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PARTICULATE MATTER POLLUTION SIMULATIONS IN COMPLEX TERRAIN: A SENSITIVITY ANALYSIS

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Abstract: Preliminary results of an annul simulation of the air quality in a region of Northern Italy is presented. The simulation was performed using a modelling system based on a meteorological model, an interface code and a transport-chemistry model. Comparisons with measured data are presented and discussed.

Key words: *Air quality, Photochemical model.*

INTRODUCTION

Comparing air quality model simulations with observations over a full or several full years, is a very challenging task in predicting the atmospheric pollution. Concerning the long range air quality models, Johnson *et al.* (2006), using a photochemical trajectory model simulated the chemical evolution of air masses during late July and August 2003, a period which included a widespread and prolonged photochemical pollution episode. Observations were quantitatively verified by 13-year long simulations over the whole period using a regional chemistry-transport model and the EMEP emission inventory by Vautard *et al.* (2006). Modelling systems including emission pre-processor, meteorological model, dispersion and chemical models have been developed (see for instance Sokhi *et al.*, 2006, Sokhi *et al.*, 2007) and tested. Furthermore, different large scale air quality modeling systems are in operations nowadays.

In this work, a chemical transport modelling system is used for simulating airborne dispersion and chemical reaction on a regional scale domain (250X250 km^2) in the North-West of Italy, where the main urban industrial areas are located in the Po Valley surrounded by very complex terrain. Indeed the Po river valley is very industrialised and heavily populated and it is characterised by strong urban, industrial and traffic emissions; moreover, the presence of the Alps often gives rise to weak circulation and stagnant conditions. The model resolution is 5 km and the emissions are derived from different regional and national inventories for the year 2005. The simulation is performed using the RAMS meteorological model in order to provide meteorological input to the Eulerian chemical transport model CAMx. The project aims at analysing the simulation lasting one year and it is focused on the comparison with measured data. In particular, the influence of the meteorological parameters (wind and dispersion coefficients) and that of the emissions is investigated.

THE MODELLING SYSTEM

The proposed modeling system includes the meteorological model (RAMS, Pielke *et al*., 1992), an emission processor, (Balanzino *et al.* 2007 a,b) and the photochemical model (CAMx, Environ, 2005).

RAMS resolves the full set of the primitive dynamic equations. The governing equations are the three momentum equations, the pressure equation, the continuity equation, the moisture conservation equation and the potential temperature equation. It solves these equations using a two time step procedure whereby a small time step is utilized to stably integrate the high-speed sound waves, while the most part of the computations are carried out over a larger time step. In this study, the model has been used in its non-hydrostatic version and the Coriolis force was considered. RAMS includes a parameterization of the sub-grid scale turbulence, which entails an horizontal deformation scheme and the Mellor and Yamada 2.5 turbulence closure (Mellor and Yamada, 1982) in the vertical direction, while the local deformational scheme is used for horizontal mixing. The topography is introduced using a terrain-following vertical coordinates. As lateral boundary conditions, the Klemp and Wilhelmson (1978) conditions, are activated. About the radiation parameters the options for evaluating short-wave radiative transfer and long-wave radiation are set to Chen and Cotton (1983) parameterization. This scheme does account for condensate in the atmosphere, but not whether it is cloud water, rain or ice. The convective parameterization is used to vertically redistribute heat and moisture in a grid column when the model generates a region which is super-adiabatic or convectively unstable and when the horizontal grid resolution is too coarse for the model to develop its own convective circulation. Surface layer and soil parameterization are used. We have selected the higher moisture complexity level, which activates the bulk micro-physics parameterization, which includes cloud water, rain, pristine ice, snow, aggregates, graupel, and hail, or certain subsets of these. This parameterization includes the precipitation process. The model is driven by means of the nudging technique using the ECMWF (European Centre for Medium Range Weather Forecasts) analysis as initial and boundary conditions, with 0.5^o space resolution and 6 hours time resolution. Emission input data are prepared starting from different inventories: within the Italian borders, the INEMAR regional emission inventories of Piemonte and Lombardia, the Italian official inventory for European areas and for the portion of Mediterranean Sea emission data have been derived by the EMEP inventory that provides an emission assessment over Europe based on cells of 50X50 km^2. Inside each inventory, emission data are subdivided by activity and organized using the SNAP (Selected Nomenclature for Sources of Air Pollution) classification scheme, which is, in our case, composed by 554 different sectors. The emission processing system was designed by our group (Balanzino *et al.* 2007a and b) to produce emission fields according to the model needs: we have developed an emission processor, based on emission data collected from the different inventories. As the data provided by emission inventories are unsuitable for air quality modeling purposes (Seinfeld, 1988), the emission processor performs spatial disaggregation (allocating the territorial unit information onto grid cells), the temporal modulation (calculating hourly emissions from the annual emission), the hydrocarbon speciation (converting the total volatile organic compounds emission in species-group required by the model) and the particulate speciation (performing chemical speciation and dimensional splitting of the total PM mass according to the model outline). Space and time disaggregation of the inventory data were made on activity basis according to thematic data (CORINE Land Cover and high resolution vector information on studied areas) and typical modulation profiles (monthly, daily and hourly).

