Atmospheric Environment 44 (2010) 2997–3006

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

Air pollution impacts of speed limitation measures in large cities: The need for improving traffic data in a metropolitan area

José M. Baldasano [a,b,*], María Gonçalves [b], Albert Soret [b], Pedro Jiménez-Guerrero [b,1]

[a] *Environmental Modelling Laboratory, Technical University of Catalonia, Avda. Diagonal 647, Edificio H, Oficina 10.23, 08028 Barcelona, Spain*
[b] *Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC–CNS), Earth Sciences Department, Jordi Girona 29, Edificio Nexus II, 08034 Barcelona, Spain*

ARTICLE INFO

Article history:
Received 12 March 2010
Received in revised form
6 May 2010
Accepted 7 May 2010

Keywords:
Urban air quality
Air quality modelling
Traffic emissions
Atmospheric management
Barcelona Metropolitan Area

ABSTRACT

Assessing the effects of air quality management strategies in urban areas is a major concern worldwide because of the large impacts on health caused by the exposure to air pollution. In this sense, this work analyses the changes in urban air quality due to the introduction of a maximum speed limit to 80 km h^{-1} on motorways in a large city by using a novel methodology combining traffic assimilation data and modelling systems implemented in a supercomputing facility. Albeit the methodology has been non-specifically developed and can be extrapolated to any large city or megacity, the case study of Barcelona is presented here. Hourly simulations take into account the entire year 2008 (when the 80 km h^{-1} limit has been introduced) vs. the traffic conditions for the year 2007. The data has been assimilated in an emission model, which considers hourly variable speeds and hourly traffic intensity in the affected area, taken from long-term measurement campaigns for the aforementioned years; it also permits to take into account the traffic congestion effect. Overall, the emissions are reduced up to 4%; however the local effects of this reduction achieve an important impact for the adjacent area to the roadways, reaching 11%. In this sense, the speed limitation effects assessed represent enhancements in air quality levels (5–7%) of primary pollutants over the area, directly improving the welfare of 1.35 million inhabitants (over 41% of the population of the Metropolitan Area) and affecting 3.29 million dwellers who are potentially benefited from this strategy for air quality management (reducing 0.6% the mortality rates in the area).

1. Introduction

Improving air quality in urban areas is nowadays an important environmental challenge (Akimoto, 2003; Molina and Molina, 2004). In addition, worldwide epidemiological studies show a consistent increase in cardiac and respiratory morbidity and mortality from exposure to air pollution (Dockery et al., 1993; Nel, 2005; Pope and Dockery, 2006). As well as a source of local pollution, urban activities contribute to transboundary pollution and the increase of greenhouse gases (GHGs) concentration (Fenger, 1999; Baldasano et al., 2003). The public administrations are testing management strategies mainly addressed to reduce on-road traffic emissions, because this sector is the largest contributor to anthropogenic pollutants emissions in the urban environments (Colvile et al., 2001; Querol et al., 2001; Ghose et al., 2004). These strategies intend to either reduce the number of vehicles circulating on conurbations or to mitigate the unitary emissions by vehicle, either using alternative fuels or new technology vehicles (hybrids, fuel cells, natural gas, biofuels, etc.) (e.g. Schultz et al., 2003; Stephens-Romero et al., 2009). A complementary way of reducing traffic emissions consists in changing the speed circulation patterns (Gonçalves et al., 2008; Keller et al., 2008). The speed dependency of emissions varies as a function of the pollutant, depending on the vehicle age, weight and cubic capacity of the engine. Therefore a unique optimal speed circulation for atmospheric pollutants for the whole range of vehicles in an urban vehicles fleet does not exist. Nevertheless, it is a widely adopted traffic management strategy, because its benefits concern not only pollutants emissions, but also reduces congestion, noise and accidents. The evaluation of air quality management strategies requires the use of measurements and air quality models to perform quantitative impact studies (Ponche and Vinuesa, 2005). On-road traffic modules included within emission inventories need more emissions measurements from vehicle types and pollution control

---

* Corresponding author at: Environmental Modelling Laboratory, Technical University of Catalonia, Avda. Diagonal 647, Edificio H, Oficina 10.23, 08028 Barcelona, Spain. Tel.: +34 93 413 77 19.

E-mail addresses: jose.baldasano@bsc.es (J.M. Baldasano), pedro.jimenezguerrero@um.es (P. Jiménez-Guerrero).

[1] Now at: Department of Physics, University of Murcia, Ed. CIOyN, Campus de Espinardo, 30100 Murcia, Spain. Tel.: +34 868 88 8175.

1352-2310/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.atmosenv.2010.05.013

technologies to parameterize emissions (Carslaw and Beevers, 2005).

2. Methodology

We explore the changes in urban air quality by using a novel methodology combining traffic assimilation data and a third generation modelling system (WRF + HERMES + CMAQ + BSC-DREAM8b) (see Baldasano et al., 2008a,b for further details) when introducing a maximum speed limit to 80 km h^{-1} (Gonçalves et al., 2008) in the access motorways of a large Mediterranean city, the Barcelona Metropolitan Area (Fig. 1), which may be considered as representative of a large European conurbation. Albeit the methodology has been non-specifically developed and can be extrapolated to any large city or megacity, the case study of Barcelona is of particular interest since the Mediterranean region is especially sensitive to air pollution owing to cloud-free conditions and high solar radiation intensity (Lelieveld et al., 2002; Rodríguez et al., 2003). This management strategy for the improvement of air quality has been planned by the regional administration and extensively applied in the area. Simulations take into account the entire year 2008 (when the 80 km h^{-1} limit has been introduced) vs. the traffic conditions for the year 2007 using the same meteorology to isolate the effect of changing traffic emissions. One of the added values of this study is the unprecedented high resolution applied (1 km^2, 1 h) for a large conurbation and the vertical extension of the modelling system (30 layers covering the whole troposphere and the low stratosphere). This resolution, together with the techniques for traffic assimilation data, requires of a large capacity of high-performance computing; hence the methodology developed is based upon the availability of the MareNostrum supercomputer hold in the Barcelona Supercomputing Center—Centro Nacional de Supercomputación (BSC—CNS). The advances in the parallelization of air quality model codes for their implementation in these high-performance computing infrastructures have allowed the simulations performed here on medium- and long-term periods (e.g. the needed time for integrating both hourly annual air

