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**THE COUPLED CHEMISTRY-METEOROLOGY MODEL BOLCHEM: AN APPLICATION
TO THE AIR POLLUTANTS LEVEL IN THE PO VALLEY (ITALY) HOT SPOT**

Rita Cesari¹, Tony C. Landi² and Alberto Maurizi²

¹Institute of Atmospheric Sciences and Climate, CNR, Lecce, Italy

²Institute of Atmospheric Sciences and Climate, CNR, Bologna, Italy

Abstract: We present the model performance of the online Coupled Chemistry-Meteorological Model BOLCHEM on seasonal period in an air pollution hot spot. The simulation domain is the Northern Italy where a large amount of agricultural, livestock, industrial activities are present, together with big city, as Milan, Turin and Bologna. Simulated surface concentration of Particulate Matter (PM_{10} and $PM_{2.5}$) have been compared with measured concentrations at Airbase Stations for a winter period, while for the summer period also Ozone (O_3) has been considered. Results show that the model well reproduces observed concentrations, with similar correlation coefficient for particulate and ozone.

Key words: CCMM model, BOLCHEM, air pollution, hot spot, Po Valley

INTRODUCTION

In recent years, many efforts have been done in the development of numerical models that couple meteorological, dynamical and chemical atmospheric processes. Basically, this interest comes from the consolidated evidence related to the strong relationship between air quality and meteorology. In this frame, we present the online Coupled Chemistry-Meteorological Model (CCMM) BOLCHEM, and an application to the Po Valley hot spot area, both for a winter than for a summer period.

The Po Valley, the major plain of Southern Europe, is one of the most polluted areas in Europe. It extends approximately 650 km in the east-west direction in the Northern part of Italy, from the Western Alps to the Adriatic Sea, including part of different regions, namely Piemonte, Lombardia, Emilia-Romagna and Veneto. It covers an area of about 47000 km² and it is a highly populated area, with about 20 millions of inhabitants. Different factors contribute to the elevate pollutants level and composition (Ricciardelli et al., 2017): industrial activities and road transport, agricultural activities, livestock farming responsible for ammonia emission. In addition, the topography of the Valley, surroundend by the Alps and the Appennines, causes air stagnation with consequent low pollutant dispersion and high formation of secondary aerosols (Sandini et al., 2016). Furthermore, the contribution of emission located outside the hot spot is not negligible, as investigated by Maurizi et al. (2013). The authors presented numerical experiment, using the BOLCHEM model at horizontal resolution of about 50 x 50 km², pointing out that, due to the orography of the Valley, the entrainment at the boundary layer layer top and vertical mixing play a major role than the advection on the budget near the ground. It is then of particular interest to test model performance in a such complex area. Pernigotti et al., 2013, presented a model inter-comparison in order to explore the impact of emissions on air quality. All the participating models showed relatively good performance in reproducing O_3 concentration, while PM_{10} concentration is underestimate, specially in wintertime. This is mainly due to an overestimation of wind speed, specially during stagnant conditions.

Materials and method

Simulations have been perfomed using the online CCMM model BOLCHEM. The model is based on the hydrostatic meteorological model BOLAM (Buzzi et al. 2003), the gas module SAPRC90 (Carter 1990) extended to describe the formation of condensable organic products (Silibello et al. 2008) and the aerosols module AERO3 (Binkowski et al. 2003), coupled with the inorganic thermodynamic equilibrium

model ISORROPIA (Nenes et al. 1998) and with the partitioning model SORGAM (Schell et al. 2001) for secondary organic aerosol.

In the present study, the model has been used in a one-way nested grid configuration. The parent domain has horizontal resolution of $0.4^\circ \times 0.4^\circ$ and covers Europe domain (15° W – 35° E ; 30° N – 60° N) while the nested domain, over Italy, has horizontal resolution of $0.1^\circ \times 0.1^\circ$ and covers the area (6° E – 20° E; 36° N – 48° N). The model run covers the period december 2009 - november 2010, with a spin-up period of 30 days (November 2009). The parent run was driven by initial and boundary conditions for meteorology provided by ECMWF. The simulations were re-initialised every 24 hours with the ECMWF fields and lateral boundary conditions are updated every 6 hours. Climatological boundary conditions were used for chemistry. The anthropogenic emission data were based on TNO-MACC_II emission inventory inventory for the 2010 year (Kuenen et al. 2014), both in parent and nested run. In both simulations, biogenic emissions, calculated run time by the model, were based on an inventory providing potential emissions and generated by NKUA (National and Kapodistrian University of Athens) in the frame of the GEMS project (Symeonidis et al. 2008).

