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COMPARISON OF COMPUTED AND MEASURED AEROSOL OPTICAL DEPTH (AOD) OVER EUROPE FOR A YEAR LONG CHEMICAL TRANSPORT MODEL SIMULATION

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Abstract: The evaluation of Air Quality (AQ) models is very important for checking their applicability. Within MEGAPOLI Project, model simulations over Europe were performed for the full year 2005 and evaluation results are presented here for the chemical transport model FARM. The model results have been verified at several regional monitoring sites across Europe by comparing its monthly averaged Aerosol Optical Depth (AOD) predictions with data provided by the MODIS satellite sensor and AERONET photometer observations. As for PM10 and ozone, surface concentration fields have been compared with observed data across Europe made available at EMEP Chemical Coordinating Centre at NILU. As for PM10 we have compared daily concentrations during June and December; while as for ozone we have limited the analysis to June comparing calculated and observed daily 1 hour maxima. Such evaluation has evidenced an excellent agreement between observed and predicted ozone levels; as for PM10 and AOD, a better agreement has been observed during warmer season and an overestimation of measured data during colder periods particularly at northerly sites. The use of statistical indicators, suggested in the frame of FAIRMODE benchmarking activities, corroborated these results.

Key words: *Aerosol Optical Depth, MODIS, AERONET, Chemical-Transport Model, FARM, model evaluation, FAIRMODE, MEGAPOLI.*

INTRODUCTION

The evaluation of megacities and large conurbations emissions effects on the air quality and climate at regional scale is one of the main objectives of MEGAPOLI Project. Within the project a regional model ensemble has been constructed following the setup of COST-728 Action and covering the baseline year 2005. All the models participating to the exercise performed European scale simulations using an unified emission dataset, provided at a resolution of 1/8° longitude x 1/16° latitude (Kuenen *et al.*, 2010). In this context the chemical transport model FARM (Flexible Air quality Regional Model, Gariazzo *et al.*, 2007; Silibello *et al.*, 2008;), implementing the *SAPRC99* gas-phase chemical mechanism (Carter, 2000) and the *aero3* aerosol module of CMAQ (Binkowski, 1999), has been applied. FARM implements Rosenbrock and LSODE chemical kinetics solvers that are automatically generated by the Kinetic PreProcessor (KPP, Damian *et al.*, 2002). In this study we have applied the KPP-generated Rosenbrock gas-phase chemistry solver (ROS3) that involves, for the SAPRC99 mechanism, 85 species in 215 reactions. The CTM has been driven by ECMWF meteorological analyses and by boundary condition derived from MPI-MATCH time varying concentration fields for gas-phase species and GOCART climatological monthly fields for aerosol species. Natural emissions of isoprene and terpenes from vegetation and PM (fine and coarse fractions) from aeolian resuspension and sea salts have also been included in the simulations. The CTM has been applied to an area 4650x4100 km^2 wide (Figure 1) with an horizontal resolution of 25 km, covering Europe and including the 4 main MEGAPOLI target megacities (London, Paris, Ruhr-Rein and Po Valley). The vertical domain depth of the computational domain is 10000 m, with lower atmospheric level at 20 m a.g.l. To evaluate the performance of the CTM, a continental-wide comparison of modelled and observed concentrations and Aerosol Optical Depth (AOD) has been performed. MODIS satellite sensor and AERONET photometer observations have been used to compare AOD spatial patterns and time series, while data available at EMEP Chemical Coordinating Centre at NILU have been used to compare ozone and particulate matter at several regional monitoring sites across Europe (Figure 1).

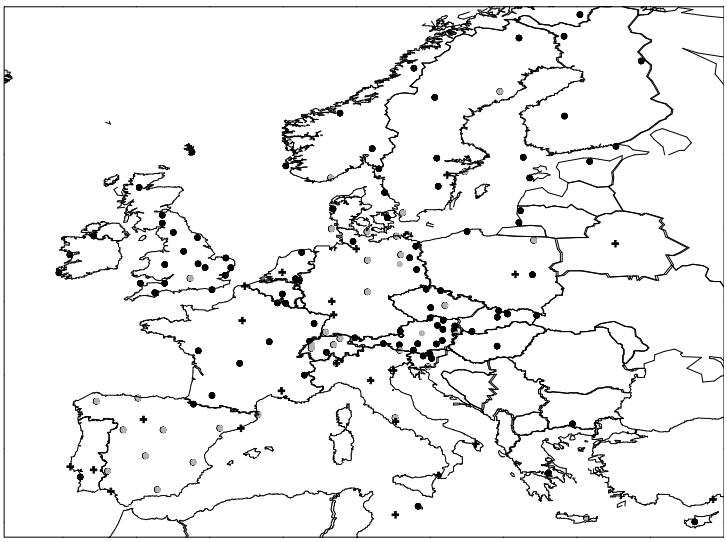

Figure 7; MEGAPOLI modelling domain and location of PM_{10} (grey circles), ozone (black circles) and AERONET stations (black crosses) considered in the study.

