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APPLICATION OF A PHOTOCHEMICAL MODEL TO THE ASSESSMENT OF REGIONAL AIR QUALITY LEVELS IN SOUTHERN ITALY: PROCEDURES AND RESULTS

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Abstract: A modelling system based on FARM photochemical model was applied to assess the air quality (AQ) levels over the Apulia region (Southern Italy) for the 2013 year. FARM implements the SAPRC99 gas-phase chemical mechanism and the AERO3 aerosol module, derived from CMAQ model. Simulations were performed on a 316 km x 248 km domain, covering the entire region with 4 km grid spacing. The meteorological fields necessary for dispersion simulations came from the meteorological model RAMS. Emission data were derived from the regional INEMAR inventory, updated to the year 2013, while the emissions from the neighbouring regions were taken from the Italian national emission inventory. Initial and boundary conditions were provided by a national-scale simulation performed by the Air Quality Forecasting System QualeAria. According to the INEMAR emission inventory, the most relevant pollutant sources in the region are a steel plant, the largest in Europe (in Taranto area), a coal fired plant, the second most powerful in Italy (in Brindisi area) and biomass burning for residential heating. Simulation results evidenced exceedances for PM_{10} daily limit value and BaP annual limit values occurring at some areas. To evaluate the model performance, hourly and daily data, measured by the 35 monitoring stations belonging to the regional air-monitoring network, were compared with the simulation results, for the main pollutants regulated by the European Directive 2008/50/EC. The comparison between simulated and experimental data evidenced a good capability of the modelling system to reproduce the spatial distribution and the temporal variability of the observations. Some exceptions occurred, probably due to the adopted model spatial resolution, the uncertainties in emission inventories and the spatial representativeness of air quality monitoring stations. The interesting results obtained suggest the use of this modelling strategy for further source apportionment studies, in order to identify and to implement proper emission control strategies.

Key words: *air quality assessment, photochemical model, model evaluation tool.*

INTRODUCTION

Humans can be adversely affected by exposure to air pollutants in ambient air. In response, the European Union has developed an extensive body of legislation which establishes health based standards and objectives for a number of pollutants in the air. These standards and objectives are considered by the Italian Legislative Decree 155/2010, which adopted the European Directive 2008/50/EC.
The application of numerical models for air quality assessment is allowed by the legislation of European Community (EU) that establishes the possibility of using modelling techniques in combination with air quality observations. This work showed the air quality modelling assessment results over the Apulia region with 4 km grid spacing for the year 2013; for this purpose, the three-dimensional Eulerian model FARM (Mircea et al., 2015) was applied and evaluated. The modelled concentrations obtained by the simulations, were also compared with the threshold limit values. Finally, the model performances were analysed by using the DELTA Tool, an Interactive Data Language-based evaluation software, developed within FAIRMODE as support in the application of the EU Air Quality Directive. Such tool was helpful among the modellers community in fast identifying problems with model performance and indicating potential weaknesses (Georgieva *et al.*, 2015).

Model description, simulation setup and emission data

A modelling system, based on FARM model, was applied to a domain covering an area of 316x248 km^2, including the entire Puglia region (Southern Italy) with a grid spacing of 4 km and a vertical extent of 5330

