concentrations.

1. INTRODUCTION

Studies on atmospheric circulations over the Iberian Peninsula have shown particularities concerning summer dynamics (Millan et al., 1992). Frequently, there is the development of a low thermal pressure area in the centre of the Peninsula, which allows mesoscale processes enhancement such as land-sea breezes. This type of circulations encourages photochemical production of air pollutants leading to smog episodes, which can cause health problems to the population and environmental degradation.

Global numerical weather prediction can provide information about the present and time evolution of the atmospheric situation (wind speed, wind direction, temperature, humidity, etc.). This information is fundamental to estimate the transport, production, dispersion and removal of air pollutants.

Nevertheless, global meteorological models are not suitable for regional studies of transport of pollutants due to their coarse resolution (1º ≈ 100 km). These models do not simulate properly mesoscale and regional phenomena, but their results may be refined with mesoscale models using dynamical downscalling. In dynamical downscaling, GCM simulations are used to drive regional climate models, which simulate mesoscale circulation and physical processes in the land-atmosphere system. The knowledge and characterisation of mesoscale atmospheric flow patterns, as well as, the description, by mathematical models, of dispersion and transformation mechanisms of photo-oxidants are fundamental.

The main purpose of this work is to describe the application of two numerical systems; the meteorological model (MM5) and the air quality model (MARS), to the NW of the Iberian Peninsula. These systems simulated the dispersion of pollutants in the atmosphere, during two summer days, in North part of Portugal. It is important to mention that the achieved results should be considered as pilot, because MARS model is very sensitive to the initial and lateral conditions of chemical species concentrations as well as to the selected MM5 parameterisations. This represents a considerable field of research in order to better integrate both models.

2. THE APPLIED NUMERICAL SYSTEMS: MM5/MARS

Version 3 of the Pennsylvania State University/ National Center for Atmospheric Research Mesoscale Meteorology Model (MM5V3.4), is a powerful meteorological model that contains comprehensive descriptions of atmospheric motions; pressure, moisture, and temperature fields; momentum, moisture, and heat fluxes; turbulence, cloud formation, precipitation, and atmospheric radiative characteristics.

MM5 is a non-hydrostatic prognostic model with a multiple nesting capability, applying one way or two-way nestings. The most interesting features in MM5V3.4 are related with its different physics parameterisations that can be selected by the user and being capable of running in different computational platforms (Dudhia et al., 2001).

MARS model describes the dispersion and chemical transformation of air pollutants in a three dimensional region (Moussiopoulos, 1992). This model is directed towards the photo-oxidants simulation, from which ozone (O_3) is the major component. It is a fully vectorised model that solves the concentration parabolic equation system for known meteorological variables. KOREM and RADM2 can be used on MARS as chemical mechanisms. The first one, which has been chosen to this work, includes 39 chemical reactions with 20 reactive pollutants.

In addition, MARS model needs daily variable chemical species emissions as inputs. These are calculated based on proper approaches depending on the emissions of air pollutants emitted by anthropogenic or biogenic sources.

MARS model numerically simulates photo-oxidants formation considering the chemical transformation process of pollutants together with its transport in the atmospheric boundary layer (Moussiopoulos et al., 1995). The model solves the parabolic differential concentration transport equation system in terrain-following co-ordinates, with the meteorological variables calculated by MM5, e.g., the mass conservation equations are driven by the momentum equation.

These two models have been applied by a variety of entities and the achieved results are acceptable by the scientific community. MM5 is a wide spread community model with strong user support, that is being tested all over the world (Stockwell et al., 2000; Elbern and Schmidt, 2001). In Iberian Peninsula several institutions are applying MM5 as a real time weather forecast tool (http://meteo.usc.es). On the other hand, MARS is also a well-tested model, in Europe (Baldasano et al., 1993; Moussiopoulos, 1994; San José et al., 1997; Borrego et al., 1998).

3. METHODOLOGY

The primary work on the numerical system of models MM5/MARS was applied to 15 and 16 June 2000. During the 15th of June the Iberian Peninsula was under the influence of an anticyclone located southern Bretagne, promoting southeastern winds at surface, over the study area. This evolves to a low surface pressure gradient situation in the middle of the afternoon. This kind of meteorological pattern promotes surface O_3 production. The surface pressure charts are similar in both days (http://www.wetterzentrale.de/topkarten/fsavneur.html;http://www.infomet.am.ub.es/arxiu/mapes_fronts/).

