Real time air quality forecasting systems for industrial plants and urban areas by using the MM5-CMAQ-EMIMO

R. San José[1], J. L. Pérez[1], J. L. Morant[1] & R. M. González[2]
[1]*Environmental Software and Modelling Group,*
Computer Science School, Technical University of Madrid (UPM),
Campus de Montegancedo, Boadilla del Monte 28660 Madrid, Spain
[2]*Department of Meteorology and Geophysics, Faculty of Physics,*
Complutense University of Madrid; Ciudad Universitaria,
28040 Madrid, Spain

Abstract

During the last five years, we have been working intensively with the new generation of air quality modeling systems such as MM5-CMAQ (PSU/NCAR/EPA, US) and using our own emission model, EMIMO (UPM, 2006), the first version of which was developed several years ago and is in the process of continuous adaptation. Recently we have incorporated an adapted version of the CFD model MIMO (University of Karlsruhe, 2000) which includes a sophisticated cellular traffic model, CAMO (UPM, 2006), to model street level pollution with the numerical Eulerian models approach with a few meters of spatial resolution. The integrated system formed by an adapted version of MIMO and CAMO is called MICROSYS. The mesoscale air quality model MM5-CMAQ-EMIMO produces air concentrations in real-time and forecasting mode for urban and regional areas with 1 km spatial resolution. The MICROSYS model is implemented to simulate the air concentrations in one 1 km grid cell with 5–10 m spatial resolution and up to 200–300 m in height (over the maximum building heights in the 1 km grid cell). The MICROSYS model is run in diagnostic mode and uses the boundary and initial conditions from MM5-CMAQ-EMIMO. The system MM5-CMAQ-EMIMO-MICROSYS produces reliable air quality forecasts for urban areas with street level detail over the Internet. In this contribution we will show the special example applied to Las Palmas (Canary Islands, Spain). Additionally, the MM5-CMAQ-EMIMO has been used to find the air quality impact of several industrial plants such as combined cycle power and cement plants. The system uses sophisticated cluster technology to take advantage of distributed and shared memory machines in order to perform the parallel runs in an efficient and optimal way since the process should operate on a daily basis. We will also show the methodology and results of these applications in two industrial complexes in the surrounding area of Madrid City.

WIT Transactions on Ecology and the Environment, Vol 116, © 2008 WIT Press
www.witpress.com, ISSN 1743-3541 (on-line)
doi:10.2495/AIR080241

1 Introduction

There has been an increased interest in managing and controlling the air quality in regional and urban areas during the last five years. The interest in understanding and knowing the air quality over large domains and with high temporal and spatial resolution is growing rapidly together with the interest in knowing the relative quantitative and qualitative impacts on a specific area (grid) and time. The advances in air quality modeling have been substantial in the past decade. The third generation of air quality modeling systems use the so-called "one-atmosphere" approach which means that the dispersion and chemical transformation of the different pollutants emitted to the atmosphere is treated in an integrated and unique way. The first approaches – first and second generation – are related to the treatment of point emissions insolated from the surrounding atmosphere. The third generation of air quality modeling systems is representing the reality that occurs in the transport and transformation of chemical pollutants in a more realistic way. The further development of these models will move to integrate the effects of water and other ecosystems and feedback effects on the atmosphere and vice versa. The increase in computer power generated in the last 20 years has contributed substantially to this parallel advance in knowledge and efficiency.

The information technology progress has played an essential role in this spectacular advance in air quality modeling systems. Since the computer power required to run the complex FORTRAN codes which are developed to incorporate the complexity of the atmospheric dynamics is phenomenal, the technology involved to carry out complex air quality impact assessments and furthermore the real-time and forecasting application is quite important.

