EVALUATION OF THE CMAQ5.0 IN THE FRAMEWORK OF THE CALIOPE AIR QUALITY FORECASTING SYSTEM OVER EUROPE

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1. INTRODUCTION

Over recent decades, there has been a clear progress across Europe towards reducing anthropogenic emissions (EEA, 2010). However, poor air quality remains an important public health issue, especially in urban environments. Airborne particulate matter (PM), tropospheric ozone (O_3) and nitrogen dioxide (NO_2) are the main problematic pollutants in Europe.

Accurate air quality forecast system can offer tremendous societal and economics benefits by enabling advanced planning for individuals, organizations, and communities in order to reduce pollutant emissions and their adverse health impacts (Zhang et al., 2012). In this sense, the current European directive 2008/50/EC establishes the possibility of using modeling techniques to assess air quality (EEA, 2011).

Several operational air quality forecasting systems already exists for Europe (http://www.chemicalweather.eu). In the Spanish context, the Earth Science Department of the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS) has established the CALIOPE air quality system to forecast air pollution (O_3, NO_2, SO_2, and PM10) with high spatial resolution over Europe (12 km x 12 km) and the Iberian Peninsula (4 km x 4 km). The CALIOPE system consists in a set of models (Baldasano et al., 2008): the WRF-ARW meteorological model; the HERMES emission model, the BSC-DREAM8b natural dust model and the CMAQ Chemical Transport Model (CTM).

The CALIOPE system is advancing our understanding about atmospheric pollution dynamics in Europe. A number of studies based on CMAQv4.5 support the confidence on the system. On the one hand, it has been full-year evaluated in Europe (Pay et al., 2010, 2012a; Basart et al., 2012) and Spain (Baldasano et al., 2011; Pay et al., 2012b). On the other hand, it is near-real time (NRT) evaluated against air quality measurements on an hourly basis using a post-process to correct systematic bias based on Kalman filter technique (Sicardi et al., 2012).

A lot of efforts have been done in order to improve CALIOPE PM forecast by means of the inclusion of desert dust, sea salt and resuspended PM emissions from paved road. Evaluation studies (Pay et al., 2012a; Basart et al., 2012) show that modeled organic aerosols are significant underestimations partly related to the state-of-the-science concerning the secondary organic aerosol (SOA) formation pathway implemented in CMAQv4.5(AERO4) which does not include biogenic SOA formation from isoprene and sesquiterpenes. The absence of the isoprene-SOA route for SOA modeling in the domain of study may impact significantly air quality during summer, when elevated biogenic volatile organic compounds (bVOC) emissions combine with an enhanced photochemistry.

Currently a new version of CMAQ is being tested in the CMAS community, namely CMAQv5.0 (CMAQ, 2012). It includes substantial scientific improvements over the version 4.5, especially devoted to improve SOA formation (Carlton et al., 2012) and dynamic interactions of fine and coarse aerosol.

The present contribution evaluates the CALIOPE air quality forecasting system over Europe using CMAQ CTM version 5.0 based on the main pollutants O_3, NO_2 and PM10 at ground levels from April 9th till June 7th, 2012.

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2. METHODS

2.1 The CMAQ CTM

CALIOPE is a high-resolution air quality system which provides forecast for 24 and 48h (www.bsc.es/caliope) since October 2006 for Europe (12 km x 12 km, 1h) and Spain (4 km x 4 km, 1h). It integrates a set of models. The meteorological model is the WRF-ARW model (version 3.3.1) initialized by the FNL/NCEP data. The European emissions are estimated by means a top-down approach implemented in the High-Elective Resolution Modeling Emission System (HERMES version 2.0) based on the EMEP inventory for the year 2008 (Guevara et al., 2012). The Chemical Transport Model (CTM) is the CMAQ (version 4.5) using the CB-IV chemical mechanism and AERO4 mode for aerosols. Chemical boundary conditions for European domain are provided by the global chemical transport model LMDz-INCA2 (Hauglustaine et al., 2004). The CMAQ horizontal grid resolution corresponds to that of WRF-ARW. Its vertical structure was obtained by a collapse from the 38 WRF-ARW layers to a total of 15 layers steadily increasing for the surface up to 50 hPa with a stronger density within the planetary boundary layer.

