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# Caliope: an operational air quality forecasting system for the Iberian Peninsula, Balearic Islands and Canary Islands – first annual evaluation and ongoing developments

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**Abstract.** The Caliope project funded by the Spanish Ministry of the Environment establishes an air quality forecasting system for Spain to increase the knowledge on transport and dynamics of pollutants in Spain, to assure the accomplishment of legislation and to inform the population about the levels of pollutants, topics in which the European Commission has shown a great concern. The present contribution describes the first quantitative verification study performed so far with two chemistry transport models (CMAQ and CHIMERE) for a reference year (2004) at medium spatial resolution (around 20×20 km for the Iberian Peninsula). Both models perform similarly in the case of ground-level ozone. The mean normalised gross error MNGE remains below 15–20% during summertime, when ozone episodes occur, outlining the good skills of the system concerning the forecasting of air quality in Spain. Furthermore, the ongoing developments of the system towards high resolution modelling (4×4 km for Spain, 12×12 km for Europe, 1 h temporal resolution) and the integration with observations within the Caliope umbrella are described.

## 1 Introduction

According to recent studies of the European Environmental Agency (EEA), air pollution is the environmental factor with the greatest impact on health in Europe and is responsible for the largest burden of environment-related disease (EEA, 2005). Under the current state of knowledge, the most serious air quality (AQ) problems are related to high levels of PM<sub>10</sub>, NO<sub>2</sub> and O<sub>3</sub> (De Leeuw et al., 2001; Baldasano et al., 2003). Particulate matter and especially small particles with a diameter less than 2.5 micrometers (PM<sub>2.5</sub>) are associated with increased mortality, especially from cardiovascular and cardiopulmonary diseases (e.g., Dab et al., 2001; Pope et al.,

2002). Several studies show a strong association between exposure to air pollution and the aggravation of asthma (e.g. Brauer et al., 2007).

The Caliope project has as its main objective to establish an AQ forecasting system for Spain coordinated by the Spanish Ministry of the Environment, delivering AQ related products with high resolution useful to a wide range of users for reducing the impacts of air pollution on human health. A partnership of four research institutions composes the Caliope project: the Barcelona Supercomputing Center (BSC), the CIEMAT, the Earth Sciences Institute “Jaume Almera” (IJA-CSIC) and the CEAM Foundation. This consortium deals with both operational and scientific aspects related to AQ monitoring and forecasting. BSC and CIEMAT lead the modelling developments of the project while IJA-CSIC and CEAM are in charge of retrieving experimental data for validation processes. The current experimental



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**Figure 1.** Location of EMEP stations in Spain with data available for the year 2004 used for the validation and comparison of CMAQ and CHIMERE chemistry transport models.

forecasts and a more detailed description of the system are available through <http://www.bsc.es/caliope>.

Several operational AQ forecast systems based in numerical modelling already exist in Europe (e.g., EURAD, Prev'Air, SILAM, PROMOTE, among others). However, none of them resolve AQ at a required resolution for Spain or include a full and precise description of the processes involved for particulate matter modelling, both important factors to obtain accurate results of air pollutant concentrations in a complex region as Spain (Jiménez et al., 2006). Moreover, none of these operational systems includes the influence of Saharan dust on a non-climatic basis. When considering only anthropogenic emissions, chemistry-transport model simulations underestimate the  $PM_{10}$  concentrations by 30–50%, using the current knowledge about aerosol physics and chemistry (Vautard et al., 2005). In this sense, the Caliope project focuses on these issues to improve the skill of an operational AQ forecasting system for Spain.

To achieve its main objective, the Caliope project defines a first step focused on the analysis of an AQ annual simulation with the initial state of the implementation of AQ models (AQMs). The resolution selected for this initial simulation is representative of the state-of-the-art of current AQ forecasting systems in Europe. This start point indicates the skills of AQMs to assess AQ over Spain on an annual basis. Then, further developments aim to build a high resolution modelling system coupling meteorological, emission and chemical transport models able to resolve com-

plex physico-chemical processes at fine scales to improve the skills of AQMs. In this contribution we present the first steps towards the evaluation of an annual simulation at coarse resolution performed with CMAQ (Byun and Schere, 2006) and CHIMERE (Vautard et al., 2003; Bessagnet et al., 2004) chemistry transport models (CTMs) applied at 18-km and  $0.2^\circ$  (aprox. 22-km) resolution, respectively. They constitute the basis of the Caliope system and the design of the high resolution Caliope modelling system (described in Sect. 3).