The cluster approaches open new scenarios for many applications and particularly in the atmospheric dynamics simulations. The atmospheric models have also reached highly sophisticated levels that include the simulation of the aerosol processes and cloud and aqueous chemistry. These models include sophisticated land use information and deposition/emission models [10]. The atmospheric models traditionally include two important modules: a) meteorological modeling and b) transport/chemistry modules. These two modules work in a full complementary mode, so that the meteorological module provides full 4D datasets (3D wind components, temperature and specific humidity) to the transport/chemistry modules. CPU time is mainly used for transport/chemistry (75%). This modeling system requires important initial and boundary data sets to simulate properly specific time periods and spatial domains, such as landuse data, digital elevation model data, global meteorological data sets, vertical chemical profiles and emission inventory data sets. In this experiment we have used AVN (NCEP/NOAA, USA) global meteorological information as input for the MM5 meteorological model. The emission inventory for the proper spatial domain and for the specific period of time (at high spatial and temporal resolution) is possibly the most delicate input data for the sophisticated meteorological/transport/chemistry models. The accuracy of emission data is much lower than the accuracy of the numerical methods used for solving the partial differential equation systems (Navier–Stokes equations) for meteorological models [5] and the ordinary differential equation system for the chemistry module [9–11]. Typical uncertainty associated to emission data is 25–50%. However, in our application it is more important to see the relative impact of the industrial emissions in the mesoscale domain – where the tested industrial plant is located – than to quantify and qualify the absolute pollutant concentrations in the atmosphere due to the emission uncertainty.

The emission inventory is a model that provides in time and space the amount of a pollutant emitted to the atmosphere. In our case we should quantify the emissions due to traffic, domestic sources, industrial and tertiary sector and also the biogenic emissions in the three model domains with 9 km, 3 km and 1 km spatial resolution. The mathematical procedures to create an emission inventory are essentially two: a) Top-down and b) Bottom-up. In reality a nice combination of both approaches offers the best results. Because of the high non-linearity of the atmospheric system, due to the characteristics of the turbulent atmospheric flow, the only possibility to establish the impact of the part of the emissions (due to traffic or one specific industrial plant, for example) in air concentrations, is to run the system several times, each time with a different emission scenario.

Examples of "state-of-the-art" meteorological models are: MM5 (PSU/NCAR, USA), RSM (NOAA, USA), ECMWF (Redding, U.K.), HIRLAM (Finnish Meteorological Institute, Finland), etc. Examples of "state-of-the-art" of transport/chemistry models – also called "third generation of air quality modeling systems" – are: EURAD (University of Cologne, Germany), [13], EUROS (RIVM, The Netherlands), (Langner et al. [7]), EMEP Eulerian (DNMI, Oslo, Norway), MATCH (SMHI, Norrkoping, Sweden), [2], REM3 (Free University of Berlin, Germany), [14], CHIMERE (ISPL, Paris, France), [12], NILU-CTM (NILU, Kjeller, Norway), [3], LOTOS (TNO, Apeldoorm, The Netherlands), [8], DEM (NERI, Roskilde, Denmark), [4], STOCHEM (UK Met. Office, Bracknell, U.K.), [1]. In USA, CAMx Environ Inc., STEM-III (University of Iowa) and CMAQ model are the most up-to-date air quality dispersion chemical models. In this application we have used the CMAQ model (EPA, U.S.) which is one of the most complete models and includes aerosol, cloud and aerosol chemistry.

The OPANA system is an air quality modelling system developed in the 90's by the Environmental Software and Modelling Group of the Computer Science School of the Technical University of Madrid (ESMG-FI-UPM). The system is used in forecasting and historical modes. The system includes different state-of-the-art mesoscale meteorological and chemical transport models such as MM5 and/or CMAQ. In the 90's the meteorological module was the MEMO model (University of Karslruhe (Germany), 1994) and the chemistry was included on-line in the meteorological model by using the CBM-IV scheme [6,7]. Further versions of the model included MM5 and CMAQ as part of the meteorological module and chemistry transport module. The system includes and emission model, EMIMO, which has also different version which includes biogenic and anthropogenic emissions with different updated version of the global or