AirBase data AIRBASE (<https://www.eea.europa.eu/data-and-maps/data/airbase-the-european-air-quality-database-2>) was used for the model verification in the study area (7.5° E – 13.5° E; 44.0° N – 46.0° N). Only stations with altitude not exceeding 300 m. above sea level have been selected. AirBase is the European air quality database maintained by the EEA through its European topic centre on Air pollution and Climate Change mitigation. It contains air quality monitoring data submitted by participating countries throughout Europe, under 97/101/EC Council Decision establishing a reciprocal exchange of information (EoI) and data from networks and individual stations measuring ambient air pollution within the Member States. Due to model horizontal resolution, stations classified as traffic and industrial have been not used, but only data of background stations, separated in three types of area: rural, suburban and urban. A qualitatively model assessment is shown by scatter plots, while the Taylor diagrams show how three complementary model performance statistics vary simultaneously: they are the correlation coefficient R, the normalized standard deviation (SD) and the centred root mean square error (RMSE).

The analysis has been performed for two different period: winter period from december 2009 to february 2010, ad summer period, from june to august 2010. For the winter period we have focused on daily averaged Particulate Matter (PM₁₀ and PM_{2.5}) surface concentration, while for the summer period also hourly averaged Ozone (O₃) surface concentration has been contemplated.

Results and discussion

Fig. 1 shows the used Airbase station over the simulation domain for the different pollutants: Fig. 1a for PM₁₀, Fig. 1b for PM_{2.5} and Fig. 1c for O₃.

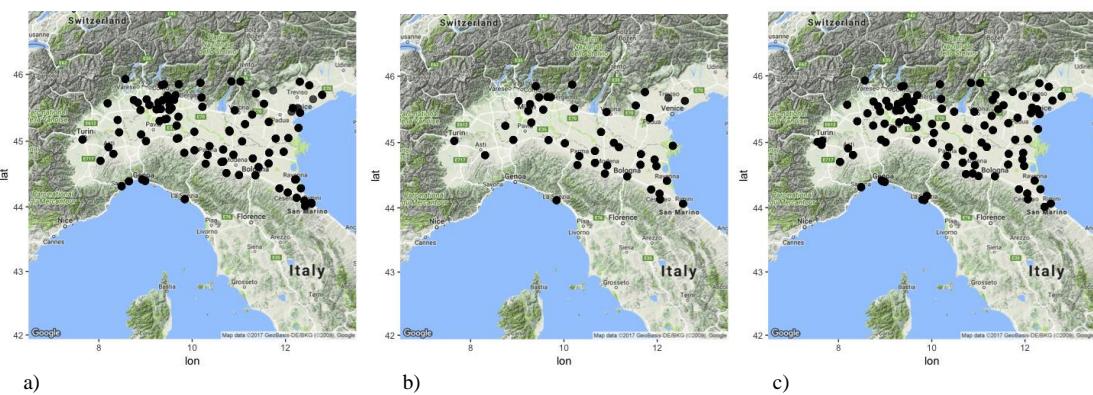


Figure 1. Airbase Stations over the study domain for PM₁₀ (a), PM_{2.5} (b) and O₃ (c)

For the winter period, the scatterplot for daily averaged PM₁₀ and PM_{2.5} ground concentrations ($\mu\text{g m}^{-3}$) is shown in Fig. 2. In the legend, counts indicates the number of data falling in each hexagon. Both pollutants are slightly underestimated. The Taylor diagrams for daily averaged PM₁₀ and PM_{2.5} ground concentration over all the stations for winter period are shown in Fig. 3. We recall that the axes are normalized by the observations standard deviation. The correlation coefficient for PM₁₀ varies from 0.5 to

0.6, and for PM_{2.5} it varies from 0.4 (suburban station) to 0.6 (urban station). The normalized SD < 1 shows that the model data have less variability than the measurement, and centered RMSE < 1 (apart for PM_{2.5} at suburban stations) means that the model is a better predictor of the observations, compared to the mean of the monitoring data.