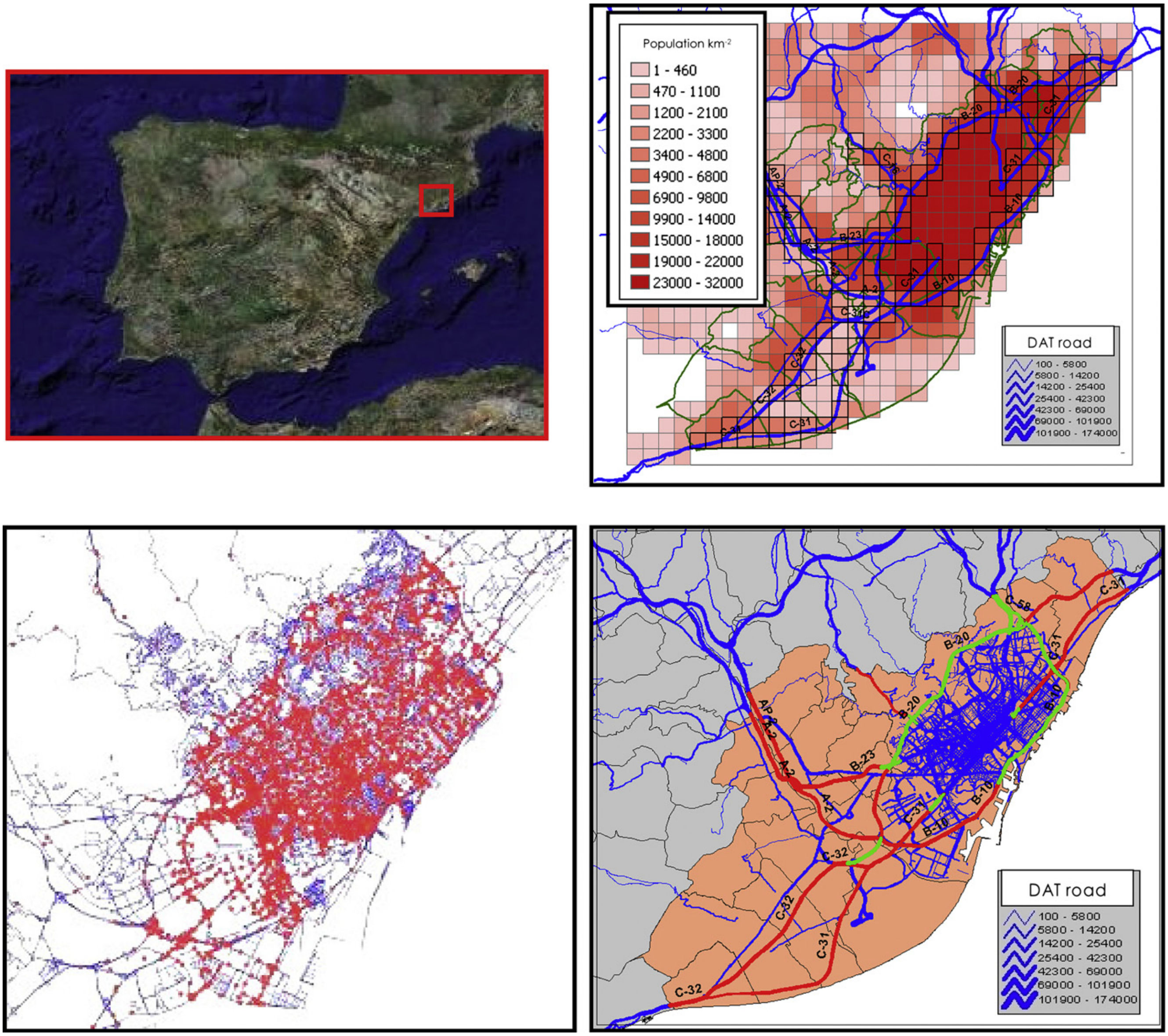


Fig. 1. (Left-up) Location of the domain of study; (right-up) population density in the areas affected by the 80 km h^{-1} limit; (left-down) points with daily average traffic information in the city of Barcelona; (right-down) roads limited to 80 km h^{-1} (red), roads with speed under 80 km h^{-1} before the implementation of the limit (green) and not-affected roads (blue).

quality simulations with traffic-assimilated data for the years 2008 and 2007 has reduced from 908.3 days with a single-processor machine to 2.5 days using 512 processors at MareNostrum).

The model used presents a novel approach for emission estimates, including the definition of the road network, dividing it in stretches with specific temporary disaggregating profiles (distinguishing day-type: weekday-holiday, and month), specific average speed, daily average traffic (number of vehicles per day), stretch length, route type (highway, road or urban) and circulation zones. For the implementation of the 80 km h^{-1} limit, data coming from 125 measurement points have been assimilated within the emission model; these points are located in the access roads to the area of study and contain hourly detailed information of average circulation speed and hourly traffic intensity.

3. Results and discussion

3.1. Validation of the simulations

Air quality station hourly data, averaged over the domain of study were used to evaluate the performance of the modelling system for predicting ground-level nitrogen dioxide and particulate matter during the year 2008. Measurements of ambient pollutants were reported by 15 air quality surface stations in the Barcelona Metropolitan Area, which are part of the Environmental Department of the Catalonia Government (Spain). This network provides air quality data for urban, industrial and background areas with an accurate territorial distribution, and it represents one of the most dense air quality networks in Europe. The European Directive 2008/50/EC assumes an uncertainty of 50–60% for the air quality objective for modelling assessment methods. This uncertainty is defined as the maximum error of the measured and calculated concentration levels. In addition, the US Environmental Protection Agency has recently developed new guidelines (US EPA, 2005) for a minimum set of statistical measures to be used for these evaluations in regions where monitoring data are sufficiently dense. These guidelines indicate that it is inappropriate to establish a rigid criterion for model acceptance or rejection (i.e., no pass/fail test). These statistical measures considered are the mean bias (MB); the mean normalized bias error (MNBE) and the mean normalized gross error (MNGE) for concentrations above a prescribed threshold, among others. With respect to particulate matter evaluation, Boylan and Russell (2006) indicated that MNBE and MNGE may not be appropriate and suggested mean fractional bias (MFB) and mean fractional error (MFE) instead. They propose that a model performance goal is met when both the MFE and MBE are less than or equal to 50% and ±30%, respectively, and a model performance criterion is met when both MFE $\leq$ 75% and MFB $\leq \pm$75%. The results presented below summarise the evaluation of the annual average values during the year 2008 for air quality simulations, since the validation of the performance of the meteorological model over the area of study can be found in Jiménez-Guerrero et al. (2008a).

For nitrogen dioxide, the concentration of this pollutant is accurately predicted in the stations of the greater Barcelona Area (MB, −5.7 μg m^{-3}; RMSE, 9.2 μg m^{-3}; MNBE, −11.8, MNGE, 14.0%; MFE, 15.6%) (Fig. 2). The value of the correlation coefficient is significant ($r = 0.798$). In this domain, the on-road traffic pervasive emissions and local photochemistry dominate vs. other contributions such as e.g. advective or convective transport. The underestimation in the values may be caused because a relatively coarse vertical resolution of the lower troposphere leads to artificial vertical exchange between the boundary layer and the free troposphere, which enhances nitrogen oxides venting from the planetary boundary layer (Wang et al., 1998). The statistical values meet the reference values for uncertainty air quality modelling set in the European Directive 1999/30/EC and 2008/50/EC.

In the case of particulate matter PM10, the model underestimates the annual average concentration observed in the conurbation (MB, −10.1 μg m^{-3}; RMSE, 13.0 μg m^{-3}; MNBE, −24.0%; MNGE, 24.2%, MFB, −29.4%; MFE, 29.7%). The results of the evaluation indicate that the model performs accurately, taking into account the performance goal and criteria and considering that current 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 slight underestimation in the Barcelona Metropolitan Area is produced since the emission model does not consider the re-suspension from soils and paved roads in urban areas (Lenschow et al., 2001; Viana et al., 2005), which may exert a limited influence in the PM10 levels in the area especially during the peak traffic hours.

A summary of the evaluation results is given in Fig. 2. The underestimation (mainly in the case of primary pollutants) is caused because the average volume defined by the model horizontal grid spacing must be sufficiently small to allow the air quality to be reproduced accurately, especially on urban scales. It appears that a finer grid is important for addressing air pollution processes in urban areas, whereas for rural areas larger grids may be allowed, for example, to capture the non-linearity of the secondary aerosol formation as a function of precursor concentrations.