European emission database. Actually, OPANA V4 includes a sophisticated CFD code (based on the MIMO model (University of Karslruhe (Germany), 1996)), which runs in diagnostic mode over a 1 km x 1 km model domain over highly dense populated areas in cities (Madrid, Las Palmas de Gran Canaria, etc.). The CFD code is called MICRFOSYS and has a resolution 1-10 m receiving traffic emission data from a sophisticated cellular automata model (CAMO) – also developed by the ESMG-FI-UPM. This CFD code receives the initial and boundary conditions from the mesoscale part of the model (typically MM5-CMAQ-EMIMO). OPANA V3 is used in several forecasting applications for urban and industrial sites but it does not include the CFD part. The CMAQ model is implemented in a consistent and balanced way with the MM5 model [4]. The CMAQ model is fixed "into" the MM5 model with the same grid resolution (MM5 grid cells are used at the boundaries for CMAQ boundary conditions). The system can be implemented in any domain over the world. As an example a domain architecture is shown in Figure 1. MM5 is linked to CMAQ by using the MCIP module which is providing the physical variables for running the dispersion/chemical module (CMAQ) such as boundary layer height, turbulent fluxes (momentum, latent and sensible heat), boundary layer turbulent stratification (Monin-Obukhov length), friction velocity, scale temperature, etc. We have run the modeling system (MM5-CMAQ) with USGS 1 km landuse data and GTOPO 30'' for the Digital Elevation Model (DEM). The system uses EMIMO model (EMIssion Model) to produce every hour and every 1 km grid cell the emissions of total VOC's (including biogenic), SO_2, NO_x and CO. This model uses global emission data from EMEP/CORINAIR European emission inventory (50 km spatial resolution) and EDGAR global emission inventory (RIVM, The Netherlands). In addition the EMIMO model uses data from DCW (Digital Chart of the World) and USGS land-use data from AVHRR/NOAA 1 km satellite information. The EMIMO model includes a biogenic module (BIOEMI) developed also in our laboratory based on the algorithms for natural NO_x, monoterpene and isoprene emissions in function of LAI (leaf Area Index) and PAR (photosintetic active radiation).

2 Results

Different applications have been carried out over different domains and emission sources. We show different applications: (1) Different simulations to know the air quality impact of a combined cycle power plant in Madrid area; (2) Similar application than in Madrid (Spain) area but in Andalusia (Spain); (3) A study of the impact of the emissions of an incinerator in the Basque Country (Spain) and (4) A real-time air quality forecasting system for Las Palmas de Gran Canaria (Canary Islands, Spain).

2.1 Combined cycle power plant in Madrid domain

In this section we show results for an application over Madrid domain designed for a specific study of the impact of a future power plant construction for different years. Several studies of this type have already been conducted at different areas in the Iberian Peninsula for different industrial type plants as mentioned above. In Figure 1 we showed the scheme designed for the study in the Madrid domain. Similar architecture has been used for different areas. Figure 2 shows the comparison between observed and modelled data in the Alcalá monitoring station in Madrid Community (Spain) for the year 2005. We observe that the comparison is excellent, particularly if we consider that the maximum concentration in this particular period of time (July, 9–15, 2005) is quite important. Values near 200 μgm^{-3} are found for 12th of July 2005. The modelled data and observed data are particularly satisfactory. On 14th of July, during the night time the model reproduces values higher than observed.

Figure 3 shows the impact at 15:00 GMT on July 25, 2006 for ozone concentrations. The map is produced by making the differences between ON and OFF scenarios, so that the only difference between both scenarios is the air concentrations produced as consequence of the emissions of the power plant. The nonlineal process in the atmosphere produces increases (4%) and decrease (28,5%) in the air concentrations. The changes are important hour per hour, so that, a real-time air pollution system is considered essential in order to control the important changes due to the atmospheric dynamics and chemical process.