The processor performs first the spatial splitting using a "surrogate (or proxy) variables" approach. Each emission activity is allocated according to one or more appropriate proxy variables: cultivated areas, industrial areas, urban areas, highways, railways, roads, rivers, lakes, sea, forests (subdivided in three different mixed proxy on the basis of the kind of tree) and two mixed river-lake variables. Secondly the processor makes the temporal modulation, using three modulation factors (monthly, daily and hourly). The hydrocarbon speciation is then carried out starting from the total volatile organic compounds emissions and defining a speciation profile. According to the speciation profile (Passant, 2002), total VOC emissions of a specific source are split into single organic species and then lumped into the aggregated classes handled by the model. Finally the particulate speciation (CARB, 2000) is performed according to the aerosol mechanism options chosen for treating the aerosol size distribution. The scheme actually implemented divides the size distribution into two bins (coarse and fine).
CAMx (Environ, 2005) is a Eulerian photochemical dispersion model that simulates the emission, dispersion, chemical reaction and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids. CAMx requires inputs to describe photochemical conditions, surface characteristics, initial/boundary conditions, emission rates, and the meteorological fields over the entire modeling domain. The grid projection may be selected as Cartesian (fixed physical distance coordinates on a flat plane) or curvi-linear geodetic (following the curved surface of the Earth). The Cartesian options include different projections. The geodetic option performs the simulation on a latitude/longitude grid. All the input files are defined on the grid projection specified for the CAMx simulation. For gas phase chemistry the following chemistry solvers are available: CMC (Chemical Mechanism Compiler), IEH (Implicit-Explicit Hybrid), or LSODE (Livermore Solver for Ordinary Differential Equations). The nested grids are specified in terms of the range of master grid cells that each nested grid spans. The domain chosen for the dispersion simulation extends over a 250X250 km^2 area. Two nested grid were used for the meteorological simulation, the larger one covered a 540x540km^2 domain and the inner grid, having a resolution of 5 km, coincided with that of the dispersion and chemical model.

