Contribution of Saharan dust in an integrated air quality system and its on-line assessment

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[1] Nowadays none of the operational daily forecasts in Europe includes the influence of Saharan dust on a non-climatic basis. In order to account for this, the BSC-CNS currently operates daily photochemical forecasts in the Iberian Peninsula with MM5-EMEP-CMAQ modelling system and Saharan dust forecasts over Southern Europe with Eta/DREAM. The necessity of coupling both modelling systems is addressed by the study of a long summer episode combining regional re-circulations and Saharan dust covering from June 19 to July 12, 2006. As a first approach, the natural dust contribution from Eta/DREAM is added on-line to the anthropogenic output of CMAQ. The performance of the model has been quantitatively evaluated with discrete and categorical (skill scores) statistics by a fully operational on-line comparison of the first-layer simulations results of CMAQ and CMAQ+DREAM and the values measured in two different stations located in the Mediterranean part of the domain. The results indicate a remarkable improvement in the discrete and skill-scores evaluation (accuracy, critical success index and probability of detection) of PM10 exceedances set in regulations when using CMAQ+DREAM compared to CMAQ- or DREAM-alone simulations. **Citation:** Jiménez-Guerrero, P., C. Pérez, O. Jorba, and J. M. Baldasano (2008), Contribution of Saharan dust in an integrated air quality system and its on-line assessment, *Geophys. Res. Lett.*, *35*, L03814, doi:10.1029/2007GL031580.

1. Introduction

[2] The most serious air quality problems are related to high levels of PM10, NO_2 and O_3 [*De Leeuw et al.*, 2001; *Baldasano et al.*, 2003]. The case of southern Europe is more critical since some of the objectives proposed by the EU Directives related to air quality for year 2010 are less well attained than in the more northern latitudes, especially in summer when the threshold levels are exceeded. In these cases, the regulation demands a detailed diagnosis of those areas where the exceedances are found and a forecast of the evolution of ground-level concentrations; and it establishes the possibility of using modelling techniques to assess air quality.

[3] Indeed, atmospheric chemistry transport model simulations and observations have shown that summertime aerosol levels in the entire Mediterranean troposphere are among the highest in the world [e.g., *Lelieveld et al.*, 2002]. Under weak synoptic forcing, air-mass coastal re-circulations become large natural photo-chemical reactors where most of the NO_x emissions and other precursors are transformed into oxidants, acidic compounds, aerosols and O_3 [*Jiménez et al.*, 2006a, 2006b]. In addition, the contribution of mineral aerosols is very high due the poor vegetation soil coverage, the re-suspension of loose material on the road surface and the frequent occurrence of Saharan dust events which decisively contribute to the exceedances of the PM10 limit values of Directive 1999/30/CE [*Rodríguez et al.*, 2001; *Querol et al.*, 2004].

[4] However, nowadays, to the authors' knowledge, none of the available operational daily forecasts in Europe includes the influence of Saharan dust in a non-climatic basis. When considering only anthropogenic emissions, chemistry-transport model simulations underestimate the PM10 concentrations by 30–50%, using the current knowledge about aerosol physics and chemistry [*Vautard et al.*, 2005]. The same authors demonstrated through diagnostic simulations that the introduction of boundary conditions for Saharan dust is necessary in order to model correctly the PM mass over southern Europe. However, the boundary conditions were derived from monthly averages of a global dust model simulation. Although background dust present at the southern boundary was fairly well simulated, dust peaks could not be represented due to the highly episodic nature of the events in the region (1-4 days average duration).

[5] In order to account for the local/regional pollution and the Saharan dust contribution, the Barcelona Supercomputing Center (BSC-CNS) currently operates photochemical forecasts in the Iberian Peninsula and all Europe with MM5-EMEP-CMAQ modelling system (http://www.bsc.es/projects/earthscience/aqforecast-en) and Saharan dust forecasts over Europe with the Eta/DREAM model (http://www.bsc.es/projects/earthscience/DREAM) on a daily basis.

[6] The objective of this work is to provide an operational PM10 product for air quality forecasting by on-line adding the Saharan dust contribution from DREAM to the anthropogenic output of CMAQ (Figure 1a and 1b). This addition is performed by using a bi-linear interpolation of CMAQ and DREAM integration grids into a unique common grid (Figure 1b). The necessity of coupling both aforementioned systems in an integrated framework is addressed by the analysis of a study case of a long summer event (June 19–July 12, 2006) of Saharan dust transport towards Europe, focusing on the Iberian Peninsula, and its analysis and evaluation against the on-line ground observations available during the period.