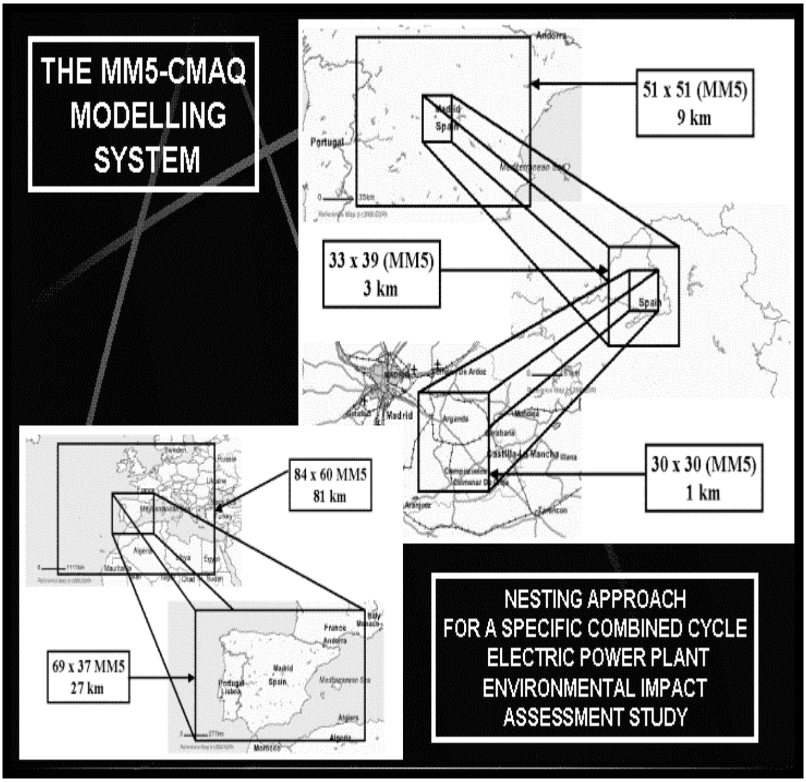

Figure 1: MM%_CMAQ-EMIMO modelling architecture for use in forecasting and historical modes.

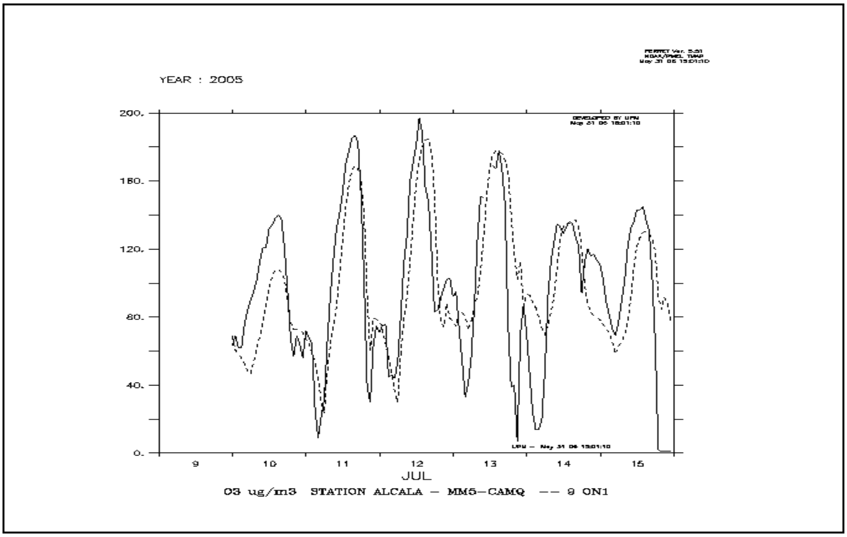

Figure 2: Comparison between observed and modelled ozone data for Alacalá monitoring station in Madrid Community area (located about 35 km east of the Madrid metropolitan area). The comparison between both data sets is particularly good taking into account the high values observed during such a period of time.