## 2 Evaluation of an annual simulation of AQ

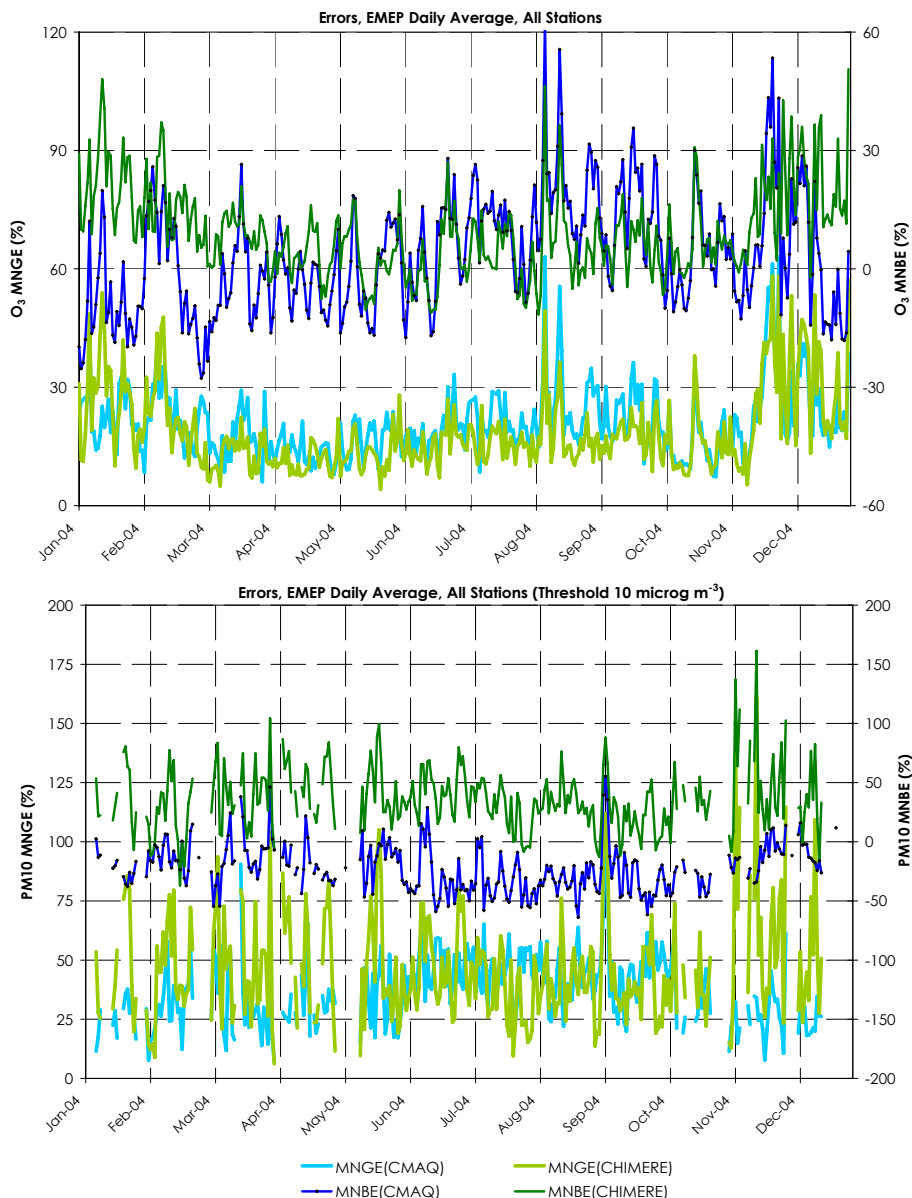
Two AQMs are compared on a yearly basis: WRF-ARW/EMEP/CMAQ and MM5/EMEP/CHIMERE. The first qualitative and quantitative verification studies performed so far for the modelling system for a selected year (2004) have outlined the reasonably good skill of the CMAQ and CHIMERE models for concentrations of gaseous pollutants and aerosols in Spain. Model results for the Iberian Peninsula domain are compared against data from the EMEP observation network of Spain (see Fig. 1) provided by IJA-CSIC and CEAM that have performed a quality assurance and quality control on the data. The AQMs have been configured at medium-resolution for a first evaluation of the year 2004. Two sets of spatial domains were set up: (1) CMAQ: European domain of  $54 \times 54$  km horizontal resolution and a domain centred in the Iberian Peninsula of  $18 \times 18$  km, 12 vertical layers; (2) CHIMERE: European domain of  $0.5^\circ \times 0.5^\circ$