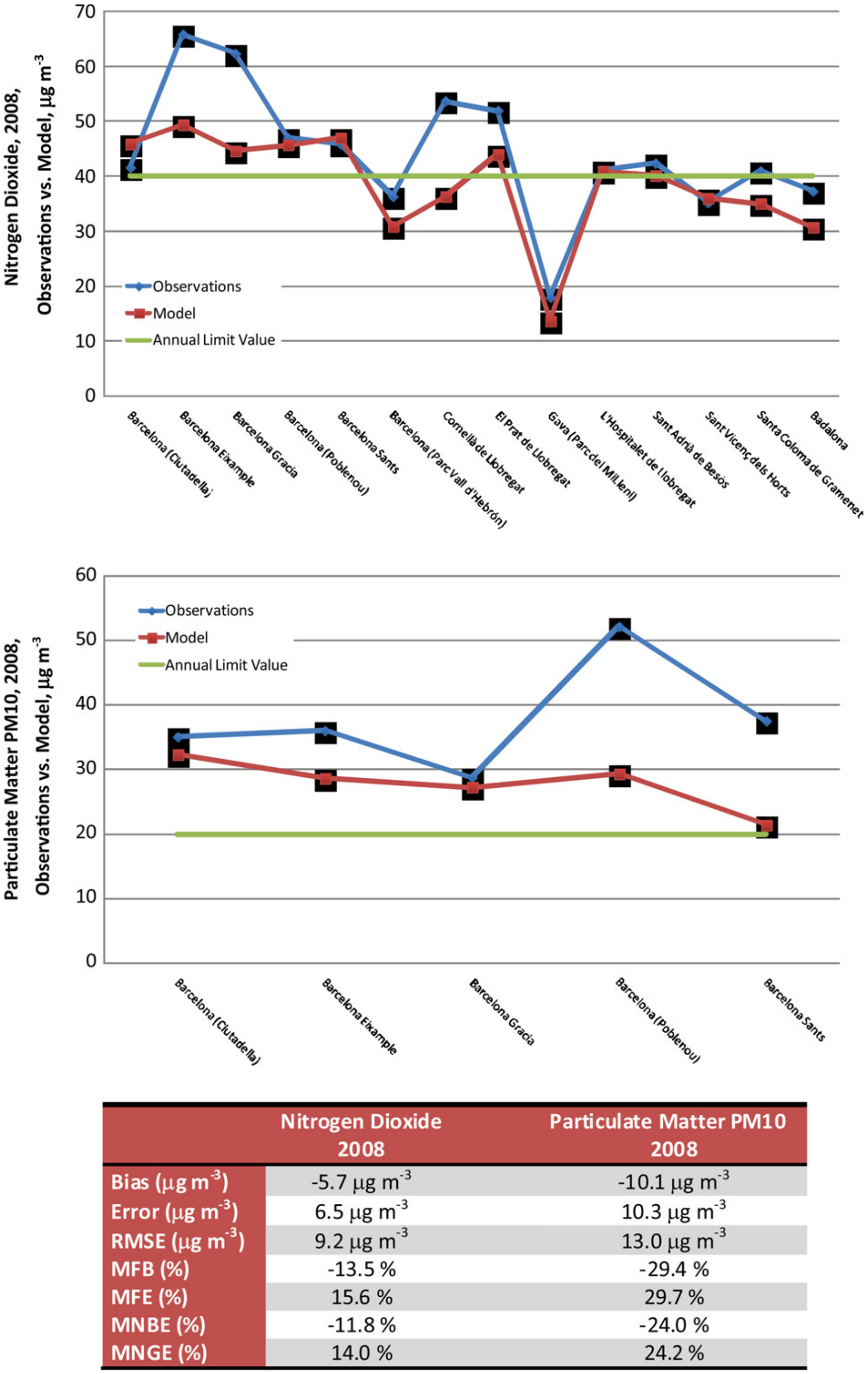
If the results of the evaluation are compared to the skill scores of previous works for several European models under the framework of the CityDelta project (Vautard et al., 2007; Cuvelier et al., 2007; Thunis et al., 2007), the modelling system used here exhibits consistent scores for NO_2. The high resolution applied in the area of study improves the results from previous studies (underestimations by 80% in the cited works); the errors obtained in this work for the entire conurbation are in the order of 10%. Also, the NO_2 correlation coefficient is 0.80 vs. 0.2–0.6 for the aforementioned studies. Last, for PM10, the results fully agree with previous works (biases of −20 to −50% vs. −24% for this work) and meet the goals and criteria established by Boylan and Russell (2006).

3.2. Speed limitation managing strategies in the area

The measure of speed limitation (80 km h^{-1}) is applied to the access roads of the Barcelona Metropolitan Area, formed by Barcelona and other 19 municipalities, with high levels of NO_x and PM10 emissions (Baldasano et al., 2008a,b). The maximum speed allowed in these roads was 100 km h^{-1} (in 63.2% of affected stretches) and 120 km h^{-1} in 20.4% of the considered stretches.

The population directly affected by the measure (that is, city dwellers adjacent to the roads where the limit of 80 km h^{-1} is implemented) is 1.35 million inhabitants, but 3.29 million dwellers potentially benefit from speed limitation. The measure involves the average reduction of speed in the indicated roads from 92 km h^{-1} to 78 km h^{-1}. On the contrary, the intensity of traffic has been similar for both years analyzed (47 859 daily average traffic – DAT – during January–August 2007 and 47 606 DAT in the period January–August 2008). For September–November there is a decrease in DAT of 5.9% (49 795 vs. 46 883 DAT for the years 2007 and 2008, respectively) which is partly caused by the economic crisis; this effect accumulates to the change due to the strategy for air quality management (speed limitation).

Therefore it should be highlighted that the differences in emissions and air quality are caused by the limitation of the speed and not because of modifications in the intensity of traffic. However, several monthly differences in the DAT (both increases and decreases) are caused by the temporal variation of holidays (Eastern, summer holidays, etc.) and their corresponding special traffic patterns.



	Nitrogen Dioxide 2008	Particulate Matter PM10 2008
Bias (μg m^{-3})	-5.7 μg m^{-3}	-10.1 μg m^{-3}
Error (μg m^{-3})	6.5 μg m^{-3}	10.3 μg m^{-3}
RMSE (μg m^{-3})	9.2 μg m^{-3}	13.0 μg m^{-3}
MFB (%)	-13.5 %	-29.4 %
MFE (%)	15.6 %	29.7 %
MNBE (%)	-11.8 %	-24.0 %
MNGE (%)	14.0 %	24.2 %

Fig. 2. Observations vs. modelled concentrations of nitrogen dioxide (top) and particulate matter PM10 (center) for the different air quality stations in the Barcelona Metropolitan Area; summary of the evaluation results for both pollutants (down).

The limitations of the speed together with the reduction in the congestion lead to a diminution in the fuel consumption (Fig. 3). The fuel consumption is reduced in 40.8 t day^{-1} for gasoline and 46.6 t day^{-1} for diesel; that is, an annual reduction of 4% in the Barcelona Metropolitan Area (over 30 000 tons of fuel per year). Since the CO_2 emissions are directly proportional to the fuel consumption, the reduction in the emission of this greenhouse gas by 4% is also important for a large city (over 94 000 tons per year). The peaks of the differences in Fig. 3 come conditioned by the dates of beginning and end of local holidays in the Barcelona Metropolitan Area, which are not coincident in consecutive years and involve a dense traffic. For instance, the date for the beginning of summer holidays is the same every year and therefore there are not such large differences during summertime from year to year; however, e.g. the dates for Eastern holidays varies from the year 2007–2008 and therefore,

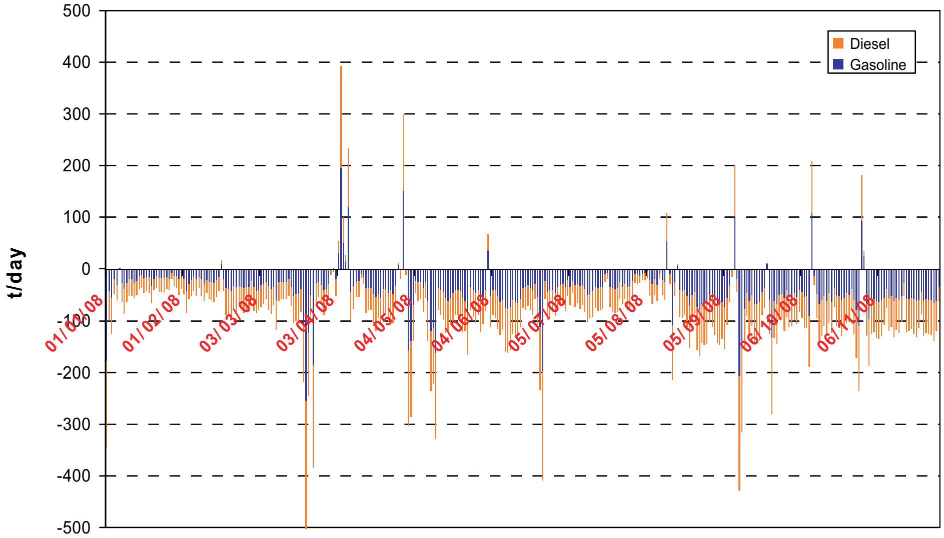


Fig. 3. Difference in the fuel consumption (year 2008–2007) for the Barcelona Metropolitan Area (tons per day).

one labor day for 2008 can coincide with a non-working day for 2007 (and viceversa).