These results show an excellent agreement between observations and modeling results in the calibration phase (before running the simulations adding the emissions from the planned industrial power plant). This agreement is essential for the reliability of the final results although the differences between the concentrations in ON and OFF modes are the most important relative results in these types of studies. We should underline that the amount of information obtained for a typical air quality impact study of an industrial and power plant for 120 hours periods along 12 month a year and for five criteria pollutants, 3 different nesting levels (9 km, 3 km and 1 km) produces an amount of information (every hour analysis) of about 5 Gbytes and 400000 images (examples are shown in this contribution). The whole system should be controlled by the corresponding scripts running in automatic mode over several weeks in different PC platforms. In real-time mode we should carefully design our architecture (generally over a cluster platform) and assure that the simulations of ON, OFF and all emission reduction scenarios (X%) run on a daily basis for a period of 120 hours and obtain the differences between ON and X% runs with OFF mode to obtain the best performance emission reduction scenario for the next 48–72 hours. The X% emission reduction scenarios are simulated by applying this emission reduction over the last 48–72 hours. This operational architecture requires – as we said – cluster platforms. Our tests over a cluster with 20 nodes (2,4 GHz.) and one main PC (with 2,4 GHz) show a speed increase of about 10 times. This test was performed at a cluster in the University of Iowa (USA).

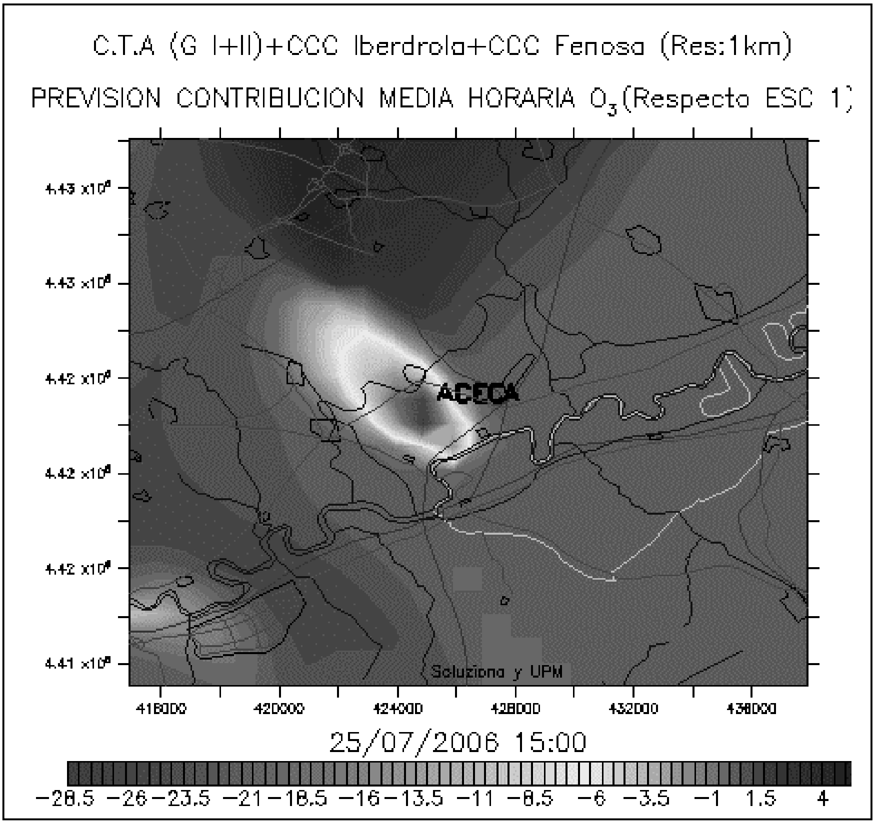

Figure 3: The map shows the impact of the emissions of the power plant by making the differences between ON and OFF scenarios for ozone on July 25, 2006 at 15:00.

2.2 Combined cycle power plant in Andalusia (South of Spain)

Similar cases have been performed for air quality impact assessment studies in Andalucia (Huelva area)

2.3 Incinerator in Basque Country (North of Spain)

In this particular air quality impact study we had to modify the CMAQ model to implement a dioxin/furna models together with the implementation of metals and B[a]P. Figure 4 shows an example of the calibration process in Basque Country (Spain). The comparison shows a good pattern between both data sets.

2.4 Real-time and forecasting application: urban application in Las Palmas de Gran Canaria (Canary Islands, Spain)

Finally, a real-time and forecasting application by using MM5-CMAQ is shown in this section. The system is mounted in our laboratory and provides the air quality forecasts through the Internet under daily basis by using a specific script automatic programme. In Figure 5 we observe the internal web presentation for the city of Las Palmas de Gran Canaria, which is accessed internally by the environmental experts in the Municipality of Las Palmas de Gran Canaria under daily basis. The model and the web interface are located in our laboratory in Madrid (Spain).