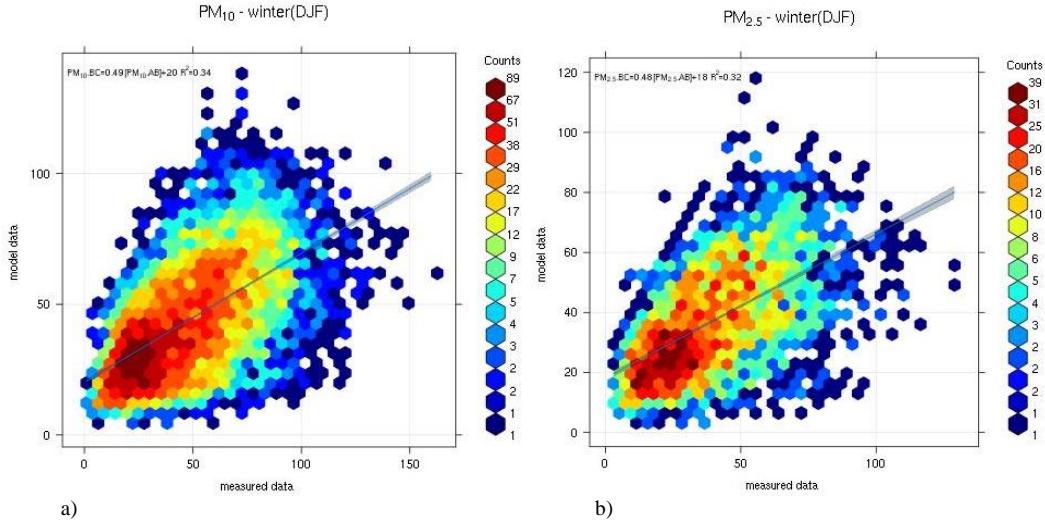


Figure 2. Modeled daily averaged concentration vs the observed one for PM₁₀ (a) and PM_{2.5} (b) at AirBase background stations for the winter period. Units are $\mu\text{g m}^{-3}$.

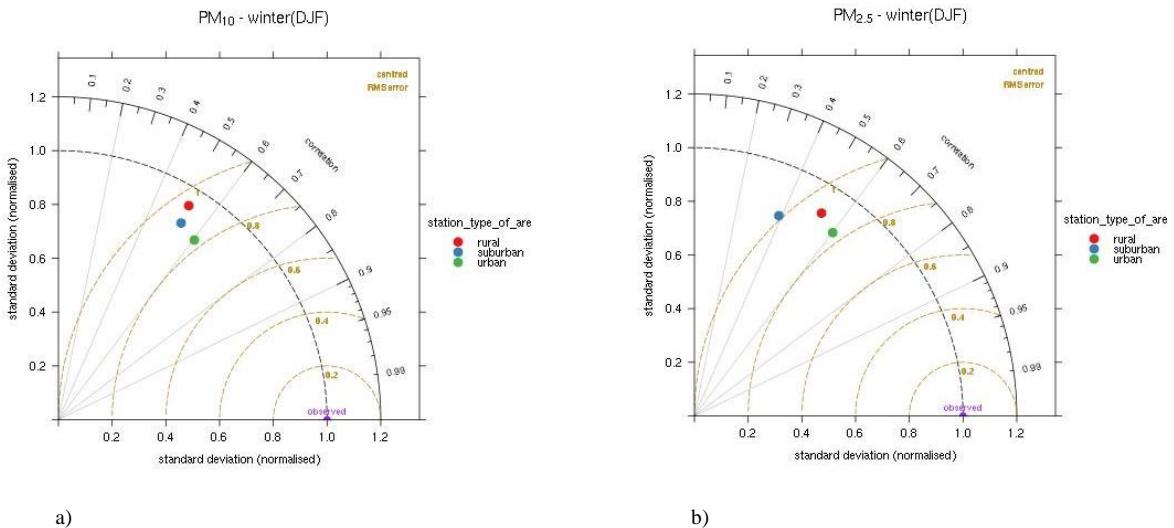


Figure 3. Taylor diagram for daily averaged PM₁₀ (a) and PM_{2.5} (b) ground concentration for the winter period.

Fig. 4 and Fig. 5 show the scatterplot and Taylor diagram for daily averaged PM₁₀ and PM_{2.5} ground concentrations ($\mu\text{g m}^{-3}$) for the summer period. The correlation coefficient varies from 0.5 to 0.6 both for PM₁₀ than for PM_{2.5}. PM_{2.5} model data have more variability than the measurement, and centered RMSE is > 1, except for rural stations. For hourly averaged O₃ ground concentrations in the summer period, the correlation coefficient ranges between 0.7 and 0.8 (Fig. 6).