In parallel to the aforementioned configuration, the CALIOPE system is currently forecasting air quality with the new CMAQ version 5.0 over the European domain. The CMAQv5.0 configuration in this study uses the CB-05 chemical mechanism and AERO5 mode for aerosols.

This work analyzes the impact of updating the CMAQ version from 4.5 to 5.0 in the framework of the CALIOPE system in forecast mode over Europe. Although CALIOPE forecast based on CMAQv5.0 is available since April 9th 2012, the present work only analyzes the period till June 7th 2012 (60 days) as preliminary results.

2.2 Air Quality Observation

The comparison between both CMAQ versions is done in terms of gaseous and aerosol concentrations (O_3, NO_2, and PM10) at the lowest level. Forecast concentrations are compared against observations on an hourly basis from the European air quality database (AIRBASE) which classifies stations as background rural/suburban. A number of 167 stations were selected to evaluate O_3, 128 for NO_2, and 74 for PM10, respectively. Fig. 1 shows the location of selected stations.

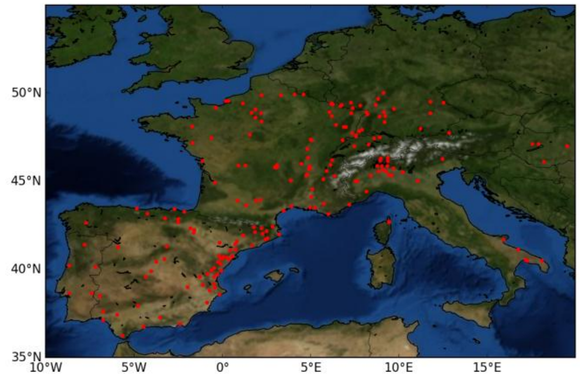

Fig. 1. Location of selected AIRBASE stations

The evaluation method is based on the analysis of temporal series and statistics, both performed on an hourly basis. The influence of the environment of the stations is also taken into account in the present evaluation. Statistics, correlation coefficient (r) and Root Mean Square Error (RMSE) are calculated according to different categories: over all stations (“All”), over rural background stations (“RB”), and over suburban background stations (“SB”). Note that the evaluation is done in NRT, and observations are not validated.

3. RESULTS AND DISCUSSION

3.1 Operational Evaluation

Model performance is quantified according the type of environment, RB and SB. Table 1 shows statistics calculated at selected AIRBASE stations for O_3, NO_2 and PM10 from April 9th till June 7th, 2012.

Statistics for modeled O_3 presented here are sensitively lower than those discussed in Pay et al. (2010) using CALIOPE system (CMAQv4.5) for the European domain. Several reasons contribute to these differences. First, the present work is run routinely in a forecast mode. Second, observations used here are not validated in a QA/QC protocol. Third, the present evaluation is performed on an hourly basis.

Despite the model performance in terms of statistics, the main idea of the present evaluation exercise is to show the first result about the relatively behavior between CMAQ4.5 versus

CMAQ5.0 working in a forecast mode, both integrated in the CALIOPE system.

Table 1. NRT statistical evaluation of the CALIOPE forecasting system against selected AIRBASE stations. Statistics, correlation coefficient (r) and Root Mean Square Error (RMSE), are on an hourly basis. #n indicates the number of stations. Type of environment is indicated as rural background (RB) and suburban background (SB).