2. Description of the Forecasting System

[7] The MM5 model [*Dudhia*, 1993] is used to operationally provide the meteorology parameters to CMAQ

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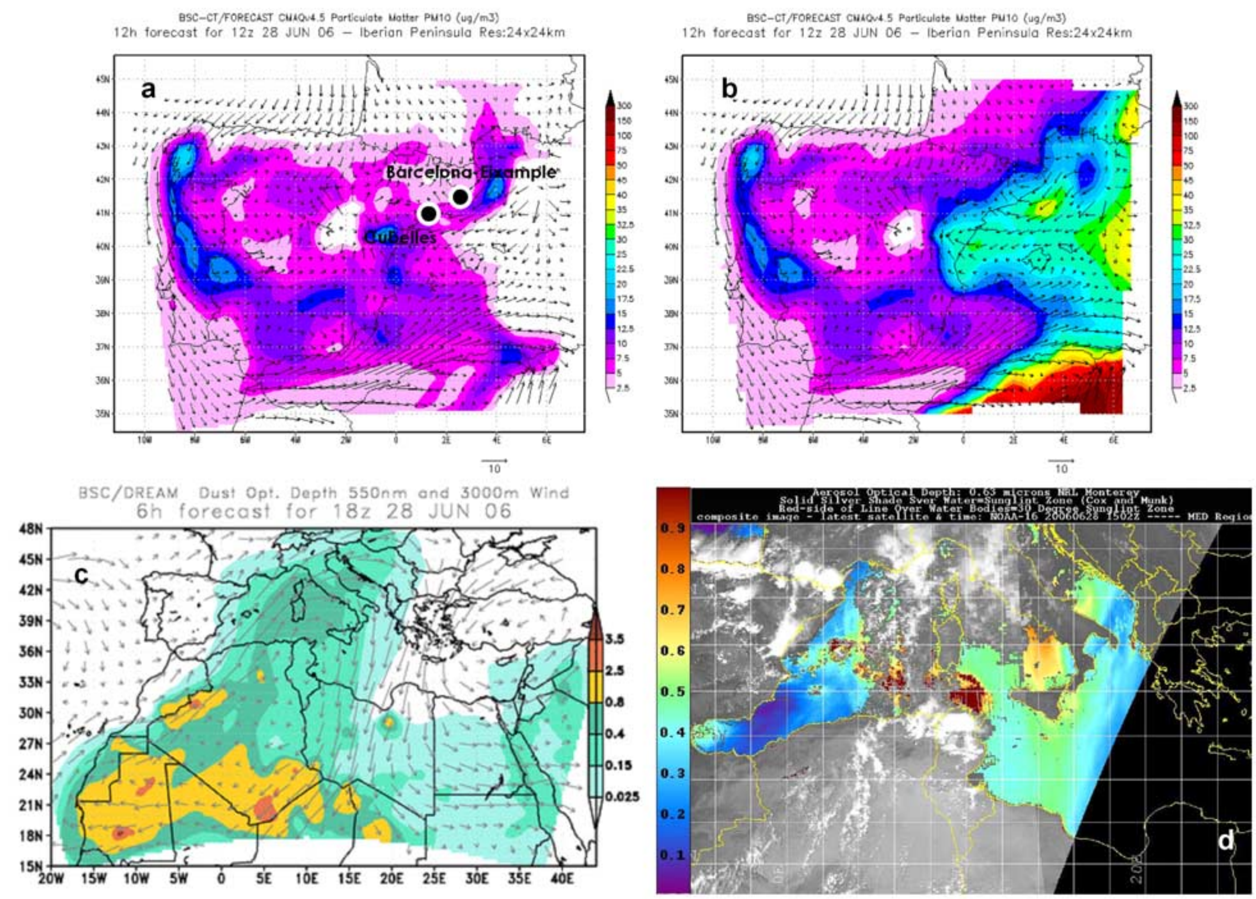

Figure 1. Operational forecast for particulate matter (PM10, μg m^{-3}) at 12 UTC of June 28, 2006 in the (a) CMAQ-alone version and (b) CMAQ+DREAM forecasting system; (c) dust optical depth (550 nm) in the DREAM-alone version; and (d) NPS/NRL AOD satellite-based image over the Mediterranean domain.