We conclude that the model is able to reproduce the observed concentrations on seasonal period. A selection of the statistical performance based on daily data for PM₁₀ and PM_{2.5} and hourly data for O₃ is reported in Table 1a (winter period) and in Table 1b (summer period). Values are in accordance with those reported in Pernigotti et al., 2013. We point out that the number of AirBase stations available for PM_{2.5} is not equal to that of PM₁₀. For example, in the winter period, the number of background station is 95 (62 urban, 22 suburban, 11 rural) for PM₁₀, while it is 42 for PM_{2.5} (26 urban, 3 suburban, 13 rural).

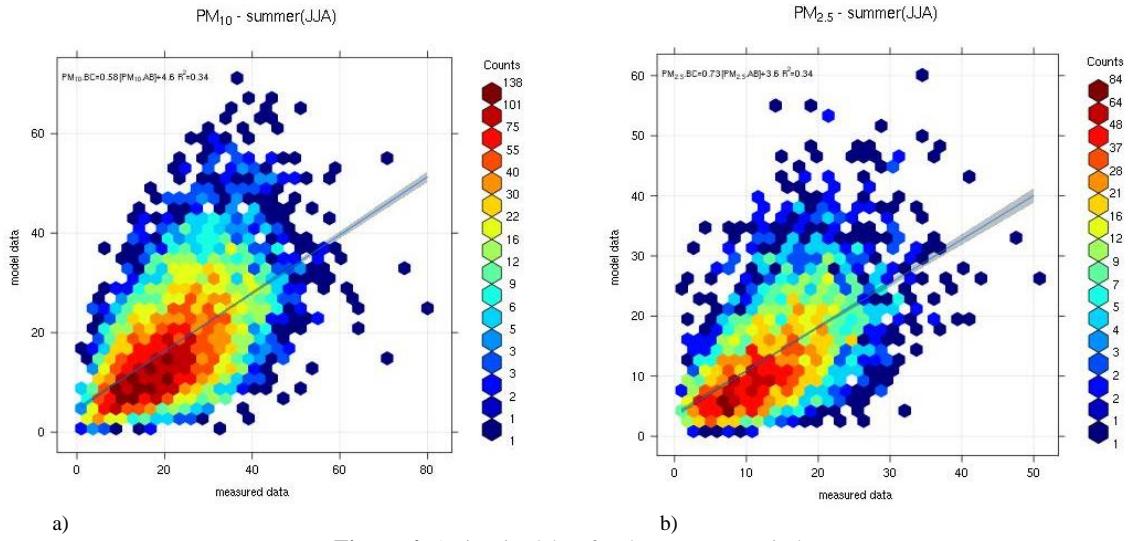


Figure 4. As in Fig. 2 but for the summer period.

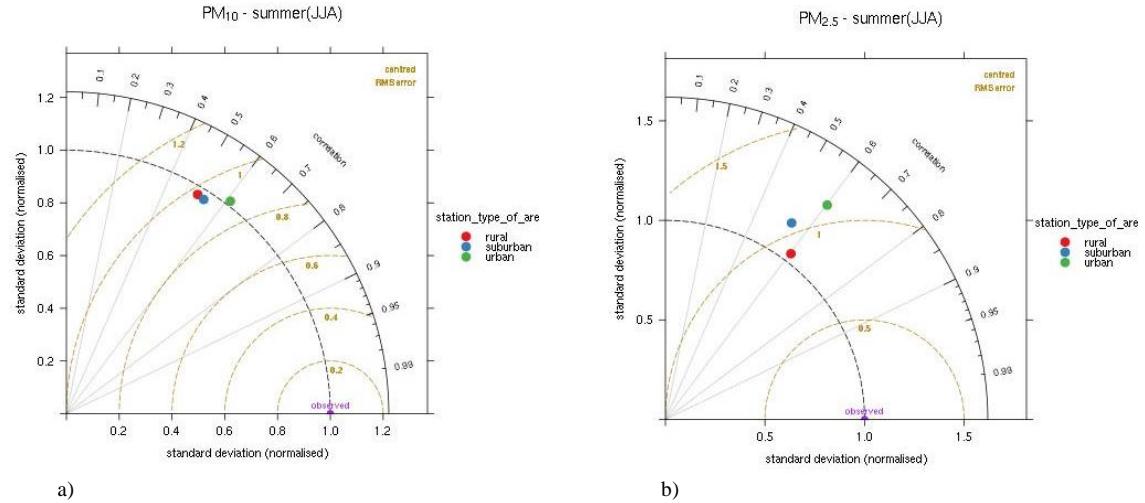


Figure 5. As in Fig. 3 but for the summer period.