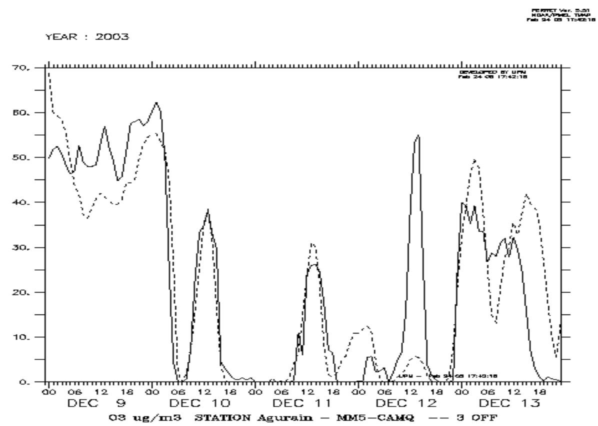

Figure 4: Comparison between O_3 observed and modeled data for Agurain monitoring station (Basque Country, Spain).

3 Conclusions

In this contribution we have shown several applications and studies by using the sophisticated MM5-CMAQ modeling system. The system has been proved to be very robust and reliable. The results assure us that it is possible to have in real-time and forecasting mode tools over the Internet that provide air quality impact forecasts for different industrial plants and urban areas and take emission reduction actions on time. Further work is currently under development to determine the best strategy to identify the best emission reduction strategies based on air quality forecasts.

In the case of industrial plants the complete switch off of the emissions for a period of 24–48 hours is the best possible solution assuming that the impact of the emissions of the industrial plant is the main cause of exceedance of the EU legislative concentration limits (or any other world legislation). In the case of urban areas, the situation is much more complex since different emission sources and spatial locations should be studied and identify to take the optimal emission reduction strategy decision. This can only be accomplished by increasing the number of model runs by using massively the cluster approach.

The system has been proved to be reliable and suitable to identify the impact in space and time of different air pollutants in real-time and forecasting mode. Further work should be done to improve the quality of the emission inventory to optimize the agreement between observations and simulations.

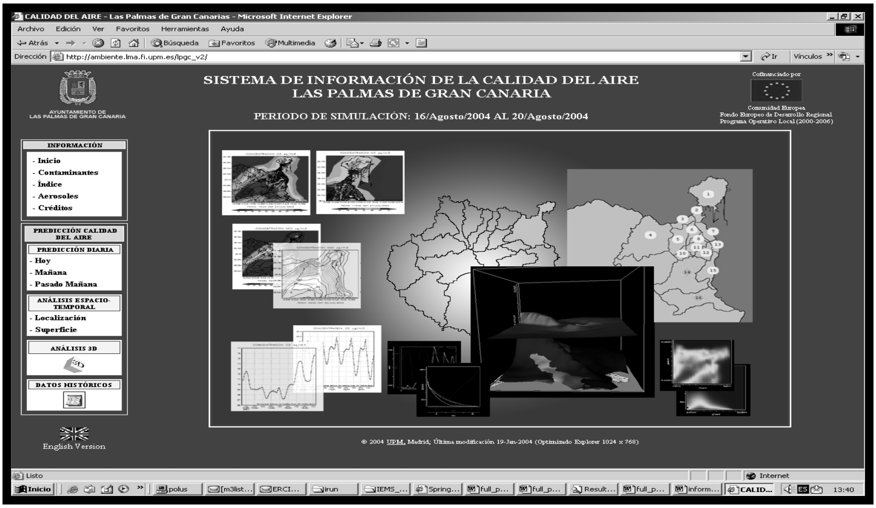

Figure 5: Home portal of the air quality forecasting system for the city of Las Palmas (Canary Islands, Spain).