chemistry transport model. The MM5 options used are described in detail by *Jiménez et al.* [2006a, 2006b]. Emissions used for the domain of Europe and the Iberian Peninsula are derived from EMEP emissions database on an hourly basis, except biogenic emissions that are estimated following the methods implemented by *Parra et al.* [2006]. The cells from the European EMEP mesh are disaggregated into a grid of 24-km resolution. The emissions of each source are speciated, according to *Jiménez et al.* [2003] in the categories of the chemical mechanism Carbon Bond-IV [*Gery et al.*, 1989]. The CMAQ System [*Byun and Ching*, 1999] simulates the main atmospheric chemistry, transport and deposition processes involved in the domain defined. The domain of operational simulations for this study case covers an area of 1392 $\times$ 1104 km^2 (Figure 1a).

[8] The model used to provide the concentrations of desert dust is the Dust REgional Atmospheric Model (DREAM) [*Nickovic et al.*, 2001]. DREAM is fully inserted as one of the governing equations in the atmospheric NCEP/Eta atmospheric model and simulates all major processes of the atmospheric dust cycle. Wind erosion of the soil is parameterized by the type of soil, vegetation cover, soil moisture content, and surface atmospheric turbulence. The resolution is set to 50 km in the horizontal and to 24 layers extending up to approximately 15 km in the vertical. For this study case, a first qualitative evaluation of the system was carried out by comparison with NPS/NRL AOD satellite-based images, observing an excellent agreement in the description of the dust dynamics over southern Europe (Figures 1c and 1d).

3. Results

3.1. Description of the Episode: June 19–July 12, 2006

[9] The major synoptic pressure forcing at surface level for the whole period (June 19–July 12, 2006) were the Azores anticyclone at middle latitudes over the Atlantic Ocean, the African thermal low extending over northern Africa, and the travel of high-latitude cyclones affecting central and northern regions of Europe. The influence of the Azores Anticyclone was present for the whole period, inducing low surface pressure gradient over the Iberian Peninsula and the Mediterranean with mean sea level pressures of 1016 hPa. This episode associated to a stagnant situation involves a low air quality in the domain of study and high local formation rates of photochemical pollutants [*Coll et al.*, 2005; *Dufour et al.*, 2005; *Jiménez et al.*, 2006b]. Furthermore, the whole period was characterized by the development of S-SW dust-enriched air pulses affecting the Iberian Peninsula and western Mediterranean