The variation in the fuel consumption leads to a reduction in the emissions of primary pollutants in the whole metropolitan area by around 4% for NO_x, PM2.5, PM10, SO_2 and CO. As an example, for the nitrogen oxides, the emissions diminish in 1.85 t day^{-1} (4.36%). For the particulate matter (PM10) emissions are reduced in 0.13 t day^{-1} (3.95%). Fig. 4 indicates a very important local pattern; the main

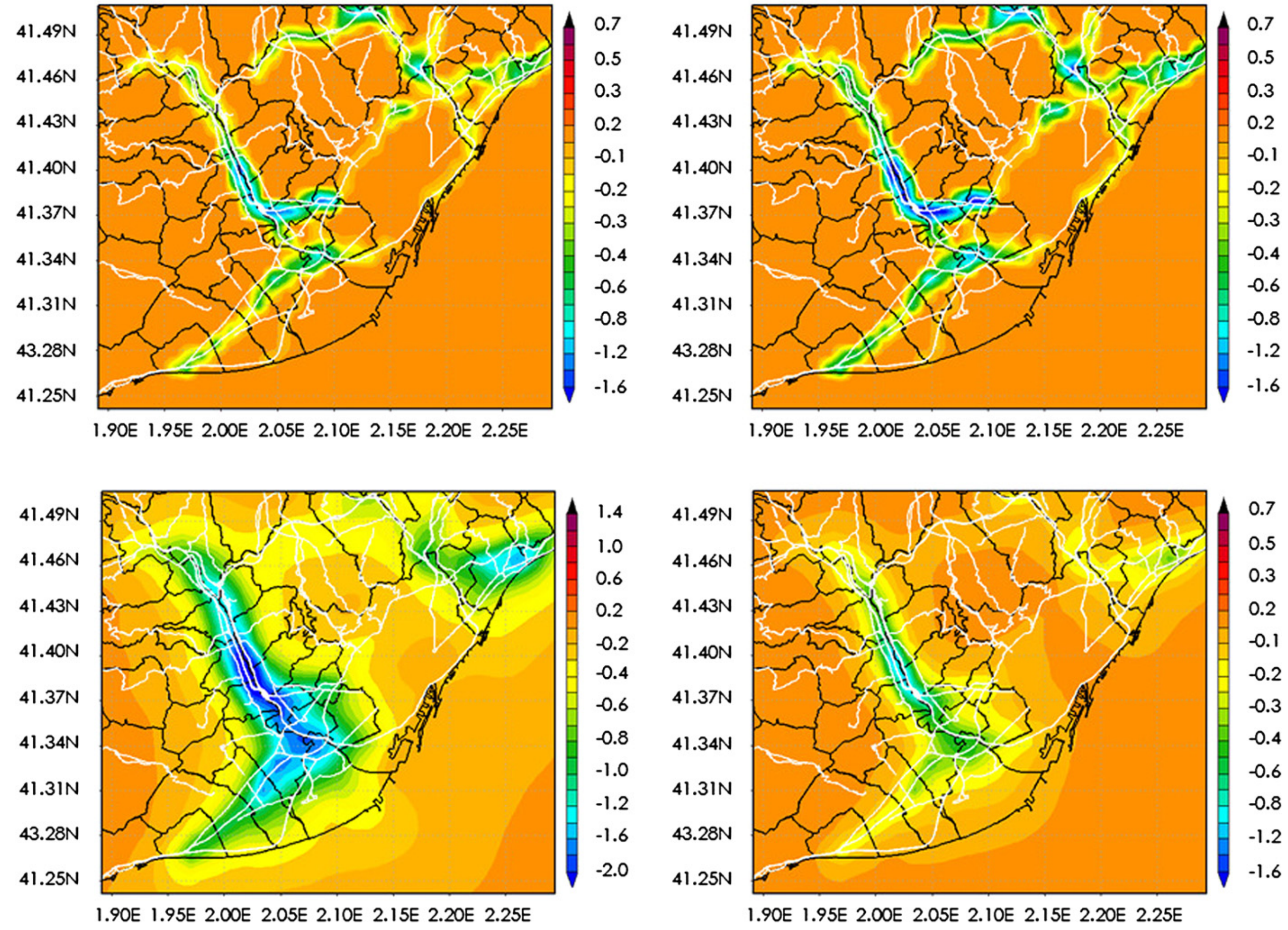
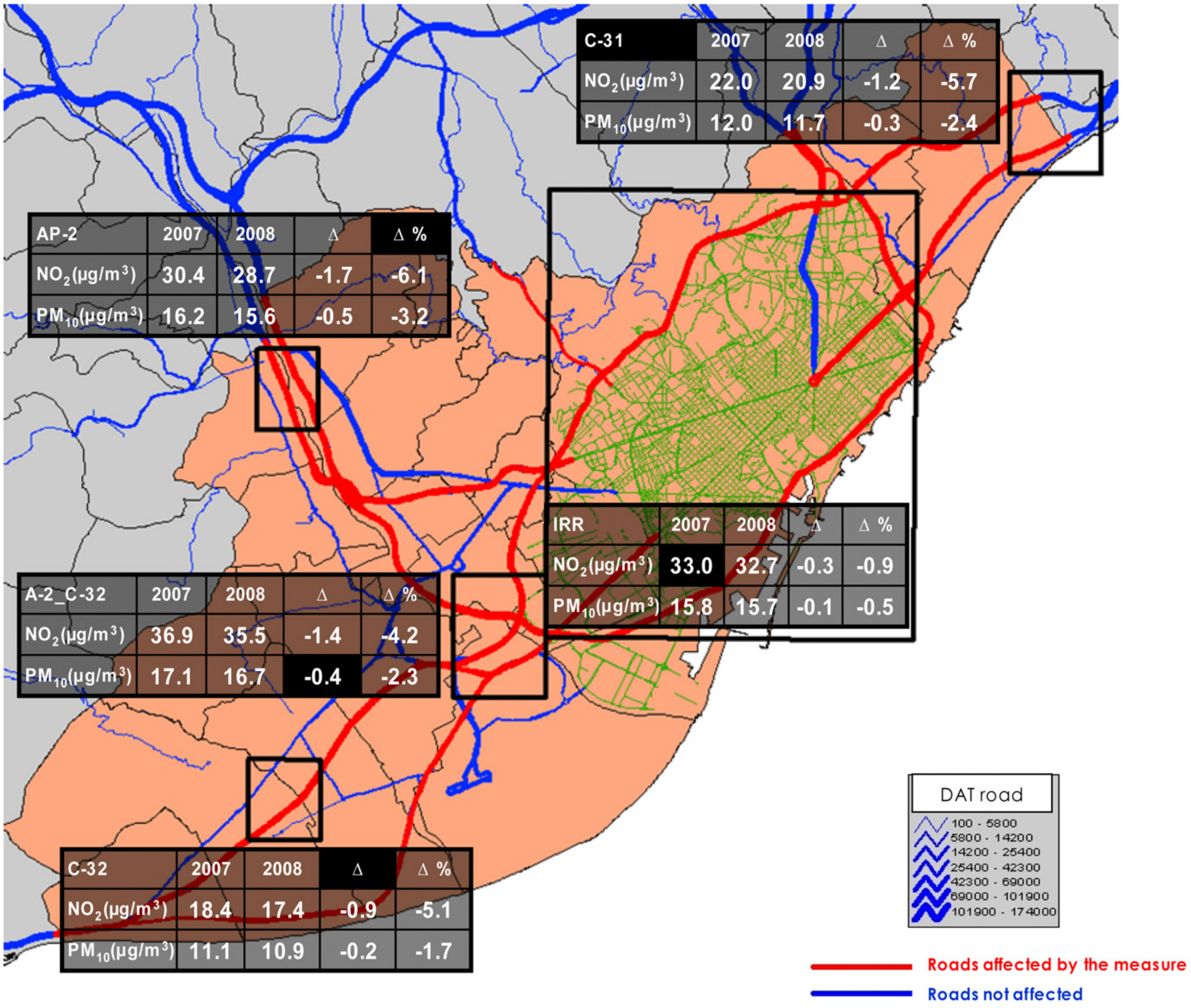