Using MM5 capability of doing multiple nestings, the meteorological model was applied with the one way nesting option and for two nests: (i) a large domain covering the Iberian Peninsula (45 km resolution), (ii) a first nest covering the Atlantic Coast of Iberian Peninsula (15 km resolution), (iii) and a second nest for the North part of Portugal (5 km resolution).

In order to analyse the photochemical production over the fine grid domain, an interface between MM5 and the photochemical model MARS was built up. With this interface all the needed meteorological parameters to calculate photochemical air pollutants advection, production and removal are fed into the photochemical mesoscale model with the necessary time-step resolution results.

MM5 simulations were initialised from the gridded NCEP/AVN analysis, producing outputs in nested 45 km, 15 km and 5 km grids. The grid sizes are 27 x 31, 31 x 43, and 40 x 40 grid points, respectively. All modelling domains have the same vertical structure with 23 unequally spaced σ levels. The 5 km grid is governed by the Warm Rain microphysics moisture scheme, no cumulus scheme, and a Blackadar boundary layer.

In order to integrate both models, the meteorological and the photochemical, a numerical tool was developed. MARS model runs for the inner domain (200x200 km^2 with 5x5 km^2 resolution) with MM5 outputs and the calculated pollutant emissions grid. Anthropogenic emissions were calculated applying a disaggregation technique from the national level to the municipal and then to the sub-municipal level. The CORINAIR 95 National Inventory was used to estimate emission data with required spatial and temporal resolution. For this purpose, disaggregation technique based on statistical indicators was applied. As a first step, national emission data are disaggregated to the municipal level using fuel consumption. Then, the data are processed jointly with population statistics in order to obtain sub-municipal resolution. In this work biogenic emissions were not considered.

4. RESULTS AND DISCUSSION

For the present study, ozone measurements were available at three different locations over the study region: Coimbra, Avanca and Teixugueira. Coimbra (see Figure 1) is an urban air quality station and, for that reason, maximum ozone concentrations were 86 $\mu g.m^{-3}$ and 88 $\mu g.m^{-3}$, both occurring at noon of the 15^{th} and 16^{th} of June, 2000. On the other hand, Avanca and Teixugueira air quality stations are located near the industrial complex of Estarreja and both present the ozone pick during the afternoon, around 17h and 18h local time, over 160 $\mu g.m^{-3}$ (see Figure 2 b)). The appearance time of these two picks, on both days, indicates that the ozone present in these locations may be due to plume production and advection from urban areas, like Coimbra.

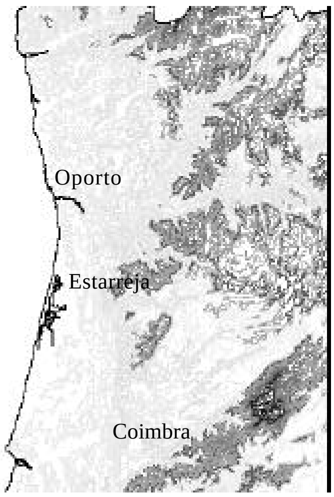
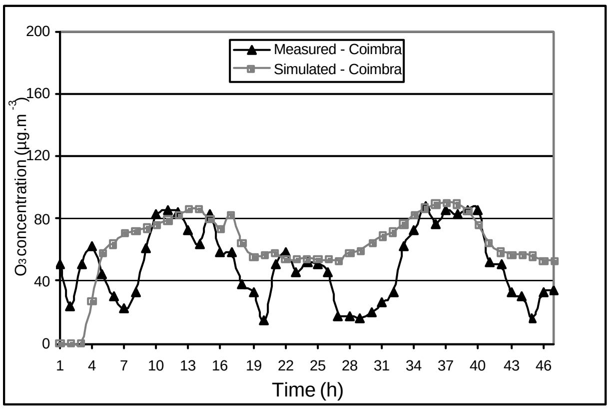
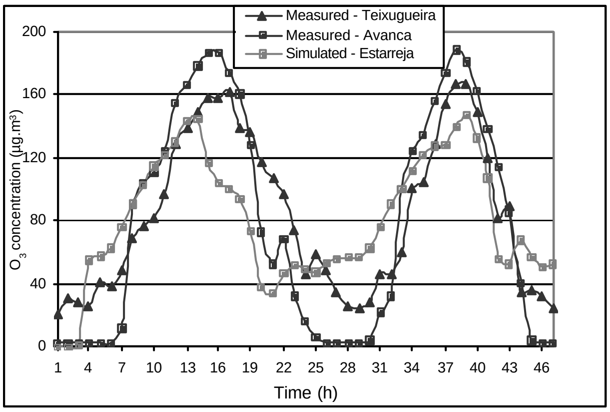