AOD ANALYSIS

The aerosol module aero3 model does not include coarse mode particles in its visual range calculations. Therefore the AOD calculation outlined below does not account for the effect of coarse mode particles. AOD, a dimensionless quantification of visibility impairment, is defined by the following equation:

$$AOD = \int_{z=0}^{z_{top}} B_{sp} dz \qquad (1)$$

where B_{sp} is the aerosol extinction coefficient in km^{-1} and z is altitude in km. B_{sp} is calculated through the extinction efficiency, a measure of light scattering efficiency, which in turn is estimated using approximations to the Mie theory (Binkowski, 1999). To evaluate the model predicted columnar AOD against observations we have used data from MODIS satellite sensor and sun photometer measurements of the direct (collimated) solar radiation (AERONET network). As for the latter data, we have derived the optical thickness data at 550 nm using following relationship:

$$\delta_{550} = \delta_{675}\left(\frac{550}{675}\right)^{-\alpha} \qquad (2)$$

where δ_{400} and δ_{675} are the optical thickness respectively from 440 and 675 nm channels and α is the Angström exponent defined as:

$$\alpha = ln\left(\frac{\delta_{440}}{\delta_{675}}\right) \Big/ ln\left(\frac{675}{440}\right) \qquad (3)$$

A comparison between observed and simulated monthly averaged AOD across Europe for the year 2005 is presented in Figure 2. To be consistent with the Terra orbit tracks over Central Europe, simulated monthly AOD are computed from daily 6-hour running averaged fields extracted at noon. The seasonal patterns and the values observed at different locations are well reproduced. The agreement is generally better during warmer months and an overestimation occurs during winter season particularly at sites located in central and eastern Europe. An underestimation of observed AOD at stations located in Po Valley (Ispra, Venice and Modena) is observed confirming the peculiarity of this area, that is one of the air pollution hot spots of major concern in Europe where about 45% of the Italian population lives.