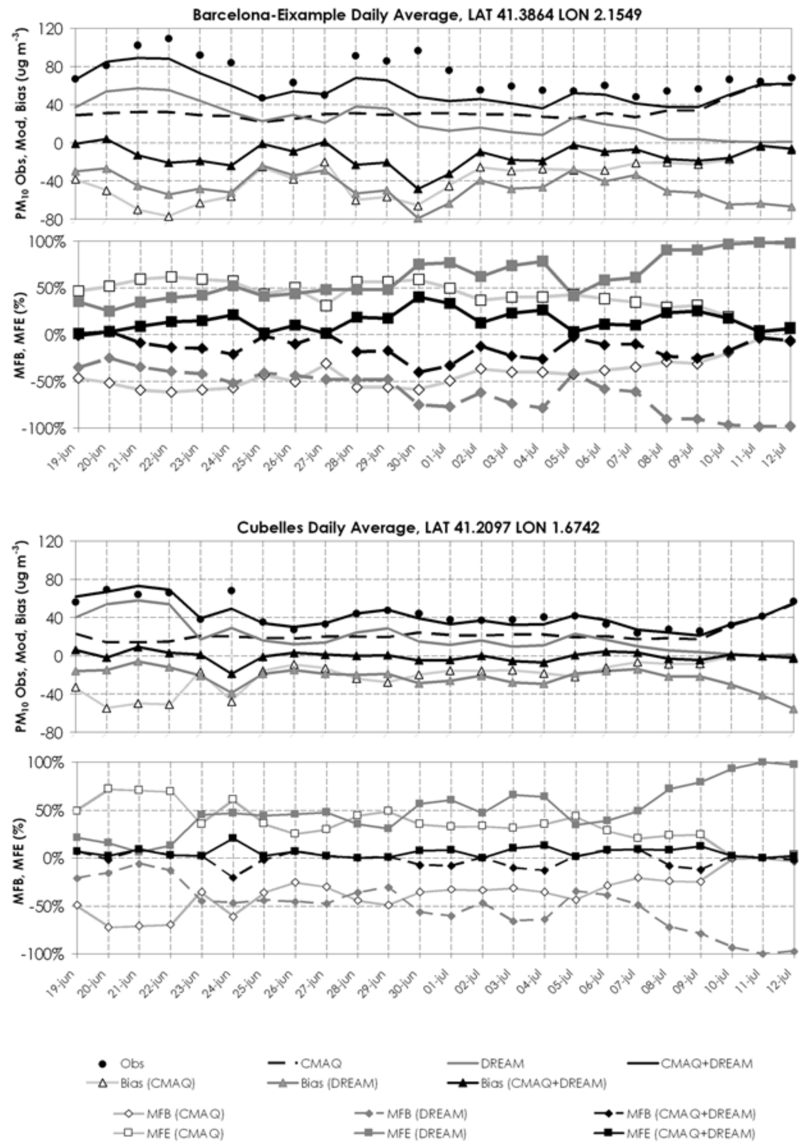

Figure 2. On-line validation results of the different configurations of the air quality forecasting system (CMAQ- and DREAM-alone versions and coupled CMAQ+DREAM) for the period June 19–July 12, 2006 in a urban station with high influence of traffic at (top) Barcelona-Eixample, LAT 41.39; LON 2.15) and (bottom) a background station (Cubelles, LAT 41.21; LON 1.67).

basin. The period June 19–28 was characterized by two SW dust pulses in the low-middle troposphere: a first pulse from June 19–25 and a second intensified pulse observed in June 26–28. Another SW pulse flows affecting the Iberian Peninsula developed from July 3–6, with the formation of a moderate westerly wave at 700 hPa interacting with a relative high-pressure region over Africa, which reflected the African thermal low observed at surface levels as a subsidence inversion (see http://www.bsc.es/projects/earthscience/visor/dust/med/dld/archive/).

3.2. Evaluation of the Models

[10] The performance of the system for predicting PM10 levels was statistically evaluated by comparison of the first-layer (vertical extent $\sim$ 86 m) simulations results of CMAQ and CMAQ+DREAM and the values measured on-line in two different stations located in the Spanish Mediterranean coast (Figure 1a): a urban station with high influence of traffic (Barcelona-Eixample, LAT 41.39; LON 2.15) and a background station (Cubelles, LAT 41.21; LON 1.67). The qualitative and quantitative validation studies using data from lidar stations, sun-photometers and satellites have been presented by *Ansmann et al.* [2003], *Balis et al.* [2006], *Pérez et al.* [2006a, 2006b], and *Papayannis et al.* [2007]; outlining the good skills of the model for AOD predictions and concerning both the horizontal and vertical extent of the dust plume in the region. However, because of the rising interest in on-line assessments of air quality forecasts, the number of stations used comes conditioned by the lack of available information provided in real time for the domain of study. The results of the evaluation are shown in Figure 2 and Table 1.

[11] The European Directive 1999/30/EC does not define criteria for modelling performance in the case of hourly and

Table 1. Summary of the Discrete and Categorical (Skill Scores) Statistical Evaluation of PM10 in the Forecasting System for the Stations of Barcelona-Eixample (Urban) and Cubelles (Background) During June 19 to July 12, 2006[a]

	Discrete Evaluation		
	Barcelona-Eixample	Cubelles	Average
Bias(C) (μg m^{-3})	−37	−20	**−29**
Bias(D) (μg m^{-3})	−47	−23	**−35**
Bias(C+D) (μg m^{-3})	−14	−1	**−7**
MNBE(C) (%)	−50.8	−43.6	**−47.2**
MNBE(D) (%)	−68.2	−58.1	**−63.2**
MNBE(C+D) (%)	−18.9	−1.8	**−10.3**
MNGE(C) (%)	50.8	43.6	**47.2**
MNGE(D) (%)	68.2	58.1	**63.2**
MNGE(C+D) (%)	19.5	8.4	**14.0**
MFB(C) (%)	−41.8	−35.7	**−38.7**
MFB(D) (%)	−60.7	−50.4	**−55.6**
MFB(C+D) (%)	−14.0	−1.5	**−7.7**
MFE(C) (%)	41.8	35.7	**38.7**
MFE(D) (%)	60.7	50.4	**55.6**
MFE(C+D) (%)	14.4	5.8	**10.1**