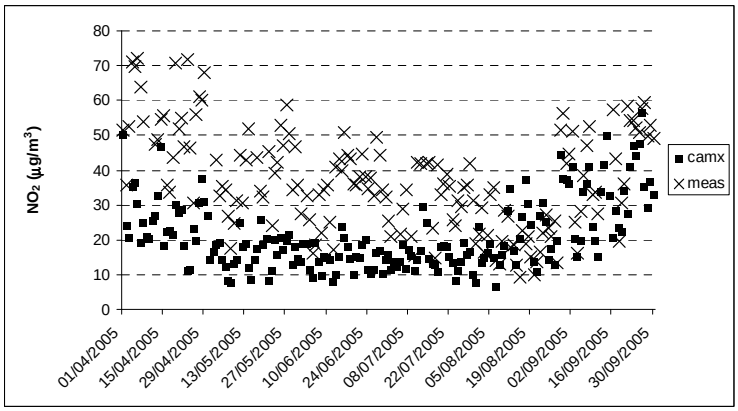

Figure 7. Six months daily mean NO_2 concentrations at the urban station

SIMULATION RESULTS

The first parameter we account for is the stations environment. To this aim we compare the results obtained for two measurement locations, the first one refers to urban environment (station 1), while the second one to rural environment (station 2). Figure 1 shows the comparison between measured and simulated daily mean NO_2 concentrations at station 1 for the period from 1st April to 30th September. It appears that the measured concentrations are underestimated by the model, but the seasonal trend seems to be captured, the average level decreases in the middle of the summer and increases going towards the autumn. This behaviour may be due, in the spring, to the effect of the residential heating that is not active during the hot season and to the higher solar radiation in the late spring and summer. However the NO_2 reduction is limited due to the urban traffic. The model seems to be able reproduce this modulation. The underestimation thus seems to be linked to the meteorology, as for example to an overestimation of either vertical dispersion or wind velocity, because the model does not properly account for the urban effect.

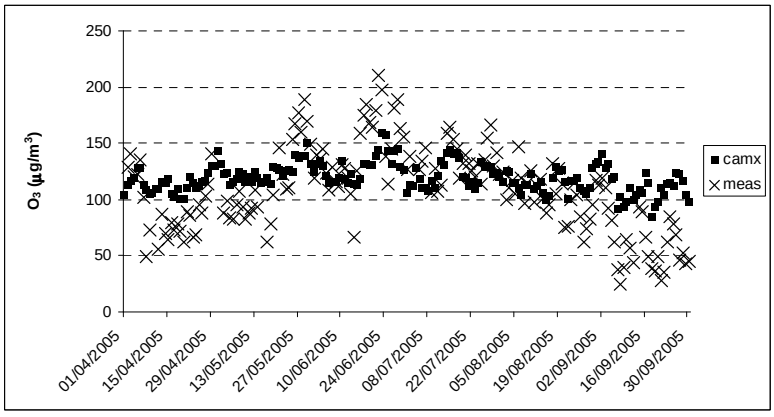

Figure 2. Six months daily maximum 8-h average O_3 concentrations at the urban station

In figure 2 the comparison between simulated and measured daily maximum 8-h average O_3 concentrations at the same urban station 2 can be observed. In this case the mean values seem to be better predicted than the trend during the period, as a matter of fact the ozone concentration does not show any seasonal variation, while the measurements exhibit largest values in the hottest months. Overestimation taking place in spring and fall is related to the excess of dilution already highlighted for NO2, limiting the effect of NOX titration. Summer underestimation is probably related to dispersion too. Indeed, an excess of dilution can give rise to an underestimation of precursors concentration, reducing photochemistry and ozone production.