km. Initial and boundary conditions were provided by the national-scale Air Quality Forecasting System (AQFS) “QualeAria” (http://www.aria-net.it/qualearia/en/).
FARM was configured with an updated version of SAPRC99 gas-phase chemical mechanism (Carter, 2000), that includes PAHs and Hg chemistry, and the Aero3 modal aerosol module, implemented in CMAQ model (Binkowski, 1999). Aero3 aerosol module includes ISORROPIA (Nenes et al., 1998) and SORGAM (Schell et al., 2001) models for the calculation of secondary inorganic and organic aerosols.
Input meteorological fields for all 2013 have been generated by the prognostic, non-hydrostatic model RAMS (Cotton et al., 2003), applied over three nested grids covering the whole Europe, Italy and the Apulia region, with spatial resolution of 60, 20 and 4km respectively.
Emission data were derived from the regional INEMAR inventory (http://www.inemar.arpa.puglia.it/), updated to the 2013, while the emissions from the neighbouring regions were taken from the Italian national emission inventory. The regional INEMAR inventory is a database developed in order to estimate on municipality level the emissions of different pollutants, grouped for activities (heating, road transport, agriculture, industry, etc.) according to the SNAP nomenclature adopted in the EMEP - CORINAIR inventory. The most relevant pollutant industrial sources in the region are the steel plant, located in Taranto area and the coal fired power plant in Brindisi area (2640 MWe). In particular regarding to the total INEMAR emissions these sources contribute respectively by 72% for SO_2, 27% for NO_x and 13% for primary PM_{10}.To reconstruct accurately with INEMAR the emissions from the biomass residential heating, it was carried out a specific survey on the biomass consumption for the residential heating in Apulia. For primary PM_{10} the total emission from this activity accounts for 30% with respect to the total regional emissions. Biogenic emissions (VOC from vegetation, soil dust, sea salts and heavy metals from soil and sea) were computed by applying the MEGAN emission model (Guenther et al., 2006) and the SURFPRO model. The contribution of Saharan dust was not modelled and no assimilation data was performed.

Monitoring data and model evaluation

The regional air-monitoring network, managed by the Regional Environmental Protection Agency (ARPA), is equipped with 71 stations of different type, all active in the year 2013. In order to evaluate the performances of the adopted modeling system, the NO_2, O_3, BaP, PM_{10} and $PM_{2.5}$ predictions were compared with the observation satisfying following requirements: the stations should have a spatial representativeness similar to the model horizontal resolution and a data availability greater than 75%. Table 1 shows the number of stations, distinguished for type, as defined by conventional classification established by the Italian regulation.

Table 1. Number of stations per type and pollutant for 2013

Number of Stations	NO_2 hourly	O_3 hourly	PM_{10} daily	$PM_{2.5}$ daily	BaP monthly
Urban-background	3	1	2	-	6
Suburban	25	11	19	3	4
Rural	7	4	7	3	2
Number of stations with more than 75% of available data	32	16	28	6	12

Delta Tool was used to compute the following statistical indicators: root mean square error (RMSE), correlation coefficient (R), mean bias (Bias), mean standard deviation (SD) and centred root mean square error (CRMSE). These statistics have the peculiarity in DELTA to be normalised by the observations uncertainty $U(O_i)$ (Thunis et al., 2013; Pernigotti et al, 2013), in particular by the quadratic mean of measurement uncertainty, defined as:

$$RMS_U = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(U(O_i))^2} \qquad (1)$$

With the simple principle of allowing the same margin of tolerance to both model and observations, the Model Quality Objective (MQO) is defined by comparing the error between observed and modelled values to the absolute measured uncertainty:

$$MQO = \frac{1}{2}\frac{RMSE}{RMS_U} = \frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(O_i - M_i)^2}}{2RMS_U} \leq 1 \qquad (2)$$

If MQO ≤ 0.5 the model results are within the range of $U(O_i)$, if 0.5 <MQO≤ 1 RMSE is larger than RMS_U, but model results could still be closer to the true value than the observations; if MQO > 1 the observation and model uncertainty ranges do not overlap and model and observation are more than 2 RMS_U apart.
To identify the fulfilment of the performance criteria, MQO can be visualized for every monitoring stations on an adapted target diagram, named target plot, where X and Y axes represent CRMSE and BIAS, normalised by observation uncertainty.