**Table 1.** Configuration of the Air Quality Modelling systems for the 2004 annual simulation.

| CMAQ                                   |                                      | CHIMERE                       |   |   |
|--|--------------------------------------|-------------------------------|---|---|
| Domains                                |                                      |                               |   |   |
|  | Europe                               | Iberian Peninsula             | Europe  | Iberian Peninsula                                 |
| NX                                     | 55                                   | 94                            | 88 (meteo),<br>67 (chemistry)                                 | 88 (meteo),<br>80 (chemistry)                     |
| NY                                     | 55                                   | 82                            | 79 (meteo),<br>46 (chemistry)                                 | 69 (meteo),<br>46 (chemistry)                     |
| NZ                                     | 32 (meteo),<br>12 (chemistry)        | 32 (meteo),<br>12 (chemistry) | 32 (meteo),<br>8 (chemistry)                                  | 32 (meteo),<br>8 (chemistry)                      |
| Horizontal resolution                  | 54 km                                | 18 km                         | 36 km (meteo), 0.5°<br>(approx. 55 km;<br>chemistry)          | 19 (meteo), 0.2°<br>(approx. 22 km;<br>chemistry) |
| Meteorology                            |                                      |                               |   |   |
| Meteorological driver                  | WRF                                  |                               | MM5   |   |
| Dynamics                               | ARW                                  |                               | MM5   |   |
| Microphysics                           | WSM-3 class                          |                               | Reisner graupel   |   |
| Radiation                              | RRTM, Dudhia scheme                  |                               | RRTM, Cloud radiation   |   |
| PBL                                    | YSU                                  |                               | MRF PBL   |   |
| LSM                                    | Noah LSM                             |                               | Five-Layer LSM  |   |
| Cumulus                                | Kain-Fritsch                         |                               | Grell   |   |
| Initialization and boundary conditions | NCEP-GFS analysis                    |                               | NCEP-GFS analysis   |   |
| Emissions                              |                                      |                               |   |   |
| Database                               | EMEP                                 |                               | EMEP  |   |
| Chemistry                              |                                      |                               |   |   |
| Chemical transport model               | CMAQ                                 |                               | CHIMERE   |   |
| Chemical mechanism                     | CBM-IV                               |                               | MELCHIOR  |   |
| Processes                              | Aerosols and heterogeneous chemistry |                               | Aerosols and heterogeneous chemistry, resuspension, sea salt. |   |
| Initial and boundary conditions        | US EPA profiles                      |                               | Monthly climatology of LMDz-INCA                              |   |
| Natural dust transport                 |                                      |                               |   |   |
| Dust conditions                        | DREAM for Saharan dust outbreaks     |                               | DREAM for Saharan dust outbreaks                              |   |

resolution (approx. 55×55 km), and a domain in the Iberian Peninsula of 0.2°×0.2° resolution (approx. 22×22 km), 8 vertical layers. CMAQ is driven by WRF-ARW (Michalakes et al., 2005; Skamarock et al., 2005) meteorological data, while CHIMERE uses MM5 (Dudhia, 1993) as the meteorological driver. Emissions used for the domain of Europe and the Iberian Peninsula are derived from the EMEP emissions database and disaggregated on an hourly basis. However, biogenic emissions used in CMAQ are estimated following the methods implemented in Parra et al. (2006) using the land-use map derived from CORINE NATURE/LAND Cover information. The initial and boundary conditions of the system are: (1) WRF and MM5: 6h-GFS analysis; (2)

CMAQ: Climate profiles taken from US EPA (Byun and Ching, 1999); (3) CHIMERE: monthly climatology from LMDz-INCA model (Hauglustaine et al., 2004) for gases concentrations and from GOCART model (Chin et al., 2002) for particulate species, as described in Vautard et al. (2005); (4) Dust REgional Atmospheric Model (DREAM) (Nickovic et al., 2001): 6h-GFS analysis for the Eta meteorological driver and a warm start of dust concentration (the initial state of dust concentration in the model is defined by the 24-h forecast from the previous-day model run). Both CMAQ and CHIMERE use DREAM results to represent the dust contribution from North Africa. Table 1 summarises the configuration of both AQMs.



**Figure 2.** 2004 annual evolution of the daily average errors for CMAQ (blue) and CHIMERE (green) models assessed against EMEP stations for ozone (up) and PM<sub>10</sub> (down): mean normalised gross error (MNGE) (light) and mean normalised bias error (MNBE) (dark).