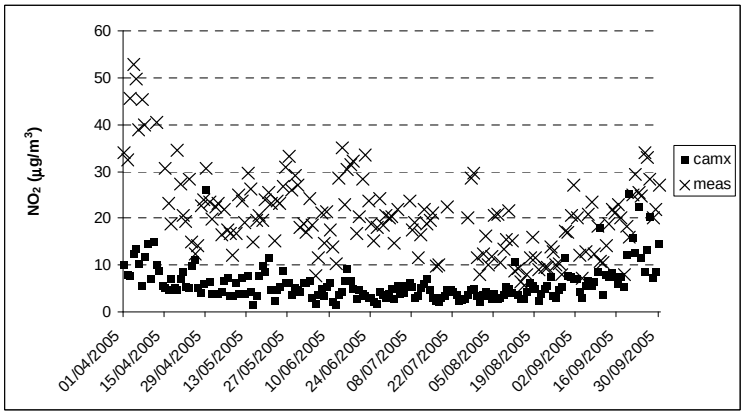

Figure 3. Six months daily mean NO_2 concentrations at the rural station

Figure 3 refers to the rural station and shows the comparison of the daily mean NO_2 concentrations. In this case the effect of the traffic is less evident in the data, which, after a decreasing in April (after the end of the residential heating) remains almost constant during the summer. The model underestimates measurements exhibiting an almost constant trend except for an increasing of the simulated values in the month of September. Also in this case, NO_2 underestimation is probably related to an overestimation of emission dilution.

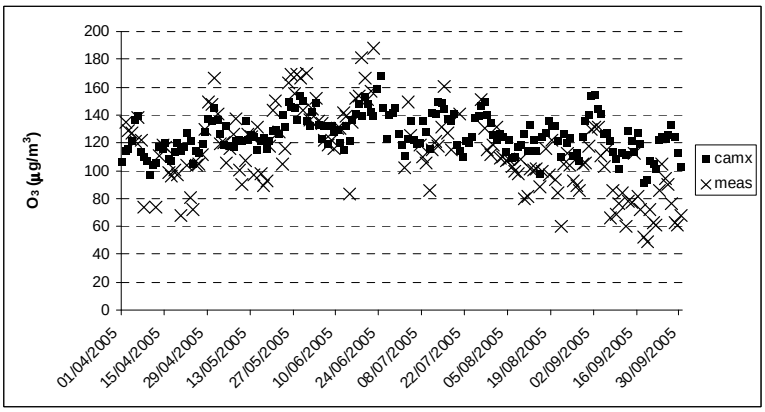

Figure 4. Six months daily maximum 8-h average O_3 concentrations at the rural station.

The daily maximum 8-h average O_3 concentrations at the rural station, depicted in figure 4, shows a rather good agreement between measurements and simulation. However the model seems to be not able to follow the extreme variations (maxima and minima) of the data gathered at station.

The statistical analysis is presented in Table 1, where mean value, Normalised Mean Square Error (NMSE), correlation coefficient (R) and Fractional Bias (FB) are considered. For NO_2 daily mean values are considered, while the daily maximum 8-h average concentrations is accounted for concerning O_3. It is possible to observe that measured NO_2 does not show differences in the mean values of the rural and urban stations. Furthermore, the predictions for O_3 agree quite well with measurements both at urban and rural station. On the contrary NO_2 values are underestimated, particularly at the rural station. In particular the reduction of the NO_2 concentrations moving from urban to rural environment, which in the measured data is less than a factor two, in the model predictions is found more than a factor three. Considering that the performance of the model is satisfactory for O_3, the unsatisfactory results for NO_2 seem to be related to local effects such as the poor emission accuracy.

Table 1. NO_2 and O_3 statistical analysis

	Pollutant	Model mean ($\mu g/m^3$)	Measur.mean ($\mu g/m^3$)	NMSE	R	FB
URBAN STATION	NO_2	21.0	36.9	0.55	0.5	0.14
	O_3	119.5	108.6	0.08	0.7	-0.02
RURAL STATION	NO_2	6.2	20.6	2.14	0.4	0.27
	O_3	125.8	112.5	0.04	0.7	-0.03

Concerning the winter semester (dived into two trimesters) we consider the comparison of the simulated daily mean PM concentration with the measurements. In Figure 5 and 6 the results at the Station 3 (urban environment) are presented for the month of January, February, March and October, November, December, respectively.