Results and discussion

Figure 1(a-d) show the predicted NO_2, $PM_{2.5}$ and BaP annual averaged concentration maps and the 90.4° percentile of PM_{10} daily means. As for NO_2 (Fig. 1a), higher levels were estimated in correspondence of larger urban areas and major traffic roads. The predicted values were, however, relevantly lower than the prescribed thresholds. As for $PM_{2.5}$, PM_{10} and BaP, the highest predicted concentrations were estimate in the Taranto industrial area and in the central southern part of the peninsula, where the biomass burning emissions due to agricultural activities and (especially) to residential heating by fireplaces are relevant. Regarding PM10, a number of daily exceedances greater than that the value allowed by the air quality directive (equal to 35) were estimated in both areas, while exceedances of the BaP annual limit value were predicted only in the central southern part of peninsula.
The model concentrations were compared with hourly and daily observed data to evaluate the modelling system performance. The statistical indicators were summarized in Table 2. Results showed a general good performance of the model in comparison with the acceptance criteria included in Delta Tool. The bias indicated an underestimation for almost all the locations and pollutants, maybe due to deficiencies in local emission estimation and in boundary conditions. The worst correlation was calculated for summer ozone in correspondence of the urban-background monitoring stations. The FA2 was greater than 50% for all pollutants, while IOA is greater than 0.5 except for O_3.
Figure 2 (a-b) gives an overview of model performance in terms of the target diagram for hourly NO_2 and daily PM_{10} concentrations. Each symbol refers to a single station, while the colours represent rural stations (orange), suburban stations (red) and urban-background stations (blue). The MQO was fulfilled for more than 90% of the stations for all these pollutants. The green area circle identifies the fulfilment of the performance criteria. The negative and positive sides of Y axis identify negative and positive biases, while the left and right zone identify errors dominated by correlation or standard deviation.
The symbols were located on the left side of diagram, except for one station for NO_2, indicating that the error for all pollutants was dominated by correlation. The bias for NO_2 was both positive and negative, while for PM_{10} daily mean concentrations the underestimation was more evident for all the stations.

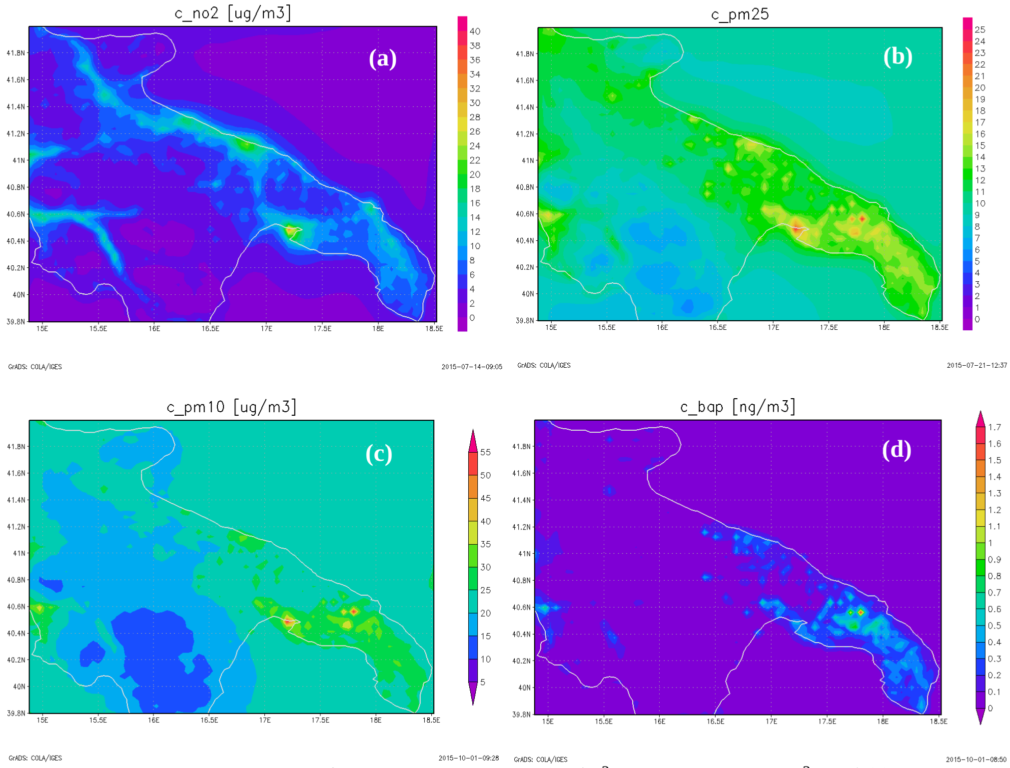

Figure 1. Annual mean concentrations for (a) NO_2, (b) $PM_{2.5}$ ($\mu g/m^3$) and (d) BaP (ng/m^3) and (c) 90.4°percentile for PM_{10} ($\mu g/m^3$)