Figure 2 shows the annual evolution of the daily average errors for the year 2004 over the Iberian Peninsula domain. The mean normalised gross error (MNGE) and mean normalised bias error (MNBE) are computed for EMEP station observations (Fig. 1) on a daily basis. These statistics are defined in US EPA (2005). The models perform similarly in the case of ground-level ozone. MNGE remains below 15–20% during summertime, when normalised errors present the most accurate scores. During wintertime, both models show a significantly different behaviour. CMAQ generally underestimates the ozone concentrations, except for some episodes, while CHIMERE over predicts them. From

April to June, the models fit better the observations, but CHIMERE shows a tendency to over predict the ozone daily values (MNBE less than 15%), while CMAQ slightly underestimates them (MNBE of –15%). This behaviour changes from July on, when both models tend to over predict daily values with a MNBE ranging between 0 and 30%. In general, CMAQ shows larger errors compared to CHIMERE. This may be explained by the different chemistry, initial and boundary conditions of both models and main monthly evolution of these conditions (larger differences during winter), and during some episodes in the differences between WRF and MM5 results. CHIMERE initialisation profiles appear



**Table 2.** Comparison of ozone and particulate matter errors for CMAQ and CHIMERE assessed against EMEP station observations in Spain (annual mean normalised bias error (MNBE), mean normalised gross error (MNGE) and unpaired peak accuracy (UPA) presented).

|        |               | Ozone    |         |          |         |         |         |
|--------|---------------|----------|---------|----------|---------|---------|---------|
|        |               | MNBE (%) |         | MNGE (%) |         | UPA (%) |         |
| Code   | Station Name  | CMAQ     | CHIMERE | CMAQ     | CHIMERE | CMAQ    | CHIMERE |
| ES0007 | Víznar        | 2.3      | 3.4     | 13.7     | 16.1    | -15.3   | -22.5   |
| ES0008 | Niembro       | 12.8     | 14.4    | 26.0     | 19.1    | 6.0     | 2.4     |
| ES0009 | Campisábalos  | 6.9      | -0.5    | 17.9     | 17.5    | -7.9    | 1.3     |
| ES0010 | Cabo de Creus | -5.8     | 0.7     | 18.2     | 12.6    | 2.8     | -11.8   |
| ES0011 | Barcarrota    | 25.1     | 28.1    | 30.6     | 32.5    | -14.3   | -17.3   |
| ES0012 | Zarra         | -4.1     | 5.9     | 13.7     | 12.1    | -9.0    | -16.0   |
| ES0013 | Peñausende    | -2.7     | 11.9    | 15.2     | 16.0    | -18.9   | -17.5   |
| ES0014 | Els Torms     | 3.3      | 15.1    | 20       | 20.2    | -5.8    | -12.5   |
| ES0015 | Risco Llano   | -23.7    | -9.9    | 24.3     | 14.0    | -21.8   | -23.6   |
| ES0016 | O Saviñao     | 24.3     | 27.4    | 32.2     | 32.6    | -6.9    | -19.7   |

|        |               | Particulate Matter PM <sub>10</sub> |         |          |         |         |         |
|--------|---------------|-------------------------------------|---------|----------|---------|---------|---------|
|        |               | MNBE (%)                            |         | MNGE (%) |         | UPA (%) |         |
| Code   | Station Name  | CMAQ                                | CHIMERE | CMAQ     | CHIMERE | CMAQ    | CHIMERE |
| ES0007 | Víznar        | -35.0                               | 43.5    | 61.2     | 59.5    | -23.1   | -4.2    |
| ES0008 | Niembro       | -37.9                               | 32.8    | 50.8     | 58.3    | -29.8   | 16.1    |
| ES0009 | Campisábalos  | -24.6                               | 51.3    | 54.9     | 65.8    | 4.2     | 22.4    |
| ES0010 | Cabo de Creus | -15.0                               | 99.4    | 45.5     | 103.2   | -2.2    | 26.3    |
| ES0011 | Barcarrota    | -40.5                               | 79.1    | 55.36    | 86.8    | -45.1   | -40.3   |
| ES0012 | Zarra         | -44.5                               | 28.1    | 48.1     | 50.2    | -20.3   | 7.5     |
| ES0013 | Peñausende    | -26.4                               | 32.9    | 51.0     | 50.1    | -17.8   | -10.2   |
| ES0014 | Els Torms     | -36.1                               | 63.3    | 47.6     | 76.0    | 16.8    | 31.2    |
| ES0015 | Risco Llano   | -48.0                               | 10.6    | 52.1     | 31.1    | -21.7   | 17.2    |
| ES0016 | O Saviñao     | 0.9                                 | 61.9    | 43.9     | 71.3    | 10.7    | 13.0    |