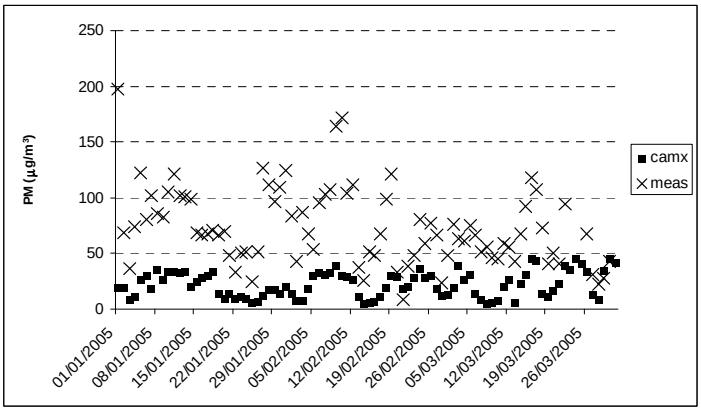

Figure 5. Three months (JFM) daily mean PM concentrations at the urban station

It can be observed that the model always largely underpredicts the measured concentrations. As a matter of fact, these last are higher than the level of 50 $\mu g/m^3$ during almost all the periods considered, while the model predictions are below this value, except for some episodes in October and November.

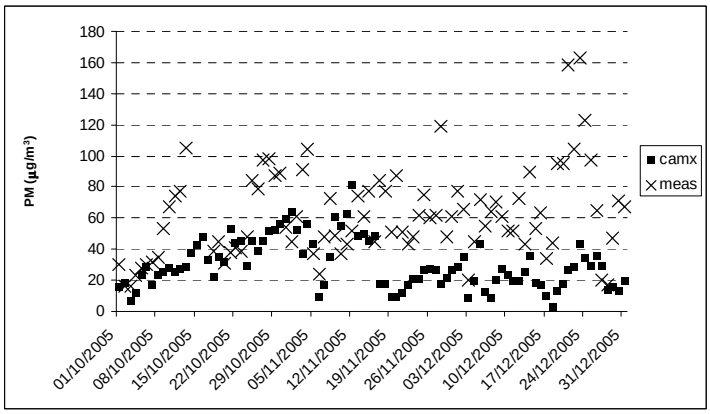

Figure 6. Three months (OND) daily mean PM concentrations at the urban station

The statistical analysis for PM daily mean concentrations is presented in Table 2. The underestimation is indicated by the positive value of the FB, as far as the large error appearing by the comparison of the mean values is confirmed by the value of NMSE. Also the temporal variation is not captured by the model which shows a low value for the correlation coefficient. Taking into account that the Station is located in an urban environment, where the effect of the emissions may be stronger than that of the transport and diffusion or those of chemical transformation, the model underestimation seems to be due to the emission inventory.

Table 2. PM statistical analysis

	Model mean	Measur.mean	NMSE	R	FB
FIRST TRIMES.	22 ($\mu g/m^3$)	74 ($\mu g/m^3$)	2.2	0.4	0.3
SECOND TRIMES.	30 ($\mu g/m^3$)	62 ($\mu g/m^3$)	1.0	0.2	0.2

CONCLUSIONS

A chemical pollution model system has been applied to simulate airborne dispersion and chemical reactions on a regional scale domain (250x250 km^2) with a grid resolution of 5 km, placed in the North-West of Italy. Simulation results over the six summer months have been compared with air quality data. The comparison between computed and measured ozone and nitrogen dioxide concentrations has highlighted some discrepancies. The simulation has also put in evidence some relevant nitrogen dioxide underestimations, mainly in the rural area, but the seasonal trend seems to be captured. This result could be linked to the meteorology (overestimation of the wind velocity and vertical dispersion). As a matter of fact, the model does not correctly reproduce the urban effect. Regarding the ozone, the mean values seem to be better reproduced than the seasonal variability. In general, the analysis of statistical indices demonstrates that the performances of the model are satisfactory for O_3 and that unsatisfactory results for NO_2 seem to be related to local scale processes as the poor emission

accuracy or vertical dispersion reconstruction. As far as the PM mean daily concentration is considered, for the winter semester, the model results show a large underestimation of the measured data at the urban station.

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