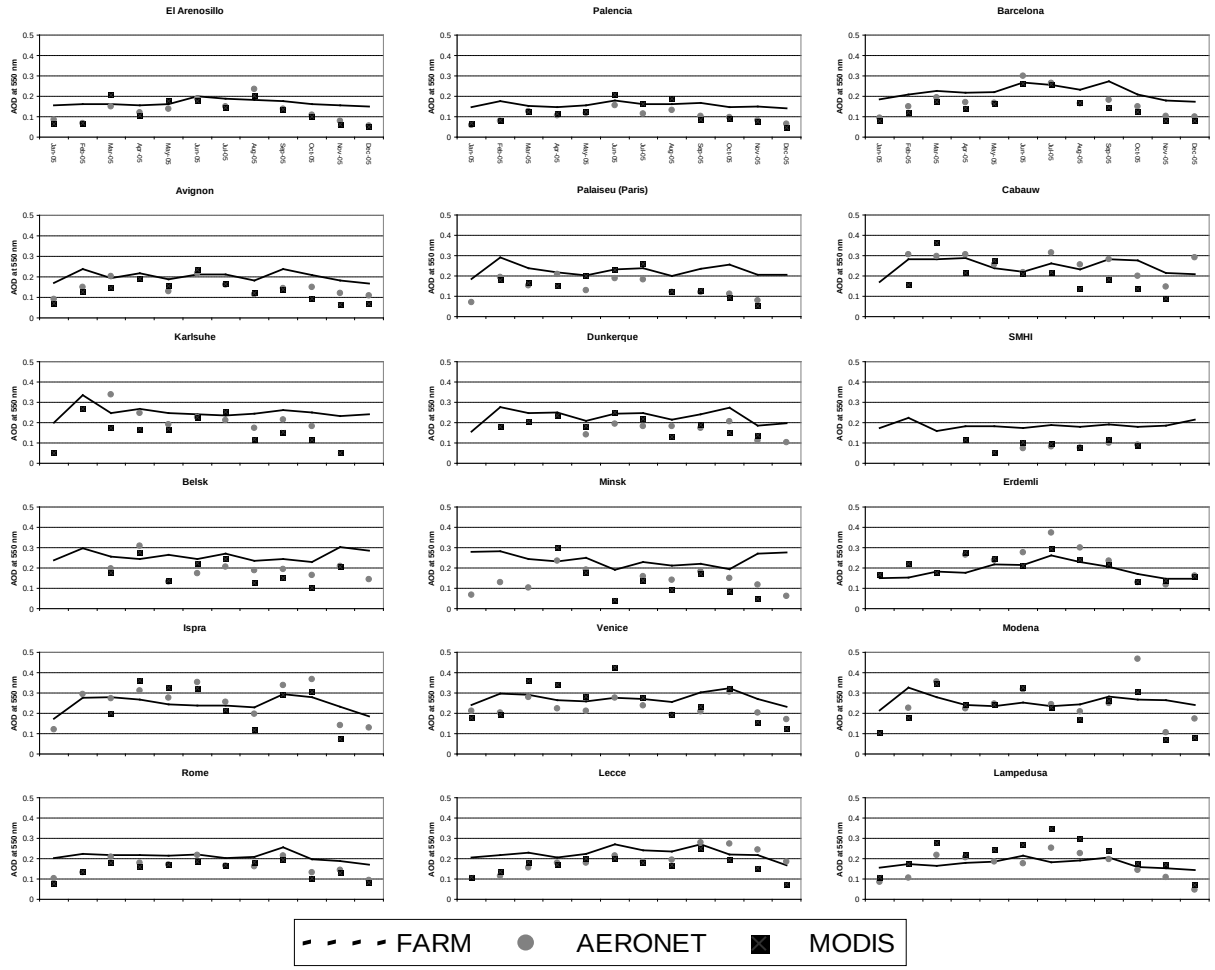

Figure 8; Comparison between simulated and observed monthly averaged AOD.

PM_{10} AND OZONE ANALYSIS

To further analyse simulation results, PM10 and ozone concentration fields have been compared with observed data across Europe made available at EMEP Chemical Coordinating Centre at NILU. As for PM_{10} we have compared daily concentrations during June and December, that recorded more typical seasonal atmospheric circulation conditions associated to summer and winter pollution episodes (Baklanov and Mahura, 2010); while as for ozone we have limited the analysis to June comparing calculated and observed daily 1 hour maxima. The scatter plots of these indicators from the monitoring

stations (see Figure 1 for their location) and FARM predictions, reported in the following Figure 3, evidences a lower performance of PM_{10} predictions during December with a general overestimation of observed levels. A better agreement occurs for the June simulation: simulated PM_{10} concentrations are generally between ±50% with a smaller overestimation of observed values with respect to the December simulation; as for O_3 an excellent performance is obtained with almost all simulated concentrations within ±50% of observed levels.

PM_{10} - daily average (December) **PM_{10} - daily average (June)** **O_3 – daily 1 hr maxima (June)**

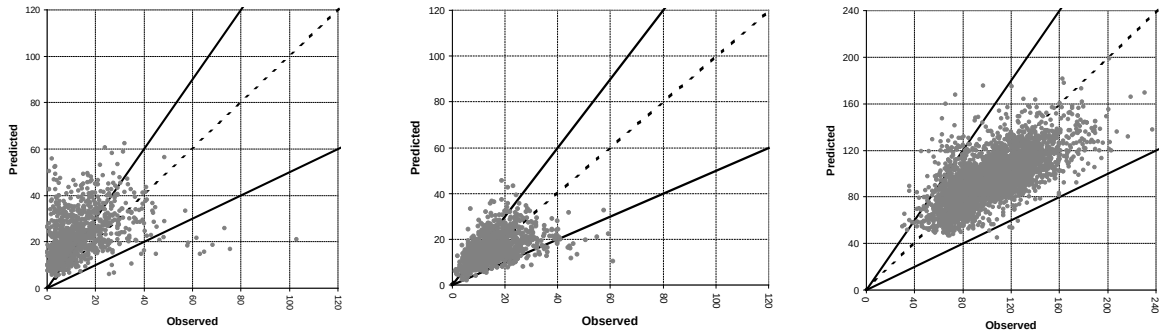

Fig. 9; Comparison between observed (EMEP network) and simulated PM_{10} and O_3 concentrations [μg m^{-3}]during December and June 2005.

The performance statistic for the two periods, shown in Table 1, confirms the above consideration: the modelling system performs better for both pollutants during summer and worse for PM10 during December. This difference of model performance for PM10 concentration between winter and summer is consistent with results obtained for AOD analysis.

Table 4. Statistical comparison between observed (EMEP network) and simulated (bold values in parenthesis) PM_{10} and O_3 concentrations during June and January 2005.