Fig. 4. (Up) Annual 2008–2007 difference in NO_2 (left) and PM10 (right) emissions (ton $year^{-1}$ $cell^{-1}$) estimated with HERMES emission model and (down) its corresponding impact on air quality; mean annual NO_x (left) and PM10 (right) differences (μg m^{-3}) in the domain of the Barcelona Metropolitan Area.

reductions of emissions are achieved over the access roads to the city of Barcelona.

If we consider just the areas with control of the circulation speed to 80 km h^{-1}, the fuel consumption reduces by about 10.4%. This also affects the emissions, which are reduced by 14.81% for CO, 10.98% for nitrogen oxides, 12.47% for PM2.5 and 10.99% for PM10.

Regarding air quality implications, the speed limitation involves a reduction in ground levels of atmospheric pollutants in the whole area where the measure is implemented. Specifically, the improvement of air quality is especially effective in the areas close to the access roads, as shown in Fig. 5, where 41.0% of the population of the Metropolitan Area lives. In order to have a better characterisation of the impacts of the management strategy on air quality, several domains have been defined according to the name of the road where they have been implemented: inside the Barcelona city ring roads (IRR), A2-C32, AP2, C31 and C32 (Fig. 5). The measure takes importance in the domains A2-C32, AP2, C31 and C32 where the levels of NO_x are reduced by 5–8% on average. For the particulate matter the reduction is around 3%. If trying to quantify the impacts on health and life expectancy, the aforementioned reduction decreases the mortality rates by around 0.6%, the number of deaths in the Metropolitan area (40 year^{-1}) and increases the life expectancy (0.15 months) according to some studies developed specifically for the area of interest (Pérez et al., 2009). Furthermore, the improvements in particulate matter-related air quality for several days may exceed 10–15%. The impacts of this latter reduction on health are noticeable, since a decrease of this magnitude in fine particulate matter levels may be associated with an estimated increase in mean life expectancy of 0.61 ± 0.20 year (Pope et al., 2009). Improvements for sulphur dioxide are lower (around 1%). Regarding tropospheric ozone chemistry, linking reductions of emissions of VOCs and NO_x to the concentrations of O_3 and other photochemical oxidants at a particular location and time is not straightforward (Finlayson-Pitts and Pitts, 1997). The NO_x emissions decrease in the city of Barcelona, which is a VOC-limited area (as shown by Jiménez and Baldasano, 2004), and therefore this reduction produces local increases of O_3 concentrations (Cohan et al., 2005; Liao et al., 2007), especially in the urban plume over the roads affected by the speed limit (up to 1%). Nevertheless the O_3 concentrations in downwind areas remain nearly constant. It is also noticeable how air quality is also improved in areas far from those roads where the speed limitation



C-31	2007	2008	Δ	Δ %
NO_2 (μg/m^3)	22.0	20.9	-1.2	-5.7
PM_{10} (μg/m^3)	12.0	11.7	-0.3	-2.4

AP-2	2007	2008	Δ	Δ %
NO_2 (μg/m^3)	30.4	28.7	-1.7	-6.1
PM_{10} (μg/m^3)	16.2	15.6	-0.5	-3.2

IRR	2007	2008	Δ	Δ %
NO_2 (μg/m^3)	33.0	32.7	-0.3	-0.9
PM_{10} (μg/m^3)	15.8	15.7	-0.1	-0.5

A-2_C-32	2007	2008	Δ	Δ %
NO_2 (μg/m^3)	36.9	35.5	-1.4	-4.2
PM_{10} (μg/m^3)	17.1	16.7	-0.4	-2.3

C-32	2007	2008	Δ	Δ %
NO_2 (μg/m^3)	18.4	17.4	-0.9	-5.1
PM_{10} (μg/m^3)	11.1	10.9	-0.2	-1.7

Fig. 5. Summary of the impacts on air quality (NO_2 and PM10) of the speed limitation measure for different areas of study within the Barcelona Metropolitan Area (in red, roads affected by the measure).

has not come into effect (IRR); here the air quality improvements are above 1%.

4. Conclusions

Our analysis of real circulation patterns by using traffic-assimilated data shows that the changes in emissions estimates range from 4% to 11% depending on the area studied. Consequently, the management strategy of speed limitation has local implications and therefore these results must be carefully extrapolated to other areas since they depend on the composition of the vehicular park and the number of circulating vehicles. If the analysis focuses on the affected roads, the reductions on primary pollutants reach up to 5–8% on 24-h average concentration, importantly improving the health and welfare of over 41% of the population of the Metropolitan Area. The NO_x emissions decrease in a VOCs limited area, such as Barcelona, and it produces local increases of O_3 concentrations, especially in the urban plume over the roads affected by the speed limit (lower than 1% in most cases); nevertheless the O_3 concentrations in downwind areas remain practically constant. The most positive effects of the management strategy are observed for CO, NO_x and PM2.5, with daily improvements in air quality reaching 10–15% and importantly affecting the life expectancy of the population. Furthermore, this study shows the importance of introducing traffic assimilation methodologies if speed limit scenarios or other management strategies are assessed in large cities or even megacities, highlighting the necessity of using hourly traffic data in emission model.

Acknowledgments

This work was funded by the Environmental Department of the Catalonia Government and CALIOPE project 157/PC08/3-12.0 of the Spanish Ministry of the Environment. Dr. Oriol Jorba and Dr. Carlos Pérez are acknowledged for the information provided and the fruitful discussions.

Appendix

The modelling system used for assessing the effects of the speed limitation measures in the study area consist in a set of meteorological, emission and chemistry-transport models included within the CALIOPE framework (Baldasano et al., 2008a,b). The Weather Research and Forecasting (WRF-ARW) model (Michalakes et al., 2005) provides the meteorology parameters as inputs to the Models-3 Community Multiscale Air Quality (CMAQ) chemistry-transport model (Byun and Schere, 2006). The WRF model represents a next-generation mesoscale numerical weather prediction system designed for operational forecasting needs. Initialization and boundary conditions for the mesoscale model were introduced with forecast data of the Global Forecast System of the National Center for Environmental Prediction (NCEP) at the standard pressure levels every 6 h. 366 simulations of 36 h have been performed (from 12 UTC of the previous day to the 00 UTC of the following day, with the aim of performing a cold initialization with 12 h of spin-up).