Figure 1. Fine grid domain over the central and north part of Portugal.



a)



b)

Figure 2. O_3 concentration values, measured and simulated, at a) Coimbra and b) Teixugueira, Avanca and Estarreja, for the simulated days (15 and 16 June 2000).

MM5/MARS system shows as results for the two simulated days the same tendency as the measured ones, although the picks of ozone are underestimated for Estarreja (the cell containing both Teixugueira and Avanca for the applied resolution of 5 x 5 km^2). Over Coimbra the system of models tends to overestimate O_3 concentrations during the night time (see figure 2 a)).

Quality indicators reflect the ability of a model to simulate real world phenomena. Applications of such indicators help to understand model limitations and provide a support for model intercomparison. It should be taken in consideration that model evaluation could not be performed on basis of a single quality indicator. A system of quantitative parameters must be identified for each task related to model developing and then, common quality indicators will be established and applied within the project. The performance of the system of models is evaluated through the application of quantitative error analysis introduced by Keyser and Anthes (1977). Consequently, if f_i and f_{iobs} were individual modelled data and observed in the same mesh cell, respectively; f_0 and f_{0obs} the average of f_i and f_{iobs} for some sequence in study, and N the number of observations, then:

$$E = \left\{ \frac{\sum_{i=1}^{N} (f_i - f_{iobs})^2}{N} \right\}^{1/2} \qquad E_{UB} = \left\{ \frac{\sum_{i=1}^{N} [(f_i - f_0) - (f_{iobs} - f_{0obs})]^2}{N} \right\}^{1/2}$$

$$S = \left\{ \frac{\sum_{i=1}^{N} (f_i - f_0)^2}{N} \right\}^{1/2} \qquad S_{obs} = \left\{ \frac{\sum_{i=1}^{N} (f_{iobs} - f_{0obs})^2}{N} \right\}^{1/2}$$

The parameter E is the root mean square error (rmse), E_{UB} the rmse after the removal of a certain deviation and S and S_{obs} the standard deviation of the modelled and observed data, respectively. Keyser and Anthes (1977), suggest that rmse decrease significantly after the removal of a constant bias. Further, according to these authors, this deviation corresponds to inaccuracy in specifications of the initial and boundary conditions. It is possible to say that the simulation presents an acceptable behaviour when:

$S » S_{obs}$, $E < S_{obs}$ and $E_{UB} < S_{obs}$.

Notice that this kind of analysis requires that the standard deviation of the measured data and the simulated data should be approximately equals, to guarantee that the natural variability presented by the measured values is simulated correctly by the numerical model. In this analysis the first five points were neglected due to the spin up of the model.

Table 1. Quantitative analysis of the system of models performance

	Quality Indicators		
Air quality stations	S/S_{obs}	E/S_{obs}	E_{UB}/S_{obs}
Avanca	0.49	0.59	0.59
Teixugueira	0.72	0.60	0.60
Coimbra	0.58	1.01	0.71

According to Table 1, it can be said that the air quality station over Coimbra presents the worst quality indicators values. This may be related to the local characteristics of this urban station, which results are compared to an average value from a 5km x 5km grid cell. The system of models is not able to simulate the natural variability of the measured ozone data due to the very low results obtained for the quality indicator S/S_{obs}. The obtained values for E/S_{obs} and E_{UB}/S_{obs}, over Avanca and Teixugueira, reveals that the model produces acceptable results. Once that Teixugueira presents the best data variability one can say that this station can be considered as a representative air quality station.