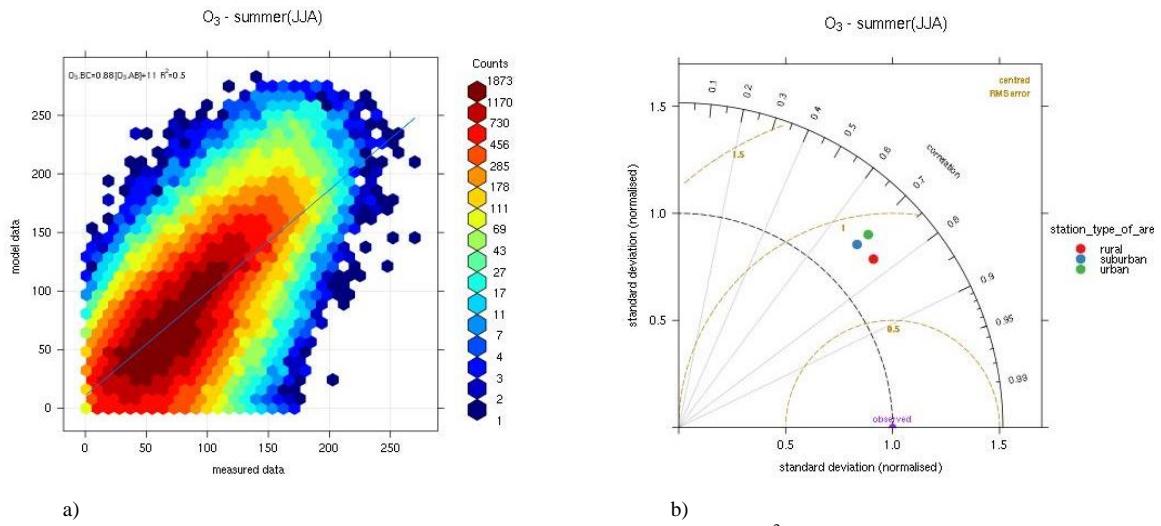


Figure 6. Modeled hourly averaged concentration vs the observed one ($\mu\text{g m}^{-3}$) (a) and Taylor diagram (b) for O_3 ground concentration

Table 1. Mean statistical indicators for PM₁₀, PM_{2.5} over winter period (a) and for PM₁₀, PM_{2.5} and O₃ over summer period (b)

| Winter | PM ₁₀ [$\mu\text{g m}^{-3}$] | | | | | PM _{2.5} [$\mu\text{g m}^{-3}$] | | | | |
|--------------|---|------|------|-----|------|--|------|-------|-----|-------|
| | Obs. | Mod. | MB | R | RMSE | Obs. | Mod. | MB | R | RMSE |
| All stations | 47.2 | 43.4 | -3.7 | 0.6 | 21.4 | 39.8 | 37.2 | -2.6 | 0.6 | 18.4 |
| Rural | 44.4 | 42.4 | -2.0 | 0.5 | 20.5 | 34.9 | 35.5 | 0.6 | 0.5 | 17.0 |
| Suburban | 45.7 | 42.0 | -3.7 | 0.5 | 21.8 | 46.6 | 34.5 | -12.0 | 0.4 | 25.3 |
| Urban | 48.3 | 44.2 | -4.0 | 0.6 | 21.4 | 41.5 | 38.4 | -3.07 | 0.6 | 18.16 |

a)

| Summer | PM ₁₀ [$\mu\text{g m}^{-3}$] | | | | | PM _{2.5} [$\mu\text{g m}^{-3}$] | | | | | O ₃ [$\mu\text{g m}^{-3}$] | | |
|--------------|---|------|------|-----|------|--|------|------|-----|------|---|-----|------|
| | Obs. | Mod. | MB | R | RMSE | Obs. | Mod. | MB | R | RMSE | MB | R | RMSE |
| All stations | 21.6 | 17.2 | -4.4 | 0.6 | 10.0 | 13.7 | 13.5 | -0.1 | 0.6 | 7.1 | 0.8 | 0.7 | 35.3 |
| Rural | 21.7 | 16.7 | -5.0 | 0.5 | 10.6 | 13.9 | 11.7 | -2.2 | 0.6 | 6.6 | 7.4 | 0.8 | 32.5 |
| Suburban | 21.4 | 16.0 | -5.4 | 0.5 | 10.5 | 16.1 | 15.1 | -1.0 | 0.5 | 7.9 | -4.8 | 0.7 | 36.5 |
| Urban | 21.6 | 17.7 | -3.9 | 0.6 | 9.7 | 13.3 | 14.3 | 0.9 | 0.6 | 7.3 | 0.3 | 0.7 | 35.9 |

b)

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