SENSITIVITY ANALYSIS OF PARAMETERS INFLUENCING ESTIMATED BY A CHEMICAL-TRANSPORT MODEL

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INTRODUCTION

According to the European Directive 96/62/EC and the Italian Legislation (D.L. 351/1999), the regional administrations are in charge to perform the air quality assessment (AQA) with the aim to classify the territory according to pollution levels and to apply action plans to improve and/or maintain the air quality. The AQA can be attained with a combination of local measurements and modelling techniques that permit to supply information for areas not covered by monitoring sites and where measurements are highly influenced by nearby emissions (poor spatial representativity). Since 2004, Piemonte authorities have charged the Regional Environmental Protection Agency (ARPA) to perform yearly AQA integrating the information provided by the regional monitoring network with concentration fields (CO, NO_x, SO_2, PM_{10}, $PM_{2.5}$, O_3 and benzene) supplied by an Atmospheric Modelling System (AMS). As foreseen by the EU Daughter Directives (1999/30/EC, 2000/69/EC and 2002/3/EC) the accuracy of the predictions given by the AMS has to be evaluated comparing modelling results with measured data. To improve the accuracy of such estimations - particularly for PM_{10}, O_3 and NO_2, the most critical pollutants in the area - a sensitivity analysis has been performed considering two episodes occurred during year 2004. The tests allowed to identify the optimal configuration for yearly runs of the following parameters: vertical diffusivities (K_z), the aeolian contribution of mineral dust to particulate emissions and the explicit treatment of benzene in the chemical mechanism. The results of this evaluation have been applied for the 2005 AQA for which a better agreement of computed fields with observed data was found with respect to previous year AQA. This result confirm the importance of a preliminary sensitivity analysis of factors influencing the performance of the AMS.

MODELLING SYSTEM AND APPLICATION DOMAIN

The Atmospheric Modelling System (AMS) used to perform the AQA over the region is Aria Regional^{TM} that is based on the 3D Flexible Air quality Regional Model (FARM, Silibello *et al.*, 2007). This model has been originally derived from STEM-II code (Carmichael *et al.*, 1991) and implements different gas-phase chemical mechanisms and two aerosol modules: the *aero3* modal aerosol module (Binkowski *et al.*, 1999) and a simplified bulk aerosol module (*aero0*) based on the approach adopted by the EMEP Eulerian Unified model (EMEP, 2003). In addition to the Chemical Transport Model (CTM), the AMS includes following subsystems to apportion data from emission inventories to grid cells, to reconstruct flows and turbulence parameters and to compute the air quality indicators required by the EC directives. This system is currently applied by ARPA over the domain described in Figure 1 covering the Piemonte and Valle d'Aosta regions, part of Liguria and Lombardia regions (the latter including Milan urban area) and portions of France and Switzerland. The domain is 220x284 km^2 wide with an horizontal resolution of 4 km; the top of the computational grid is set to 4000 m above the orography.

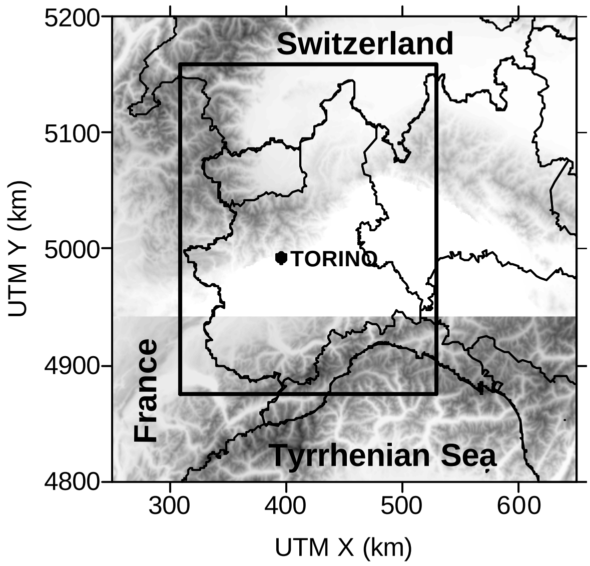

Fig. 1; Piemonte Region air quality assessment modelling system computational domain

Emission data (point, line and area sources) coming from different inventories - detailed regional (for Piemonte, Lombardia and Valle d'Aosta regions), national (for Liguria region) and EMEP (for France and Switzerland) - have been processed by the emission module EMMA (Arianet, 2005) that compute hourly, gridded, time modulated and speciated emission rates for the species considered by the chemical mechanism implemented in FARM. Meteorological fields have been reconstructed integrating analysed fields from the European Centre for Medium Range Weather Forecast (ECMWF) with observations (radiosoundings and surface data provided by the regional meteorological network) by means of the mass-consistent model MINERVE (Aria Technologies, 2001). Regional scale meteorological fields together with land cover information (e.g. roughness length) and chemical species characteristics (gas reactivity) have been then used by the interface processor SURF*PRO* (Arianet, 2004, Finardi *et al.*, 2005) to produce dry deposition velocities and turbulent diffusivity fields needed by FARM. Finally, boundary and initial conditions for all modelled species on the regional domain have been derived from daily continental runs of the CTM CHIMERE provided by INERIS Prev'Air service (http://www.prevair.org).