Type (#n)	Version	MOD (μgm^{-3})	OBS (μgm^{-3})	r	RMSE (μgm^{-3})
		O_3			
All (167)	CMAQv4.5	59.1	74.3	0.43	29.2
	CMAQv5.0	58.3	74.3	0.53	28.5
RB (89)	CMAQv4.5	60.2	78.2	0.43	29.9
	CMAQv5.0	60.3	78.2	0.50	29.2
SB (73)	CMAQv4.5	57.8	70.1	0.42	28.5
	CMAQv5.0	56.1	70.1	0.54	27.8
		NO_2			
All (128)	CMAQv4.5	4.9	9.8	0.27	12.3
	CMAQv5.0	5.8	9.8	0.26	12.5
RB (63)	CMAQv4.5	3.7	6.4	0.18	8.8
	CMAQv5.0	4.4	6.4	0.18	9.1
SB (65)	CMAQv4.5	6.0	13.9	0.20	15.6
	CMAQv5.0	7.2	13.9	0.19	15.6
		PM10			
All (74)	CMAQv4.5	7.1	14.2	0.21	20.2
	CMAQv5.0	8.8	14.2	0.26	17.5
RB (38)	CMAQv4.5	6.8	12.9	0.22	20.0
	CMAQv5.0	8.4	12.9	0.32	14.9
SB (36)	CMAQv4.5	7.4	15.8	0.19	20.5
	CMAQv5.0	9.2	15.8	0.20	20.3

Overall, O_3 statistical evaluation results (Table 1) indicate that the highest improvements with CMAQv5.0 are found at SB stations where r increases from 0.42 to 0.54 and RMSE decreases by ~1 μgm^{-3}.

The Fig. 2 shows O_3 temporal series on an hourly basis for the period 7th – 14th May 2012 at two European stations, Manlleu (Spain) in the Mediterranean Basin and Neustadt (Germany) in central Europe. Both temporal series present an O_3 daily cycle under the influence of urban emissions, with minimum during nighttime and maximum during the daytime.

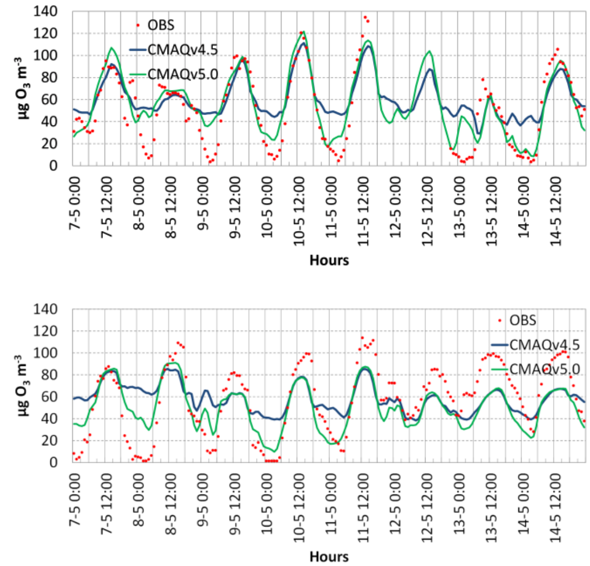

Fig. 2. Hourly O_3 temporal series for the period 7th -14th May 2012 at Manlleu station, Spain (top) and Neustadt station, Germany (bottom). Red points show observations (OBS). Continuous lines indicate the CALIOPE system forecasts: blue line using CMAQv4.5, and green line using CMAQv5.0.

O_3 peaks are higher in Manlleu (Spain) than in Neustadt (Germany). This is partly related with two facts. First, the highest concentrations over Europe are found in the Mediterranean Basin (nearly 90-105 μgm^{-3}), as this region is particularly affected by high solar radiation which hence photochemical production of O_3 and the influence of the Azores high which favors the long range transport of precursor emissions form central and northern European countries (Pay et al., 2010). Second, Manlleu station is downwind one of the biggest urban center in Spain, Barcelona city.