In order to analyse how measures correlates with simulated data scatter plots were designed. Figure 3 a), b) and c) presents the correlation for the three air quality stations. For Coimbra station the model tends to overestimate the lower O_3 concentration values. This tendency is more pronounced during night time due, probably, to the O_3 consumption by NO_x. At Avanca station, based on scatter analysis, the system of models has the tendency to underestimate the higher O_3 values and overestimates the outputs for lower O_3 concentrations. On the other hand, Teixugueira presents the best results of the three stations, as was revealed by Table 1. Although, the results achieved for the three stations were not as good as it should be, probably, this could be related to the lack of biogenic emissions as input to the photochemical model. The combined analysis of Figure 3 and Table 1 reveal that the scatter plots should not be seen *per si*, the results quality assurance is guaranteed if different kinds of jointly evaluations are executed. Based on the measured data over Teixugueira and Avanca (Figure 2 b)) it is possible to see that the air quality stations location is very important for validation studies on regional scale. Avanca presents O_3 decrease over the night, which does not occur at Teixugueira. This can be related to the fact that Avanca is closer to the industrial air pollutants sources of the study region.

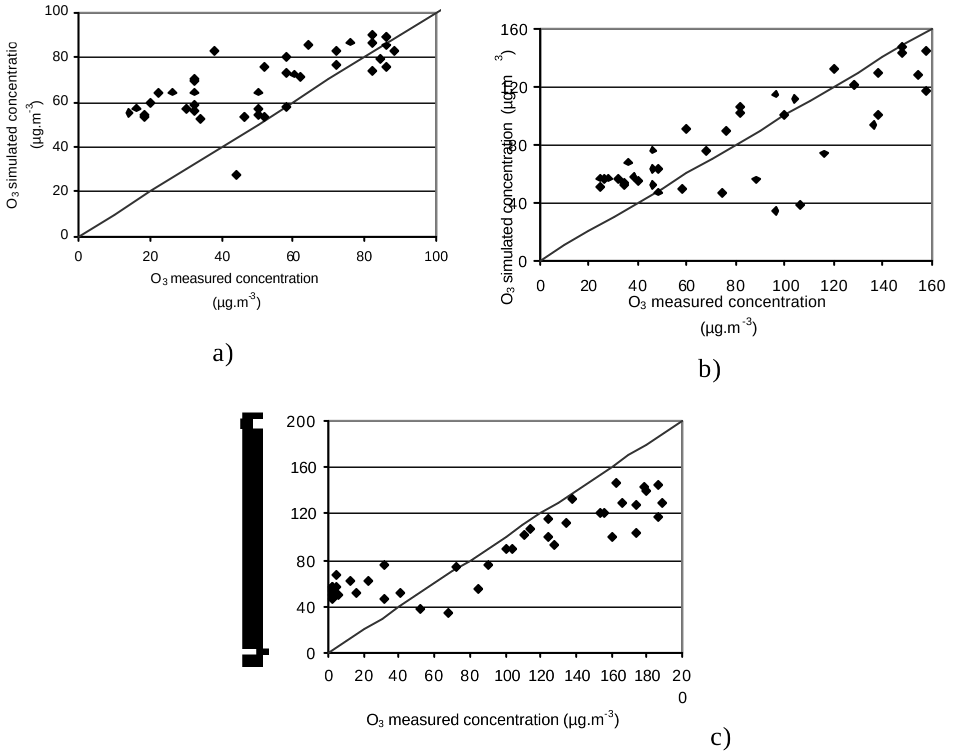


Figure 3. Scatter plots with observed data (x axis) and modeled data (y axis) for a) Coimbra, b) Teixugueira and c) Avanca air quality stations.

5. CONCLUSIONS

From this work it can be said that it will be fundamental to validate the meteorological part of the system with the necessary quality indicators. On the other hand, biogenic emissions should be considered. MARS model is very sensitive to initial and lateral conditions of chemical species concentrations as well to the selected MM5 parameterisations and this represents a considerable field of research in order to better integrate both models.

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