SENSITIVITY TESTS

To identify the optimal configuration for the AMS, some sensitivity tests have been performed to evaluate the influence of the different parameters on the estimated concentration fields. For this purpose two episodes occurred during year 2004 have been considered, characterized respectively by high concentration levels of PM_{10} (10^{th} – 20^{th} February) and ozone (20^{th} – 30^{th} June). Tests results have been compared to the so-called "base case" simulation which parameters were set as in 2004 AQA. For these applications FARM model has been applied with the SAPRC-90 (Carter, 1990) gas-phase chemical mechanism and the *aero0* aerosol module. The choice of the simplified aerosol module has been determined mainly by computational reasons (need to perform yearly simulations). The purpose of simulations were mainly aimed to improve modelling results with respect to under/over-estimation of concentration levels during specific period (day/night) occurred in different areas of the domain (rural/urban). Therefore particular attention was focused on the values assigned to parameters influencing vertical dispersion of pollutants. Table 1 summarize the sensitivity tests which will be described hereafter.

Table 1. Sensitivity tests

Test case	Note
base case	2004 AQA
1	Minimum eddy diffusivities differentiated for rural and urban cells
2	as case 1, aeolian contribution
3	as case 1, explicit benzene treatment

Minimum eddy diffusivities

Table 2. K_z^{min} values ($m^2 \cdot s^{-1}$) in test case n. 1

Land use	winter	summer
Urban	0.2	1.0
Rural	0.05	0.1

The minimum value for eddy diffusivity has an important impact on nighttime concentrations. In the "base case" this parameter has been set to 1 $m^2\ s^{-1}$ leading to overpredictions of ozone at night in rural areas, due to reduced titration, and to underpredictions of primary species in areas of high emissions (urban). To overcome such problems in the interface module SURF*PRO* is now possible to specify the minimum Kz according to the land-use. In the test case 1 the K_z^{min} values reported in Table 2 are used.

Simulation results show a decrease in ozone night levels in areas characterized by prevalent rural land use during summertime as reported in Figure 2: nighttime levels at Druento monitoring station (rural background) decrease significantly by using lower K_z^{min} values, improving the concentration profiles. No differences result in concentration levels predicted over urban areas during summer, because of same value assigned to K_z^{min}. Nevertheless, at some sites and for some pollutants (NO_2, CO) the use of these minimum vertical diffusivities at night can lead to high concentration levels; this occurs particularly for suburban background areas identified to be prevalent rural.

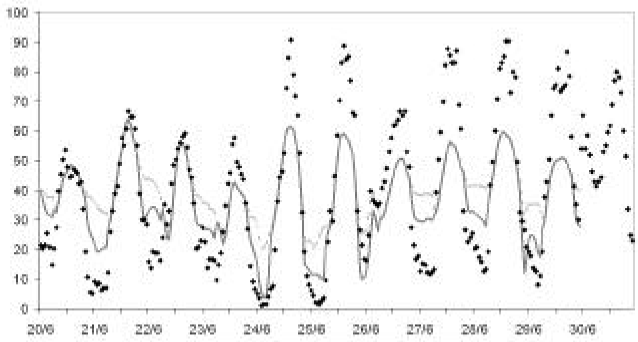

Fig. 2; Summer ozone hourly concentration levels (ppb) at Druento station; dots refer to measured values, dotted light grey line to base case and solid dark grey line to Test 1.

Mineral dust contribution

The most recent version of SURF*PRO* allows to estimate the wind related (erosion/resuspension) and marine salt contribution to particulate emission (Vautard *et al.*, 2005; Zhang *et al.*, 2005). Simulations named Test 2 allowed to estimate such contributions during different meteorological conditions. The influence of mineral dust contribution to PM_{10} concentrations turned out to be relevant particularly during summer season, due to slightly higher wind conditions. In wintertime, most of the Piemonte region is affected by low wind conditions sometimes coupled with ground based inversions, which expose the larger urbanized areas to severe pollution episodes, particularly as regards PM_{10}. Test 2 underlined that the use of this parameterisation significantly improves the estimated concentrations during summer but not in winter. Figure 3 shows the good results in estimating daily mean concentrations at two air quality monitoring stations: Borgaro (suburban background) and Druento (rural background); at urban stations, however, the increase in concentration is less evident, due to a possible underestimation of particulate primary emissions and the production of secondary components.