Acknowledgements

We would like to thank Professor Dr. Daewon Byun formerly at Atmospheric Modeling Division, National Exposure Research Laboratory, U.S. E.P.A., Research Triangle Park, NC 27711 and currently Professor at the University of Houston, Geoscience Department for providing full documentation of CMAQ and help. We would also like to thank to U.S.E.P.A. for the CMAQ code and PSU/NCAR for MM5 V3.0 code. Also, we would like to thank Soluziona S.A. for funding this project.

References

[1] Collins W.J., D.S. Stevenson, C.E. Johnson and R.G. Derwent, Tropospheric ozone in a global scale 3D Lagrangian model and its response to NOx emission controls, *J. Atmos. Chem.* **86** (1997), 223–274.

[2] Derwent R., and M. Jenkin, Hydrocarbons and the long-range transport of ozone and PAN across Europe, *Atmospheric Environment* 8 (1991), 1661–1678.

[3] Gardner R.K., K. Adams, T. Cook, F. Deidewig, S. Ernedal, R. Falk, E. Fleuti, E. Herms, C. Johnson, M. Lecht, D. Lee, M. Leech, D. Lister, B. Masse, M. Metcalfe, P. Newton, A. Schmidt, C Vandenberg and R. van Drimmelen, The ANCAT/EC global inventory of NOx emissions from aircraft, *Atmospheric Environment* **31** (1997), 1751–1766.

[4] Gery M.W., G.Z. Whitten, J.P. Killus and M.C. Dodge, A photochemical kinetics mechanism for urban and regional scale computer modelling, *Journal of Geophysical Research* **94** (1989), D10, 12925–12956.

[5] Grell, G.A., J. Dudhia and D.R. Stauffer, A description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5), NCAR/TN- 398+ STR. *NCAR Technical Note*, 1994.

[6] Jacobson M.Z. and R.P. Turco, SMVGEAR: A sparse-matrix, vectorized GEAR code for atmospheric models, *Atmospheric Environment* **28**(1994), 2, 273–284.

[7] Langner J., R. Bergstrom and K. Pleijel, European scale modeling of sulfur, oxidized nitrogen and photochemical oxidants. Model development and evaluation for the 1994 growing season, *SMHI report RMK No. 82*, Swedish Met. And Hydrol. Inst., SE-601 76 Norrkoping, Sweden, (1998).

[8] Roemer M., G. Boersen, P. Builtjes and P. Esser, *The Budget of Ozone and Precursors over Europe Calculated with the LOTOS Model*. TNO publication P96/004, Apeldoorn, The Netherlands, 1996.

[9] San José R., L. Rodriguez, J. Moreno, M. Palacios, M.A. Sanz and M. Delgado, Eulerian and photochemical modelling over Madrid area in a mesoscale context, *Air Pollution II, Vol I., Computer Simulation, Computational Mechanics Publications, Ed. Baldasano, Brebbia, Power and Zannetti,* 1994, 209–217.

[10] San José R., J. Cortés, J. Moreno, J.F. Prieto and R.M. González, Ozone modelling over a large city by using a mesoscale Eulerian model: Madrid case study, *Development and Application of Computer Techniques to Environmental Studies, Computational Mechanics Publications, Ed. Zannetti and Brebbia,* 1996, 309–319.

[11] San José, R., J.F. Prieto, N. Castellanos and J.M. Arranz, Sensitivity study of dry deposition fluxes in ANA air quality model over Madrid mesoscale area, *Measurements and Modelling in Environmental Pollution,* Ed. San José and Brebbia, 1997, 119–130.

[12] Schmidt H., C. Derognat, R. Vautard and M. Beekmann, A comparison of simulated and observed ozone mixing ratios for the summer 1998 in Western Europe, *Atmospheric Environment* **35** (2001), 6277–6297.

[13] Stockwell W., F. Kirchner, M. Kuhn and S. Seefeld, A new mechanism for regional atmospheric chemistry modeling, *J. Geophys. Res.* **102** (1977), 25847–25879.

[14] Walcek C., Minor flux adjustment near mixing ration extremes for simplified yet highly accurate monotonic calculation of tracer advection, *J. Geophys. Res.* **105** (2000), 9335–9348.