Table 2. Statistical indicators

Station	**Mean obs. ($\mu g\ m^{-3}$)**	**Mean mod. ($\mu g\ m^{-3}$)**	**BIAS ($\mu g\ m^{-3}$)**	**RMSE ($\mu g\ m^{-3}$)**	**R**	**FA2 (%)**	**IOA**
NO_2 hourly (year)							
rural	9.5	9.4	-0.12	10.0	0.33	56	0.55
suburban	13.9	12.0	-1.9	14.7	0.47	57	0.63
urban-background	19.2	20.3	1.14	15.0	0.58	72	0.75
8hDMax O_3 (summer)							
rural	111.9	86.1	-25.8	31.2	0.24	99	0.43
suburban	111.5	88.5	-23.0	28.0	0.38	100	0.46
urban-background	101.9	85.6	-16.2	20.0	0.17	100	0.38
PM_{10} daily (year)							
rural	19.3	15.8	-3.5	11.8	0.32	80	0.51
suburban	19.7	17.2	-2.6	8.5	0.43	88	0.68
urban-background	19.4	17.3	-2.1	8.4	0.46	89	0.65
$PM_{2.5}$ daily (year)							
rural	11.4	13.5	2.1	7.3	0.55	80	0.64
suburban	14.9	14.0	-0.9	6.6	0.69	89	0.81
urban-background	-	-	-	-	-	-	

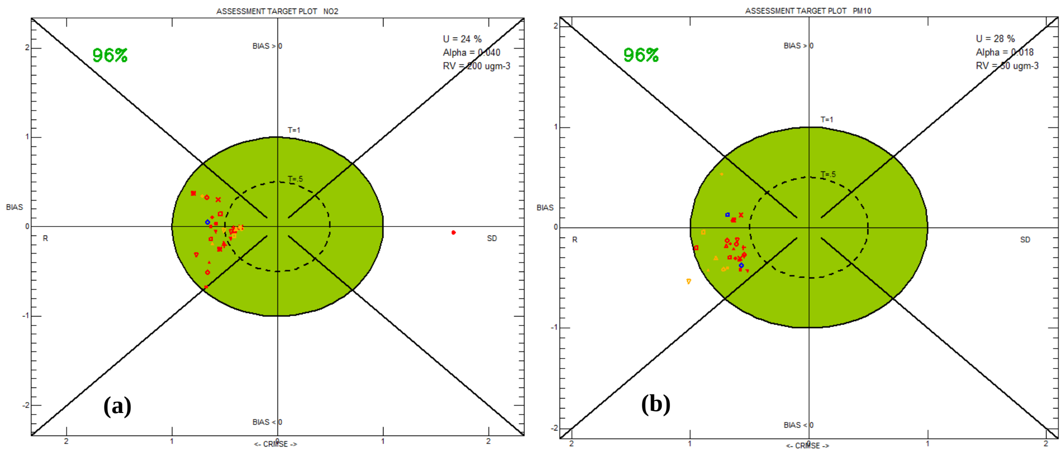

Figure 2. Target plot for NO_2 hourly values (a) and (b) daily mean PM_{10} concentrations.

Conclusions

A modelling system was applied to assess the air quality levels over the Apulia region. The simulations were performed for the year 2013, allowing the comparison between modelled data and the reference values set in the regulations. The results showed some exceeding of the limit values as regard the PM_{10} and BaP species; some of these exceeding occurred in areas where the observations are not yet available. These results suggest the need to improve the monitoring network by locating some stations in such areas.
The model performance was estimated by using the DELTA software package, showing a good behaviour of the model, with a tendency to underestimate the PM_{10} levels. Future improvements will consider the application of data assimilation/fusion techniques and source apportionment studies to better analyse the influence of different sources on air quality levels.

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