to be higher than CMAQ during winter and adjust better in summer. Moreover, the summer results show the difficulty of both models to reproduce the nocturnal depletion of ozone, even though the diurnal values are not always achieved. It is important to note the two August episodes, where both models display major errors. These are associated with an under-prediction of the meteorological cores (both WRF and MM5) of two major precipitation events over the Iberian Peninsula, which negatively impact the next days' ozone simulation.

The major differences between the models occur for particulate matter when assessed against EMEP stations. PM<sub>10</sub> results, although preliminary, show the complexity of particulate matter modelling. The CMAQ model provides lower PM<sub>10</sub> levels than CHIMERE, and are in better agreement with EMEP observations. Considering the normalised error, CHIMERE overestimates PM<sub>10</sub> levels especially during wintertime (MNBE around 30% and MNGE around 50%), while CMAQ generally underestimates them, especially during summertime, and shows a MNGE below 30% in most winter situations. The main reason for the model differences may be related to the inclusion of saltation processes and sea

salt processes in the CHIMERE configuration, not considered in CMAQ, and the different boundary conditions (see Table 1). The resuspension and sea salt parameterization are included in CHIMERE showing a tendency to produce an over prediction of the aerosols emission over the Iberian Peninsula and thus giving rise to higher modelled concentrations. In this sense, CMAQ is able to better control the cycle of PM<sub>10</sub> production, considering the anthropogenic source and only the natural part from dust outbreaks following Jiménez-Guerrero et al. (2008) methodology, which shows a reasonable good performance for winter episodes. The overall evaluation shows that two major Saharan dust outbreaks over the Iberian Peninsula are over predicted on 30 March and 5 September. The over prediction is associated with the forcing of the DREAM model, indicating the sensitivity of the system to the skill of DREAM to reproduce dust transport over the Iberian Peninsula and its impacts at surface levels. Finally, during summertime, the MNGE shows lower variability in CMAQ, but the mean values of the error are centred near 45%, higher than the mean winter errors (not considering the episodes of dust not well captured by the