	Categorical Evaluation											
	30 μg m^{-3} Threshold Forecast						50 μg m^{-3} Threshold Forecast					
	Barcelona-Eixample			Cubelles			Barcelona-Eixample			Cubelles		
	C	D	C+D	C	D	C+D	C	D	C+D	C	D	C+D
A (Accuracy)	54.2	33.3	100.0	29.2	37.5	95.8	16.7	20.8	70.8	79.2	91.7	95.8
CSI (Critical Success Index)	54.2	33.3	100.0	15.0	25.0	95.2	9.1	13.6	68.2	16.7	66.7	83.3
POD (Probability of Detection)	54.2	33.3	100.0	15.0	25.0	100.0	9.1	13.6	68.2	16.7	66.7	83.3
B (Bias)	0.5	0.7	0.9	0.9	0.8	0.9	0.9	0.9	0.9	0.8	0.3	0.9
FAR (False Alarm Rate)	0.0	0.0	0.0	0.0	0.0	4.8	0.0	0.0	0.0	0.0	0.0	0.0

[a]C+D: CMAQ+DREAM; MNBE: mean normalised bias error; MNGE: mean normalised gross error.

daily average concentration (this accuracy objective is 50% for annual average). *Boylan and Russell* [2006] have proposed model performance goals and criteria that vary as a function of particulate matter concentration. The goal has been met when both the mean fractional error (MFE) and the mean fractional bias (MFB) are less than or equal to +50% and ±30%, respectively. The criteria has been met when both the MFE and the MFB are less than or equal to +75% and ±60%. As derived from Table 1, the performance goals are not achieved by CMAQ or DREAM when applied uncoupled. For CMAQ and DREAM, the MFB exceeds the ±30% as an average behaviour during the episode; also, for DREAM, the MFE does not meet the performance goal. However, if we consider the CMAQ+DREAM system, both the performance goals and criteria accomplish with the advised values (−7.7% for MFB and 10.1% as MFE). For CMAQ+DREAM, the highest MFB and MFE is −23.9% and 23.9%, in that order, for June 30. Therefore, the performance goals are achieved for daily averages on every day during the episode just in the case of applying CMAQ+DREAM (Figure 2).

[12] Moreover, the *U.S. Environmental Protection Agency* [2005] has developed guidelines to indicate the correct performance of models against specific points where air quality stations are located. The statistics included in these guidelines that have been considered in this work are the bias error, mean normalised bias error (MNBE) and mean normalised gross error (MNGE). Both CMAQ and DREAM underestimate concentrations during the whole period of study (bias ranging from −64 to −2 μg m^{-3} for CMAQ; and −61 to −21 μg m^{-3} for DREAM). However, CMAQ+DREAM presents a clear improvement in the underprediction (bias ranging from −27 to +3 μg m^{-3}) during the period, especially in the central part of the episode when both re-circulations and Saharan dust intrusions involve an important contribution to the PM10 concentrations. The MNBE for the entire period improves from −63.2% and −47.2% (for DREAM and CMAQ, respectively) to the −10.3% (CMAQ+DREAM); this tendency is also observed for the MNGE. The forecasting modelling system combining anthropogenic and natural contributions reveals as the most accurate option for forecasting (average gross errors of 62.2% for DREAM, 47.2% for CMAQ and 14.0% in the case of CMAQ+DREAM).

[13] Furthermore, categorical statistics or skill scores [*Kang et al.*, 2005; *Eder et al.*, 2006] have been used to evaluate the different ensembles of the forecast (considering CMAQ alone, DREAM alone or coupled CMAQ+DREAM), including parameters such as the model accuracy (A), bias (B), probability of detection (POD), false alarm rate (FAR) and critical success index (CSI). With respect to the categorical forecasting for PM10 (Table 1), statistical parameters indicate that the accuracy (percent of forecasts that correctly predict an exceedance or non-exceedance) substantially improves when using CMAQ+DREAM for the particulate matter forecasts; yielding the best results (accuracy of 100% for predicting a 30 μg m^{-3} threshold) in the station of Barcelona-Eixample. In the case of considering the threshold established in the European regulations (50 μg m^{-3}, 24-hr average), for the urban station of Barcelona-Eixample the skill score accuracy improves from 16.7% with CMAQ, 20.8% with DREAM to 70.8% when using both models coupled. For the background station of Cubelles, the accuracy increases from 79.2% with CMAQ and 91.7% with DREAM to 95.8% in the case of using CMAQ+DREAM for providing daily-average forecasts. The value of the bias (B < 1 for all models) indicates that exceedances are generally underpredicted by each model,

especially in the city of Barcelona, which corresponds with the value of the MNBE obtained for discrete evaluations. This underestimation is minor for the CMAQ+DREAM configurations (bias around 0.9 for both thresholds and stations), clearly improving the bias for CMAQ and DREAM alone versions.