The High Elective Resolution Emission Modelling System (HERMES) has been developed specifically for Spain with a high resolution (1 km^2 – 1 h) and under a QA/QC protocol (Baldasano et al., 2008a,b) (Fig. 6). This model focuses on the estimation of gas and particulate matter pollutants, including the ozone precursors. HERMES (in its current version taking the year 2004 as calculation basis) considers the emissions from: (a) power generation plants, (b) industrial installations, (c) domestic and commercial fossil fuel use, (d) domestic and commercial solvents use, (e) road transport, (f) ports, (g) airports and (h) biogenic emissions. HERMES estimates the atmospheric emissions with a temporal resolution of 1 h and a spatial resolution of 1 km^2 and generates results according to the European Environmental Agency's Selected Nomenclature for Air Pollution (SNAP), which is the official activity classification system applied by the European Commission in the CORINAIR emission inventory. 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).

The traffic emissions module of HERMES (modified for implementing the speed limitation measures) considers fundamentally a bottom-up approach and takes into account 72 diesel and petrol vehicles categories (including Euro II and Euro III emission standards) according to COPERT III-EEA-EMEP/CORINAIR methodology (Nziachristos and Samaras, 2000; European Environmental Agency, 2006); divided by fuel type, vehicle weight, age of the vehicle and cubic capacity; each of them with its specific emissions factors, defined as a function of the circulation speed. The HERMES traffic module considers hot exhaust, cold exhaust and evaporative emissions. It also estimates particulate matter produced by brakes abrasion, tire wear and pavement erosion. The vehicular fleet is defined for Spain and specifically for Barcelona in this case of study using data provided by DGT (Spanish Department of Transportation, 2004), and distributed in the 72 aforementioned categories. The model includes the definition of the road network, dividing it in stretches (inside the 1 km^2 cells) with specific temporary disaggregating profiles (distinguishing day-type: weekday-holiday, and month), specific average speed, daily average traffic (number of vehicles per day), stretch length, route type (highway, road or urban) and circulation zones.

Concerning urban roads, the available information within HERMES covers the total road network for the Barcelona metropolitan area, and distinguishes five patterns of urban mobility. The road transport emissions are based on the daily average traffic (DAT) measured in over 2700 observation points throughout Barcelona and the circulation speed of each stretch, generating an attributed digital vector map with all the highways, freeways, important roads ($DAT > 200$) and urban streets. The original vector database information has been provided by Tele Atlas Multinet™ 2005. For the implementation of the 80 km h^{-1} limit, data coming from 125 measurement points have been assimilated within HERMES.

The WRF-ARW + HERMES + CMAQ + BSC-DREAM8b system was applied to the final study area with high spatial (1 km^2) and temporal (1 h) resolution. The use of fine resolution was demanded by the necessity of assessing the subtle air quality variations in urban areas; and in order to describe the transport and transformation of pollutants, as well as the dynamics on an hourly basis in very complex terrains (Jiménez et al., 2006). Four one-way nested domains were defined for the simulations, centring the final domain in Barcelona, which covers the north-eastern Iberian Peninsula (148×148 km^2) in order to assess not only the effects in the urban area, but also to detect the urban plume behaviour in downwind areas. The initial and boundary conditions for the CMAQ simulations were derived from a one-way nested simulation covering a domain of 1392×1104 km^2 centred in the Iberian Peninsula, which used EMEP emissions for the year 2004 and were disaggregated to 18 km. A 48-h spin-up was performed to minimize the effects of initial conditions for the innermost domain. The chemical mechanism selected for the simulations was Carbon Bond IV including aerosols and heterogeneous chemistry (Gery et al., 1989). The CMAQ model configuration uses the Yamartino-Blackman Cubic scheme (YAM) for the advection and convection transport and the Eddy diffusion scheme for the vertical and horizontal diffusion. The high resolution employed and the huge number of variables involved in the atmospheric integrations

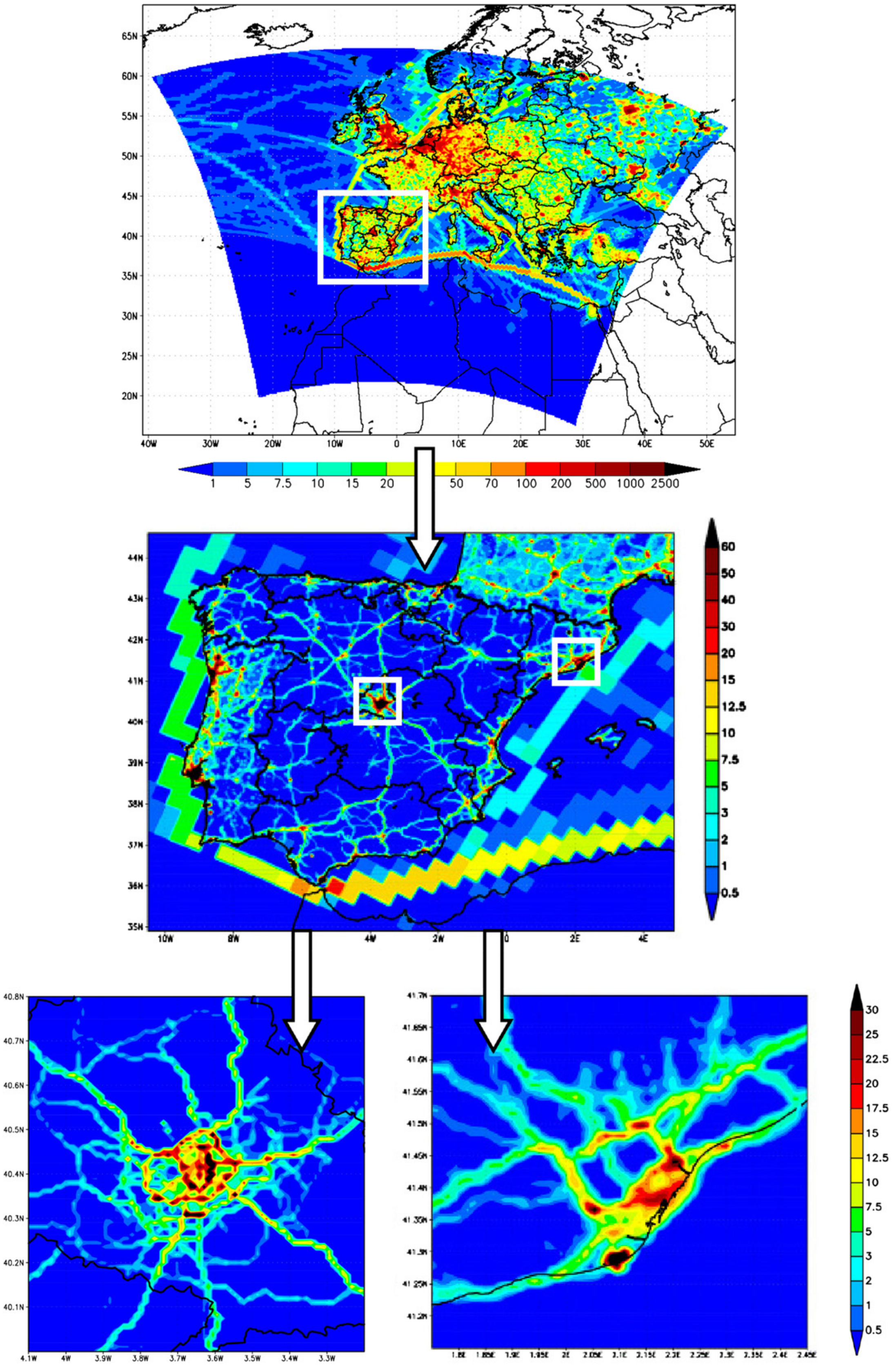


Fig. 6. Emissions implemented within the CALIOPE air quality modelling system: Europe (derived from EMEP and disaggregated to 12 km resolution, up); Iberian Peninsula (4-km resolution; estimated by HERMES for Spain and derived from EMEP for France, Portugal and maritime emissions and disaggregated to 4 km; center); and Madrid (down-left) and Barcelona (down-right) Greater Areas (calculated with HERMES).

requires high-performance computing. The availability of the MareNostrum supercomputer hold in the BSC–CNS, together with the advances in the parallelization of air quality codes, has allowed these simulations. For the integrations, 512 processors of MareNostrum have been used (64-bit), whose main features are: 94.21 Teraflops of theoretical performance peak; 10240 processors PowerPC 970 MP at 2.3 GHz (2560 JS21 blades); 20 TB of main memory; 390 + 90 TB of disk storage; Myrinet and Gigabit Ethernet interconnection networks.