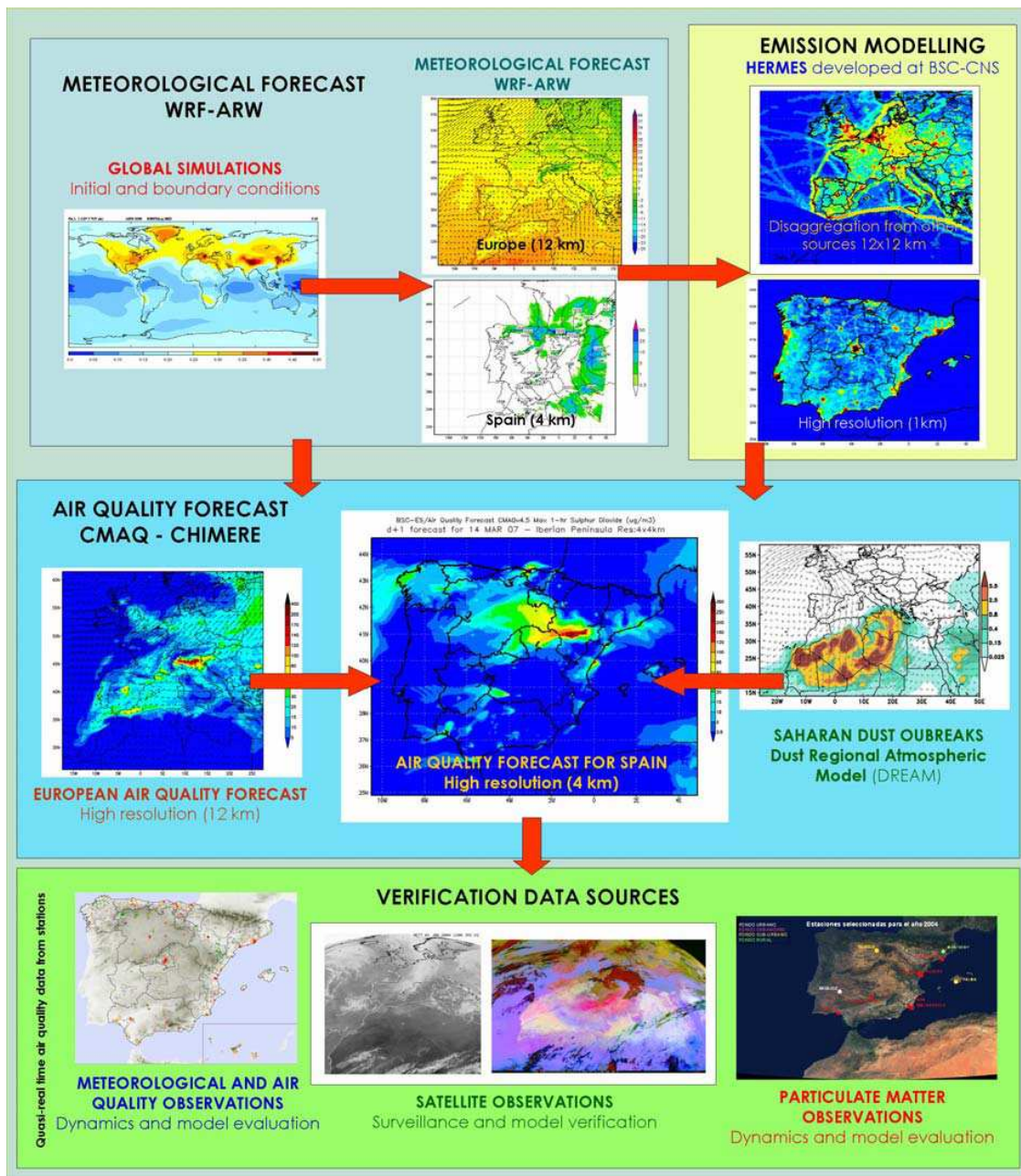


Figure 3. Caliope air quality modelling system scheme.

system). The CMAQ underestimation in summertime may be related to the needs for including local natural erosion emissions, which are not currently considered within the system. However, special care has to be taken in order to include a realistic module for natural resuspension and to improve the model skills during summertime.

A spatial comparison of ozone and particulate matter results for CMAQ and CHIMERE are presented in Table 2. The MNGE, MNBE and the unpaired peak accuracy (UPA) are computed for EMEP station observations in

Spain (Fig. 1). The largest differences between AQMs are observed at Mediterranean coastal stations, close to the land-sea transition. The AQ patterns at these stations are largely conditioned by the ability of WRF and MM5 to reproduce the mesoscale circulations in coastal areas of the Iberian Peninsula, with very marked differences between the Atlantic and the Mediterranean coasts. For ozone, the western stations witness the highest MNGE, ranging around 20–30%. MNGEs decrease to 13–20% at the Mediterranean coast and on the Iberian plateau. The ozone peaks are in general under-

estimated by both models, even though CMAQ shows better results for UPA at most of the stations (see Table 2). The results are in agreement with a previous study of Vivanco et al. (2007) that identifies the underestimation of ozone peaks during summertime of 2003–2005 especially for the centre of the Iberian Peninsula.

Particulate matter presents a major complexity and difficulty compared to ozone. MNGE ranges between 40–100% for CMAQ, and in this case CHIMERE shows noticeable lacks in modelling the observed PM<sub>10</sub> values over the north-eastern and south-western stations where an important overestimation is produced related with overestimation of sea salt aerosols and local saltation emissions, respectively. The other stations show similar results with both models. Finally, it is important to notice that the coupling of CTMs with the DREAM model produces a substantial increase in the accuracy of both discrete and categorical statistical parameters in Spain when including the Saharan dust contributions to the modelling system (e.g., Jiménez-Guerrero et al., 2008).

### 3 Ongoing developments: the Caliope modelling system

Taking advantage of the results obtained from the initial annual simulation presented in Sect. 2, the Caliope project comprises the development, implementation and validation of an integrated AQ forecasting modelling system, increasing the previous spatial resolution to 12×12 km for Europe and 4×4 km for Spain with nesting to 1×1 km for the cities of Madrid and Barcelona and a lead time of 72 h, formed by a set of models and observations taking into account anthropogenic, biogenic and natural dust pollution (Fig. 3). The modelling system is formed by the meteorological model WRF-ARW and two chemical transport models (CTMs), CMAQ and CHIMERE chemistry-transport models, being the emission core the HERMES emission model (e.g., Jiménez-Guerrero et al., 2007) developed specifically for Spain. Under the umbrella of the Caliope project, the WRFtoCHIMERE interface was created to link the CHIMERE CTM to WRF-ARW meteorology (Jorba et al., 2008).