With the present configuration, CMAQv5.0 does not improve O_3 diurnal peaks significantly. According to Fig. 2 bias reduction is less than ~5 $\mu g\ m^{-3}$. However, minimum nighttime O_3 concentration substantially improves with CMAQv5.0. Fig. 2 shows how hourly bias can be reduced till 20-30 $\mu g\ m^{-3}$ at suburban stations at nighttime.

Concerning NO_2 model performance, statistics shown in the Table 1 does not show significant improvements between both CMAQ versions. However, temporal series at several stations depict improvements in the daytime chemistry of NO_2 implemented in CMAQ5.0. Fig. 3 top shows NO_2 hourly variability at Casa de Campo station, located in the biggest city of Spain (Madrid), where simulations with CMAQv5.0 increase hourly peaks by ~5-10 µgm^{-3} compared to CMAQv4.5. In the same way, CMAQv5.0 shows a significant improvement at Paterna station (Spain) compared to version 4.5 (Fig. 3, bottom). Compared to version 4.5, NO_2 hourly peaks modelled with CMAQv5.0 increase by ~20 µgm^{-3} and show a better agreement with observations.

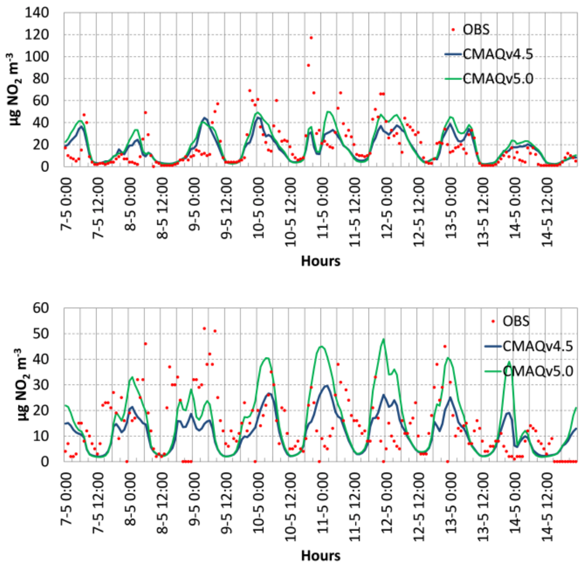

Fig. 3. Hourly NO_2 temporal series for the period May 7th -14th 2012 at Casa de Campo station, Spain (top) and Paterna station, Spain (bottom). Red points show observations (OBS). Continuous lines indicate the CALIOPE system forecasts: blue line using CMAQv4.5, and green line using CMAQv5.0.

PM10 is a pollutant which is underestimated in ~40-50% (Pay et al., 2010) (Table 1). CALIOPE forecast based on CMAQv5.0, relatively improves PM10 hourly correlation coefficient in a 24% for all the stations. The improvement is significant at RB stations, where r increases by 45%. The same tendency is found for RMSE. For all stations, RMSE is reduced by ~3 µgm^{-3} using CMAQv5.0, which represents a reduction of 13% in the error. For RB stations, CMAQv5.0 shows the highest RMSE improvement compared to version 4.5 which is reduced by ~5 µgm^{-3}, this implies a 26% reduction.

Fig. 4 shows temporal series at two SB stations in Spain. In both stations modeled PM10 background levels increase by ~10 µgm^{-3} using version 5.0 compared with version 4.5. Substantial efforts should be made in the evaluation of chemical description of PM formation and the accuracy of PM sources.