The main assumptions of the modelling system are summarized below:

(a) Net transport: It considers the sum of horizontal and vertical advection, which is the transport of pollutants due to the mean wind fields. The advection scheme used is globally mass-conserving. The horizontal advection is estimated by the piecewise parabolic method (PPM) (Colella and Woodward, 1984) scheme, deriving a vertical velocity component at each grid cell that satisfies the mass continuity equation using the driving meteorology model's air density. The vertical advection module works with no mass-exchange boundary conditions at the bottom or top of the model.
(b) Gas phase chemistry. CBM-IV mechanism is used with the Euler Backward Iterative solver (Hertel et al., 1993).
(c) Diffusion: The diffusion involves sub-grid scale turbulent mixing of pollutants. Horizontal diffusion is estimated by a diffusion coefficient based on local wind deformation. Vertical diffusion is estimated using the Eddy diffusivity theory.
(d) Dry deposition: The deposition process is simulated as a flux boundary condition that affects the concentration in the lowest layer.
(e) Clouds chemistry and wet deposition: Clouds play a key role in aqueous chemical reactions, vertical mixing of pollutants and removal of pollutants by wet deposition. They also indirectly affect the concentration of pollutants by altering the solar radiation, which, in turn, affects photochemical pollutants, such as ozone, and the flux of biogenic emissions. CMAQ models sub-grid convective precipitating clouds, sub-grid non-precipitating clouds, and grid-resolved clouds. The cloud module vertically redistributes pollutants for the sub-grid clouds, calculates in-cloud and precipitation scavenging, performs aqueous chemistry, and accumulates wet deposition amounts. The used scheme is a RADM based cloud processor that uses the asymmetric convective model to compute convective mixing.
(f) Aerosols: The third generation aerosol module takes chemical species concentrations and reactivity rates from the chemistry solvers and primary particulate concentrations from the emissions processor to compute fine and coarse particulate concentrations. The primary aerosols emissions are estimated by HERMES, not taking into account marine aerosols. The deposition velocity for particles is estimated from the aerosol size distribution, which is calculated from the mass and number concentration for each of the modes considered: Aitken (0–0.1 μm), accumulation (0.1–2.5 μm), and coarse (2.5–10 μm).

Last, the 8-bins version of the Dust REgional Atmospheric Model (DREAM) (Nickovic et al., 2001) developed at the Barcelona Supercomputing Center (BSC-DREAM8b) provides the natural dust contribution to the air quality modelling system; further details about the coupling of CMAQ and DREAM can be found in Jiménez-Guerrero et al. (2008b). The model predicts the atmospheric life cycle of the eroded desert dust and was developed as a pluggable component of the Eta/NCEP (National Centers for Environmental Prediction) model. It solves the Euler-type partial differential nonlinear equation for dust mass continuity and it is fully inserted as one of the governing prognosis equations in the atmospheric Eta/NCEP atmospheric model equations. The model simulates all the major processes of the atmospheric dust cycle. One of the key components of the dust model is the treatment of the sourcing terms in the concentration continuity equation. Failure to adequately simulate/predict the production phase of the dust cycle leads to wrong representation of all other dust processes in the model. Therefore, special attention is made to properly parameterize dust production phase. Wind erosion in the emission scheme is controlled mainly by the following factors: type of soil, type of vegetation cover, soil moisture content, and surface atmospheric turbulence.

In the latest model version (BSC-DREAM8b) (Pérez et al., 2006a,b), grid points acting as desert dust sources are specified using arid and semiarid categories of the global USGS 1-km vegetation data set. Another data participating in dust production calculations is the FAO 4-km global soil texture data set from which particle size parameters are evaluated. Other schemes in the model have been updated: (1) Eight size transport bins between 0.1 and 10 μm are considered. In this interval, the aerosol effects on solar radiation are the most significant. Within each transport bin, dust is assumed to have time-invariant, sub-bin log-normal distribution employing the transport mode with mass median diameter of 2.524 μm and geometric standard deviation 2.0; (2) Dust affects the radiative fluxes at the surface and the top of the atmosphere and the temperature profiles at every model time step when the radiation module is processed. These changes influence the atmospheric dynamics, moisture physics, and near-surface conditions. Furthermore, dust emission is modified by changes in friction velocity and turbulent exchange coefficients; dust turbulent mixing, transport, and deposition are altered by changes in atmospheric stability, precipitation conditions, and free-atmosphere winds.

References

Akimoto, H., 2003. Global air quality and pollution. Science 302, 1716–1719.

Baldasano, J.M., Valera, E., Jiménez, P., 2003. Air quality data from large cities. Science of the Total Environment 307, 141–165.

Baldasano, J.M., Güereca, P., López, E., Gassó, S., Jiménez-Guerrero, P., 2008a. Development of a high resolution (1 km × 1 km, 1 h) emission model for Spain: the High-Elective Resolution Modelling Emission System (HERMES). Atmospheric Environment 42, 7215–7233.

Baldasano, J.M., et al., 2008b. CALIOPE: an operational air quality forecasting system for the Iberian Peninsula, Balearic Islands and Canary Islands – first annual evaluation and ongoing developments. Advances in Science and Research 2, 89–98.

Boylan, J.M., Russell, A., 2006. PM and light extinction model performance metrics, goals, and criteria for three-dimensional air quality models. Atmospheric Environment 40, 4946–4959.

Byun, D.W., Schere, K.L., 2006. Review of the governing equations, computational algorithms and other components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. Applied Mechanics Review 59, 51–77.

Carslaw, D., Beevers, S.D., 2005. Development of an urban inventory for road transport emissions of NO_2 and comparison with estimates derived from ambient measurements. Atmospheric Environment 39, 2049–2059.

Cohan, D.S., Hamaki, A., Hu, Y., Russell, A.G., 2005. Nonlinear response of ozone to emissions: source apportionment and sensitivity analysis. Environmental Science & Technology 39 (17), 6739–6748.

Colella, P., Woodward, P.L., 1984. The Piecewise Parabolic Method (PPM) for gas-dynamical simulations. Journal of Computational Physics 54, 174–201.

Colvile, R.N., Hutchinson, E.J., Mindell, J.S., Warren, R.F., 2001. The transport sector as a source of air pollution. Atmospheric Environment 35, 1537–1565.

Cuvelier, C., et al., 2007. CityDelta: a model intercomparison study to explore the impact of emission reductions in European cities in 2010. Atmospheric Environment 41, 189–207.

Dockery, D.W., Arden Pope, C., Xu, X., Spengler, J.D., Ware, J.H., Fay, M.E., Ferris, B.G., Speizer, F., 1993. An association between air pollution and mortality in six U.S. cities. New England Journal of Medicine 329, 1753–1759.

European Environmental Agency, 2006. EMEP-CORINAIR Emission Inventory Guidebook – 2006 (EEA Technical Report Report n° 11. /2006). Office for Official Publications of the European Communities, Luxembourg. http://reports.eea.europa.eu/EMEPCORINAIR4/en/page002.html.

Fenger, J., 1999. Urban air quality, 1999. Atmospheric Environment 33, 4877–4900.

Finlayson-Pitts, B.J., Pitts Jr., J.N., 1997. Tropospheric air pollution: ozone, airborne toxics, polycyclic aromatic hydrocarbons and particles. Science 276, 1045–1052.