The CTMs assume gaseous species and both inorganic and organic aerosols of primary and secondary origin, including primary particulate matter, mineral dust, sulphate, nitrate, ammonium, secondary organic species and water. Southern Europe and especially Spain are strongly affected by Saharan dust outbreaks (e.g. Pérez et al., 2006a, b). To take into account this contribution into the Caliope modelling system, the DREAM model provides the concentrations of desert dust reaching the domain of study. DREAM is fully inserted as one of the governing equations in the 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 con-

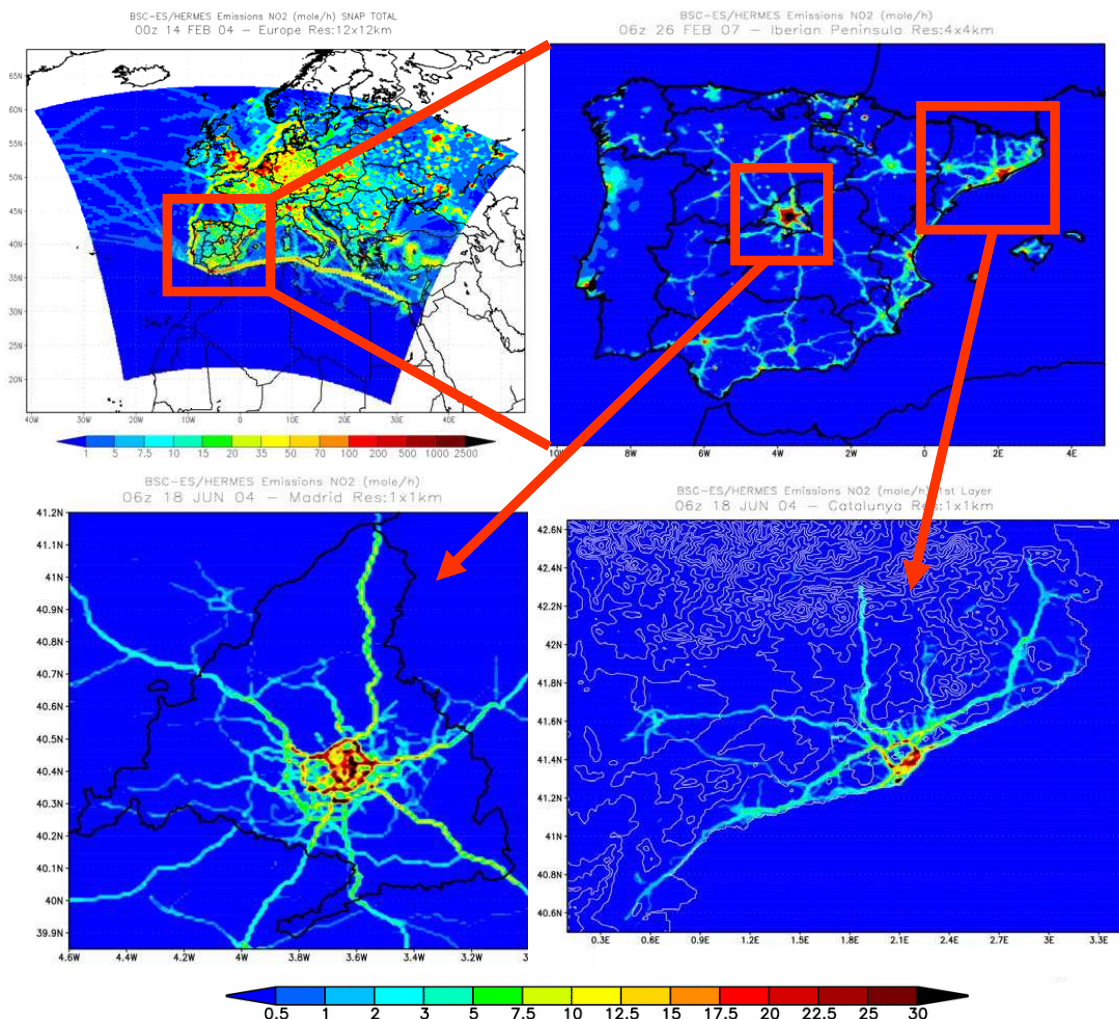
tent, and surface atmospheric turbulence. The coupling of DREAM with the Caliope system is described in Jiménez-Guerrero et al. (2008).