[14] Since the metric accuracy can be greatly influenced by the overwhelming number of non-exceedances [*Jiménez et al.*, 2006a], to circumvent this inflation the critical success index (CSI) and the probability of detection (POD) are used. Both parameters perform similarly during the whole extent of the episode, importantly increasing their score when using CMAQ+DREAM. For the 30 μg m^{-3} threshold, the POD in both stations achieves 100.0% (CSI of 100% and 95.2% in the stations of Barcelona-Eixample and Cubelles, respectively). On the other hand, for the 50 μg m^{-3} threshold as a daily average, the CSI and the POD involve identical scores, improving in the urban station from 9.1% and 13.6% for CMAQ and DREAM, in that order, to 68.2% with CMAQ+DREAM. In the background station, the scores for CMAQ, DREAM and CMAQ+DREAM increase from 16.7% and 66.7% to achieve 83.3%, respectively.

[15] Last, the fifth categorical parameter, the false alarm rate (FAR) indicates the number of times that the model predicted an exceedance that did not occur. This metric is zero for all the modelling system options, thresholds and stations; but in the case CMAQ+DREAM of the 30 μg m^{-3} threshold in the background station of Cubelles, where the FAR is 4.8%.

4. Discussion and Conclusions

[16] In this study we have coupled CMAQ anthropogenic outputs with DREAM desert dust forecasts in an operational way by on-line addition of both model outputs in the BSC-CNS Air Quality Forecast Modelling System http://www.bsc.es/projects/earthscience/aqforecast-en). This novel approach was on-line assessed against observations for a major episode of air pollution combining local/regional pollution and long range transport of Saharan dust on June–July 2006. It has been shown that the newly developed modelling system substantially increases the accuracy of both discrete and categorical (skill scores) statistical parameters in the domain of study when including the Saharan dust contributions to the forecasting system. The performance goals for PM10 simulations are achieved for daily averages on every day during the episode just in the case of applying CMAQ+DREAM system.

[17] However, there are still some development tasks for the improvement of the forecasting system; for instance, the underestimation of PM10 mass in Barcelona-Eixample (MNBE of −19% with CMAQ+DREAM modelling system) outlines the need for the inclusion of paved road resuspension during peak traffic hours, as revealed by the 1-hr modelling time series versus observations (not shown); in agreement with *Viana et al.* [2005]. Moreover, the large uncertainties in local natural erosion emissions resulting from saltation processes need further development in emission estimates and modelling, especially for the summertime ground conditions in the Iberian Peninsula.

[18] Also, the dust field is resolved in the current system in a 50 km grid which may not be fine enough to resolve the complex mesoscale circulations which would drive the dust within receptor areas. Long-range transport of dust mainly takes place in the free troposphere driven by synoptic winds. The overwhelming of the synoptic dust transport with the regional mesoscale circulations may not be accurately resolved at coarse resolutions. In this sense, we highlight the necessity for an integrated modelling system including the interaction between different scales through consistent nested grids.

[19] Finally, the definition of the horizontal grid size should be able to reproduce the atmospheric circulations of the area of study. The resolution applied in this work (24 km) is considered as adequate for addressing background air quality in the domain under study (e.g. in the case of Cubelles station where the influence of local emission sources is limited, the MNBE is under −2%). However, for urban/industrial areas as Barcelona with a pervasive influence of anthropogenic emissions on a local scale, finer grids may be needed for addressing processes related to gas-phase and aerosol secondary pollutants [*Jiménez et al.*, 2006a]. This also highlights the need for emission inventories with a bottom-up approach and fine resolutions (in the order of 1 km^2) conditioning the feasibility of high-resolution air quality forecasting systems. Indeed, several national initiatives are currently being taken into practise (e.g., France, United Kingdom, Portugal, Germany or Spain). Specifically for the Iberian Peninsula, the 1-km HERMES emission model is nowadays being developed under the framework of the CALIOPE project, a Spanish national initiative whose objective is to provide an operational service for air quality forecasting in Spain with a resolution of 4 km following the methods presented in this work.

[20] Despite the aforementioned limitations, the results of this work demonstrate that this first approach is accurate and effective in order to improve the prediction of the PM10 mass and to achieve the standards set in the regulations for modelling applications.

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