Gery, M.W., Whitten, G.Z., Killus, J.P., Dodge, M.C., 1989. A photochemical kinetics mechanism for urban and regional scale computer modeling. Journal of Geophysical Research 94, 12925–12956.

Ghose, M.K., Paul, R., Banerjee, S.K., 2004. Assessment of the impacts of vehicular emissions on urban air quality and its management in Indian context: the case of Kolkata (Calcutta). Environmental Science & Pollution 7, 345–351.

Gonçalves, M., Jiménez-Guerrero, P., López, E., Baldasano, J.M., 2008. Air quality models sensitivity to on-road traffic speed representation. Effects on air quality of 80 km h^{-1} speed limit in the Barcelona Metropolitan area. Atmospheric Environment 42, 8389–8402.

Hertel, O., Berkowicz, R., Christensen, J., Hov, O., 1993. Test of two numerical schemes for use in atmospheric transport-chemistry models. Atmospheric Environment 27, 2591–2611.

Jiménez, P., Baldasano, J.M., 2004. Ozone response to precursor controls in very complex terrains: use of photochemical indicators to assess O_3–NO_x–VOC sensitivity in the northeastern Iberian Peninsula. Journal of Geophysical Research 109, D20309. doi:10.1029/2004JD004985.

Jiménez, P., Lelieveld, J., Baldasano, J.M., 2006. Multi-scale modeling of air pollutants dynamics in the north-western Mediterranean basing during a typical summertime episode. Journal of Geophysical Research 111, D18306.

Jiménez-Guerrero, P., Jorba, O., Baldasano, J.M., Gassó, S., 2008a. The use of a modelling system as a tool for air quality management: annual high-resolution simulations and evaluation. Science of the Total Environment 390, 323–340.

Jiménez-Guerrero, P., Pérez, C., Jorba, O., Baldasano, J.M., 2008b. Contribution of Saharan dust in an integrated air quality system and its on-line assessment. Geophysical Research Letters 35, L03814.

Keller, J., Andreani-Aksoyoglu, S., Tinguely, M., Flemming, J., Heldstab, J., Jeller, M., Zbinden, R., Prevot, A.S.H., 2008. The impact of reducing the maximum speed limit on motorways in Switzerland to 80 km h^{-1} on emissions and peak ozone. Environmental Modelling and Software 23, 322–332.

Lelieveld, J., et al., 2002. Global air pollution crossroads over the Mediterranean. Science 298, 794–799.

Lenschow, P., Abraham, H.J., Kutzner, K., Lutz, M., Preu, J.D., Reinchenbacher, W., 2001. Some ideas about the sources of PM10. Atmospheric Environment 35, 123–133.

Liao, K.-J., Tagaris, E., Manomaiphiboon, K., Napelenok, S.L., Woo, J.-H., He, S., Amar, P., Russell, A.G., 2007. Sensitivities of ozone and fine particulate matter formation to emissions under the impact of potential future climate change. Environmental Science & Technology 41 (24), 8355–8361.

Michalakes, J., Dudhia, J., Gill, D., Henderson, T., Klemp, J., Skamarock, W., Wang, W., 2005. In: Zwiehofer, W., Mozdzynski, G. (Eds.), Proceedings of the Eleventh ECMWF Workshop on the Use of High Performance Computing in Meteorology, pp. 156–268.

Molina, M.J., Molina, L.T., 2004. Megacities and atmospheric pollution. Journal of the Air & Waste Management Association 54, 644–680.

Nel, A., 2005. Air pollution-related illness: biomolecular effects of particles. Science 308, 804–806.

Nickovic, S., Papadopoulos, A., Kakaliagou, O., Kallos, G., 2001. Model for prediction of desert dust cycle in the atmosphere. Journal of Geophysical Research 106, 18113–18129.

Nziachristos, L., Samaras, Z., 2000. Computer Programme to Calculate Emissions from Road Transport. Methodology and Emission Factors (Version 2.1) (Tech. Rep. N. 49). European Environmental Agency.

Pérez, L., Sunyer, J., Künzli, N., 2009. Estimating the health and economic benefits associated with reducing air pollution in the Barcelona metropolitan area. Gaceta Sanitaria 23, 287–294.

Pérez, C., Nickovic, S., Baldasano, J.M., Sicard, M., Rocadenbosch, F., Cachorro, V.E., 2006a. A long Saharan dust event over the western Mediterranean: Lidar, Sun photometer observations, and regional dust modelling. Journal of Geophysical Research 111, D15214. doi:10.1029/2005JD006579.

Pérez, C., Nickovic, S., Pejanovic, G., Baldasano, J.M., Özsoy, E., 2006b. Interactive dust-radiation modeling: a step to improve weather forecasts. Journal of Geophysical Research 111, D16206. doi:10.1029/2005JD006717.

Ponche, J.L., Vinuesa, J.F., 2005. Emission scenarios for air quality management and applications at local and regional scales including the effects of the future European emission regulation (2015) for the upper Rhine valley. Atmospheric Chemistry and Physics 5, 999–1014.

Pope, C.A., Dockery, D.W., 2006. Health effects of fine particulate air pollution: lines that connect. Journal of the Air & Waste Management Association 56, 709–742.

Pope, C.A., Ezzati, M., Dockery, D.W., 2009. Fine-particulate air pollution and life expectancy in the United States. New England Journal of Medicine 360, 376–386.

Querol, X., Alastuey, A., Rodríguez, S., Plana, F., Ruiz, C.R., Cots, N., Massagué, G., Puig, O., 2001. PM10 and PM2.5 source apportionment in the Barcelona Metropolitan Area, Catalonia, Spain. Atmospheric Environment 35, 6407–6419.

Rodríguez, S., Querol, X., Alastuey, A., Viana, M., 2003. Events affecting levels and seasonal evolution of airborne particulate matter concentrations in the Western Mediterranean. Environmental Science & Technology 37 (2), 216–222.

Schultz, M.G., Diehl, T., Brasseur, G.P., Zittel, W., 2003. Air pollution and climate-forcing impacts of a global hydrogen economy. Science 302, 624–627.

Spanish Department of Transportation, 2004. Statistical Data in the Number of Vehicles and Fuel Used for the Year 2004. http://www.dgt.es/portal (in Spanish).

Stephens-Romero, S., Carreras-Sospedra, M., Brouwer, J., Dabdub, D., Samuelsen, S., 2009. Determining air quality and greenhouse impacts of hydrogen infrastructure and fuel cell vehicles. Environmental Science & Technology 43 (23), 9022–9029.

Thunis, P., et al., 2007. Analysis of model responses to emission-reduction scenarios within the CityDelta project. Atmospheric Environment 41, 208–220 (207).

US EPA, 2005. Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-hour Ozone NAAQS. US EPA Report No. EPA-454/R-05-002. Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina, US, October; 2005, 128 pp.

Vautard, R., Bessagnet, B., Chin, M., Menut, L., 2005. On the contribution of natural Aerolian sources to particulate matter concentrations in Europe: testing hypothesis with a modelling approach. Atmospheric Environment 39, 3291–3303.

Vautard, R., et al., 2007. Evaluation and intercomparison of ozone and PM10 simulations by several chemistry transport models over four European cities within the CityDelta Project. Atmospheric Environment 41, 173–188.

Viana, M., Pérez, C., Querol, X., Alastuey, A., Nickovic, S., Baldasano, J.M., 2005. Spatial and temporal variability of PM levels and composition in a complex summer atmospheric scenario in Barcelona (NE Spain). Atmospheric Environment 39, 5343–5361.

Wang, Y., Logan, J.A., Jacob, D.J., 1998. Global simulation of tropospheric O_3–NO_x–hydrocarbon chemistry, 2., model evaluation and global ozone budget. Journal of Geophysical Research 103, 10727–10755.