A high spatial (1 km<sup>2</sup>) and temporal (1 h) resolution emissions inventory model specific for Spain (HERMES) has been developed to generate emissions (Fig. 4). This model focuses on the estimation of gas and particulate matter pollutants, including ozone precursors. HERMES considers emissions from the following sources: (1) electricity generation plants, (2) industrial installations, (3) domestic and commercial fossil fuel use, (4) domestic and commercial solvents use, (5) road transport, (6) ports, (7) airports and (8) biogenic emissions; using a bottom-up approach except for domestic and commercial fossil fuel use, where a top-down approach was adopted and regional emissions were allocated to fine grid cells by surrogate indexes. It follows the methodologies and criteria of previous emission models developed for the Eastern Iberian Peninsula: EMICAT2000 (Parra et al., 2004, 2006) and EMIVAL2000 (Arévalo et al., 2004). The reference year chosen is 2004, since it is the most recent year in which all the needed data for the HERMES development are available. HERMES estimates the atmospheric emissions with a temporal resolution of 1 h and a spatial resolution of 1 km<sup>2</sup> and generates results according to the EEA's Selected Nomenclature for Air Pollution (SNAP). Furthermore, HERMES has the capacity of presenting results according to individual installation, industrial activities, land use classification or type of pollutants or process (fugitive, evaporative, hot or cold emissions). Experimental forecasts with the Caliope system are available on <http://www.bsc.es/caliope>.

### 4 Conclusions

The fast-track development, testing and implementation of the initial operational capability of an AQ forecasting system for Spain (Caliope project) result from the close cooperation between BSC, CIEMAT, IJA-CSIC and CEAM. The annual simulation has outlined the capabilities of AQMs in their current state and resolution to model air pollution episodes in Spain. However, there are still several development tasks for the improvement of the forecasting system; the underestimation of PM<sub>10</sub> mass during summertime with CMAQ and the overestimation with CHIMERE outlines the need for the accurate inclusion of local natural erosion emissions resulting from saltation processes not well resolved by current models, especially for summertime ground conditions in the Iberian Peninsula. Moreover, the paved road re-suspension during peak traffic hours is also missing in the models and may substantially contribute to PM<sub>10</sub> concentrations (Viana et al., 2005). Also, the definition of the horizontal grid size should be able to better reproduce specific atmospheric circulations in the study area. The resolution applied in this work (18 and 22 km) is considered adequate for addressing background air quality in the domain under study. However, for





**Figure 4.** The HERMES anthropogenic and biogenic emission model has been specifically developed as a high-resolution ( $1 \text{ km}^2$  and 1 h) emission model under a GIS framework. It computes high resolution emissions for Spain and it is able to disaggregate emissions from other sources to finer resolutions (Top-left panel: disaggregation of EMEP European emissions at  $12 \times 12 \text{ km}$  horizontal resolution of total SNAP activity sectors for NO<sub>2</sub> emissions (mole/h) for 14 February 2004 at 00:00 UTC; Other panels: NO<sub>2</sub> emissions (mole/h) for 18 June 2004 at 06:00 UTC computed with HERMES model at  $4 \times 4 \text{ km}$  for the Iberian Peninsula and  $1 \times 1 \text{ km}$  for Madrid and Catalunya regions).

urban/industrial areas with a pervasive influence of anthropogenic emissions on a local scale, finer grids will be needed for addressing processes related to gas-phase and aerosol secondary pollutants (Jiménez et al., 2006). This also highlights the need for emission inventories with a bottom-up approach and fine resolutions (of the order of  $1 \text{ km}^2$ ) conditioning the feasibility of high-resolution AQ 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.

The improvement of the resolution addressed by the Caliope project in the whole region is expected to serve as a standard tool for public and private, state and local forecast-

ers who provide tailored forecasts for their communities, and will allow taking preventive measures to safeguard human health. The Caliope system also complements the data obtained in the present networks of AQ measurements managed by regional and local authorities, and in certain experimental measurement campaigns or AQ studies performed both in urban or background areas. The results of the Caliope system will allow for a better level of information for the citizenship related to AQ forecasting. Caliope results are disseminated through the web site <http://www.bsc.es/caliope>. Experimental operational forecasts for Europe and Spain are delivered on a daily basis for a 48 hour cycle. The system is qualitatively verified against satellite observations and surface stations.

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