Metric	Range / Ideal value	Units	Ozone (June)	PM_{10} (June)	PM_{10} (December)
$\overline{P} = \frac{1}{N}\sum_{i=1}^{N} P_i$		[μg m^{-3}]	102.90 **(94.88)**	16.48 **(16.34)**	13.39 **(22.66)**
$\sigma_p = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(P_i - \overline{P}\right)^2}$		[μg m^{-3}]	29.11 **(21.03)**	8.50 **(6.36)**	12.05 **(10.28)**
$SKVAR = \sigma_P / \sigma_O$		[-]	0.72	0.75	0.85
$R = \frac{\frac{1}{N}\sum_{i=1}^{N}\left(P_i - \overline{P}\right)\cdot\left(O_i - \overline{O}\right)}{\sigma_P \sigma_O}$	-1 to +1	[-]	0.70	0.44	0.32
$FOEX = \left[\left(\frac{1}{N}\sum_{i=1}^{N} i \,\middle|\, (P_i > O_i)\right) - 0.5\right]\cdot 100$	-50 to 50%	[%]	-15.44	5.41	35.73
$FAC2 = \left(\frac{1}{N}\sum_{i=1}^{N} i \,\middle|\, \left(0.5 \le \frac{P_i}{O_i} \le 2\right)\right)\cdot 100$	0 to +100%	[%]	99.54	86.12	47.57
$MB = \frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)$	Ideal value 0	[μg m^{-3}]	-8.02	-0.14	9.27
$ME = \frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$	Ideal value 0	[μg m^{-3}]	17.20	5.97	12.19
$FB = \frac{\sum_{i=1}^{N}\left(P_i - O_i\right)}{\sum_{i=1}^{N}\left(\frac{P_i + O_i}{2}\right)}$	-2 to +2	[-]	-0.08	-0.01	0.51
$FE = \frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N}\left(\frac{P_i + O_i}{2}\right)}$	0 to +2	[-]	0.17	0.36	0.68
$MNB = \frac{\sum_{i=1}^{N}\left(P_i - O_i\right)}{\sum_{i=1}^{N} O_i}\cdot 100$	-100% to +∞	[%]	-7.80	-0.84	69.21
$MNE = \frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}\cdot 100$	0% to +∞	[%]	16.71	36.21	91.02
$MFB = \frac{1}{N}\sum_{i=1}^{N}\frac{\left(P_i - O_i\right)}{\left(\frac{P_i + O_i}{2}\right)}\cdot 100$	-200 to +200%	[%]	-1.64	1.14	16.27
$MFE = \frac{1}{N}\sum_{i=1}^{N}\frac{\lvert P_i - O_i\rvert}{\left(\frac{P_i + O_i}{2}\right)}\cdot 100$	0 to +200%	[%]	4.27	9.16	18.63
$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)^2}$	Ideal value 0	[μg m^{-3}]	22.28	8.03	16.00

To further analyse such results in the following Table 2, are reported, for some statistical indicators, performance criteria and goals suggested for the regional scale in the frame of FAIRMODE (Forum for air quality modelling in Europe) benchmarking activities (Thunis *et al*., 2011).

Table 2: Regional scale performance criteria (P.C.) and goals (G.) for some statistical indicators (extracted from Thunis et al., 2011).

Pollutant	*|MFB| [%]*		*MFE [%]*		*FAC2 [%]*		*R*	
	P.C.	*G.*	*P.C.*	*G.*	*P.C.*	*G.*	*P.C.*	*G.*
PM_{10}	60	30	75	50	50	60	0.40	0.48
O_3	30	15	45	30	50	60	0.65	0.78

From these tables it results that even for December simulation the performance satisfies the PM_{10} quality criteria except for the Pearson Correlation Coefficient (*R*) and the factor of modelled values within a factor of two of observations (*FAC2*): for these indicators the values are lower than the prescribed one (respectively 0.32 and 47.57 against 0.40 and 50%). As for June simulation, both PM10 and O_3 satisfy the above criteria except for the Pearson Correlation Coefficient (*R*): for this indicator the values are lower than the prescribed one (for ozone and PM_{10} respectively 0.70 and 0.44 against 0.78 and 0.48). Nevertheless, it should be noted that the magnitude of *R* it may not be consistently related to the accuracy of the prediction: correlations between very dissimilar P and O can easily approach 1; statistically signify-cant values are often unrelated to the size of the difference between O and P; small differences between O and P can occur with low *R* values.

CONCLUSIONS

A modelling system based on FARM model has been applied to an European scale simulation, carried out in the frame of a regional model ensemble exercise performed within MEGAPOLI Project, for the baseline year 2005. The performance of the CTM has been evaluated by comparing modelled and observed PM_{10} and O_3 concentrations and Aerosol Optical Depth using EMEP and AERONET photometer observations at several regional monitoring sites across Europe. As for PM_{10} and AOD, such evaluation has evidenced a better agreement between observed and modelled data during warmer season and an overestimation of measured data during colder periods particularly at northerly sites. The possible reasons of the seasonal PM bias are presently under investigation with particular focus on wintertime PM emissions treatment, e.g. residential heating. The use of statistical indicators corroborated these results evidencing, for ozone, an excellent agreement between observed and predicted levels for the June simulation.

ACKNOWLEDGMENTS

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