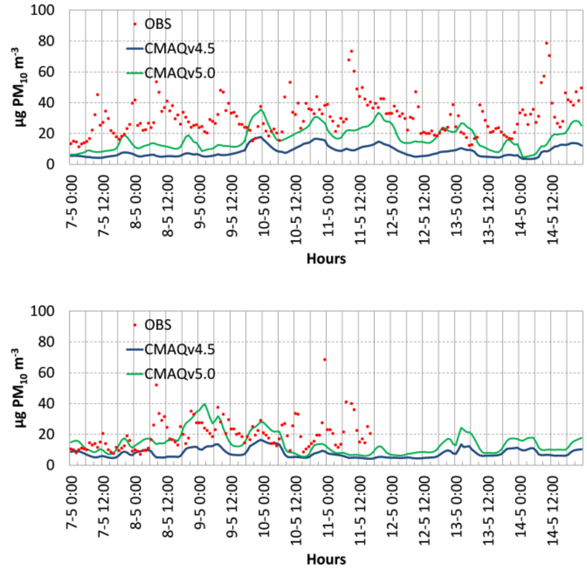

Fig. 4. Hourly PM10 temporal series for the period 7th - 14th May 2012 at El Atabal station, Spain (top) and Vilafranca del Penedes station, Spain (bottom). Red points show observations (OBS). Continuous lines indicate the CALIOPE system forecasts: blue line using CMAQv4.5, and green line using CMAQv5.0.

3.1 Bias-correction Impact

The present contribution also evaluates the effect of using the Kalman filter post-process (KF) to reduce systematic bias in both CMAQ versions. Statistics in **Table 2** show that overall the bias-adjustment technique is more effective over CMAQv5.0 than over version 4.5. The pollutant with the highest improvement is O_3. Hourly r for all stations increases till 0.53 with CMAQv5.0 after applying KF, meanwhile r reach 0.43 with CMAQ4.5 with the same bias-correction.

The NO_2 performance after applying KF demonstrate significant relative improvements compared to O_3, mostly because the original modeling system skills are lower for this pollutant.

For PM10, KF presents a higher relative improvement applied over CMAQ5.0 than over version 4.5, with an increasing of 19% in r (from 0.36 to 0.43) and a decrease of 15% in RMSE (from 18.1 µgm^{-3} to 15.4 µgm^{-3}).

Table 2. NRT statistical evaluation of the CALIOPE forecasting system against selected AIRBASE stations using Kalman filter post-process. Statistics, correlation coefficient (r) and Root Mean Square Error (RMSE), are on an hourly basis. #n indicates the number of stations.

Type (#n)	Version	MOD (μgm^{-3})	OBS (μgm^{-3})	r	RMSE (μgm^{-3})
O_3 All (167)	CMAQv4.5	59.1	74.3	0.43	29.2
	CMAQv5.0	58.3	74.3	0.53	28.5
NO_2 All (128)	CMAQv4.5	8.8	9.8	0.59	9.4
	CMAQv5.0	8.7	9.8	0.56	9.8
PM10 All (74)	CMAQv4.5	13.3	14.2	0.36	18.1
	CMAQv5.0	13.2	14.2	0.43	15.4

4. CONCLUSION

This work presents the first evaluation results after updating the CMAQ version from the 4.5 to 5.0 in the framework of the CALIOPE air quality forecasting system over Europe.

Results indicate that CMAQv5.0 improves O_3 forecast daily cycle, especially at nighttime over suburban stations, where O_3 biases are reduced between 20 and 40 μgm^{-3}. The NO_2 performance demonstrates significant relative improvements compared to O_3, mostly because the NO_2 concentrations is mainly related to emission modeling. However, the CMAQv5.0 improves the forecast of NO_2 peaks at suburban stations reducing biases ~10-20 μgm^{-3}. PM10 CALIOPE forecast improves with the new CMAQ version. Episodes of secondary aerosol formation are now reproduced (i.e. 7-14th May 2012), where bias are reduce in ~10-20 μgm^{-3}. Furthermore, PM10 hourly peaks in suburban stations are better reproduced reducing hourly biases ~5-10 μgm^{-3}.

The contribution also evaluates the effect of using the Kalman filter post-process to reduce systematic bias in both CMAQ versions. The results confirm the advantage of the application of bias correction techniques for air quality forecasts. Results show that the bias-adjustment technique is more effective over CMAQv5.0.

Current work concerning the improvement of CALIOPE system is dealing with estimation of bVOC emissions by means the MEGANv2.0 model which hence new SOA mechanism implemented in AERO5.

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