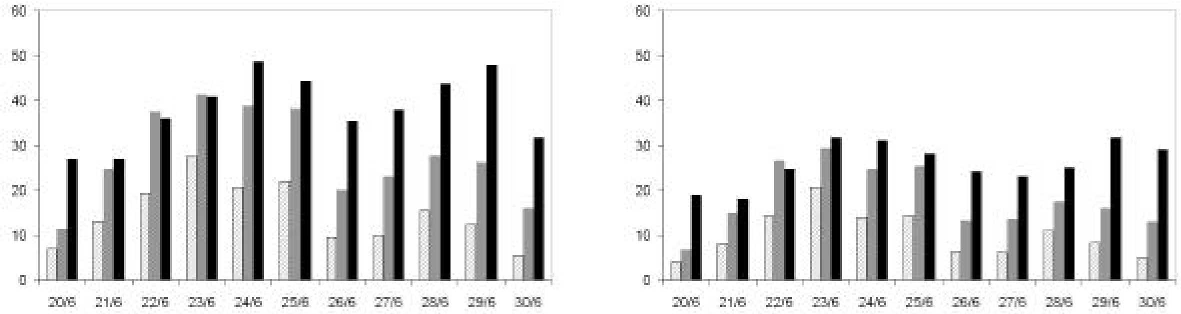

Fig. 3; summer PM_{10} daily mean concentration levels ($\mu g/m^3$) at Borgaro (left) and Druento (right) stations; black bars refer to measured values, light grey bars refer to base case and dark grey bars to Test 2.

Benzene explicit treatment

Test n. 3 simulations were finalized to evaluate the influence of the explicit treatment of benzene in the FARM chemical mechanism. In the original SAPRC-90 chemical mechanism this species is aggregated with toluene and ethylbenzene in the lumped species ARO1, while in the modified version of the mechanism its reaction with OH radical is considered (see http://www.arb.ca.gov/aqd/ethanol/ethanol.htm). In the following Figure 4 the comparison between observed and computed benzene at two urban traffic stations is given. As for the base case the benzene has been estimated, on the basis of available air quality data in the area, to be 20% of the lumped species ARO1. The analysis of such figure evidence a better reproduction of daily patterns and the reduction of the overestimation of benzene concentrations obtained in the base case.

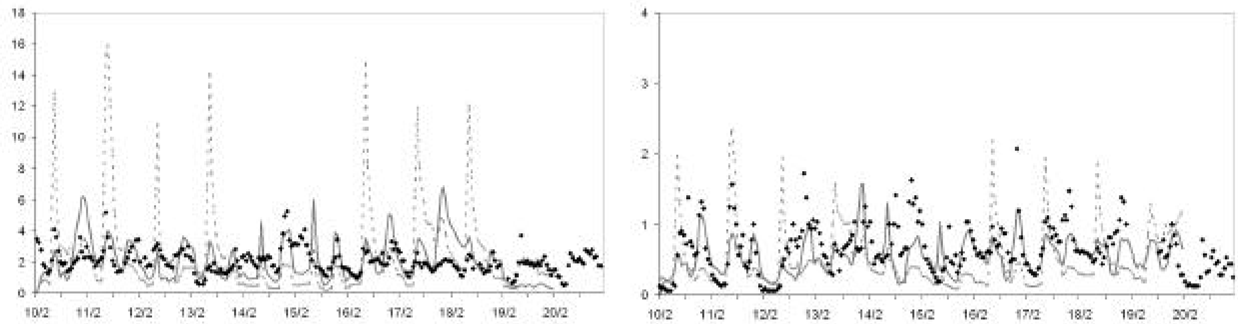

Fig. 4; winter benzene hourly concentration levels (ppb) at Torino-Consolata (left) and Cuneo (right) stations; dots refer to measured values, dotted light grey line to base case and solid dark grey line to Test 3.

CONCLUSIONS

A number of tests have been performed with the aim of improve the performance of the modelling system running at ARPA Piemonte to produce yearly the air quality assessment (AQA) over the region. The configuration used in year 2004 AQA was used as "base case" and evaluated against different settings for a number of parameters: minimum vertical eddy diffusivities according to the land-use, introduction of a module aimed to evaluate aeolian mineral dust contribution to PM_{10} concentrations and the explicit reaction of benzene with

radical OH instead of its treatment in the lumped species ARO1. The introduction of different values of K_z^{min} in urban and rural areas gives good results in the estimate of nocturnal summer ozone concentrations especially in rural areas. The contribution of mineral dust related to wind erosion/resuspension seems to be relevant particularly during summer in suburban and rural areas, while winter concentrations are not significantly affected due to lower wind speed affecting the region in the colder seasons. The SAPRC90 chemical mechanism has been partly modified to treat benzene as species, giving interesting results in improving the simulated concentration levels and their modulation.
The best configuration resulted from these tests have been successfully applied to perform the year 2005 and 2006 AQAs; the evaluation process, as foreseen by the European and Italian legislation, shows an improvement in the whole system performance with reduced difference between predicted and observed values. Future works are finalized to a better comprehension of aerosol treatment and to an improvement in the description of emissions treatment.

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