The Use of Air Quality Modelling Systems for Industrial and Urban Impact Assessment in Spain

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Abstract. The use of complex air quality modeling systems such as MM5-CMAQ is illustrated in this contribution. We have mounted and applied the system for air quality impact assessment studies and also for real-time and forecasting information services with high performance and excellent results. In this contribution we will show the results of several examples of application of the system over cities and industrial plants in historical mode (impact assessment studies) and real-time and forecasting modes. The system provide a full description of the air concentrations in time and space in the urban domain and in the surrounding areas of the industrial plants such as combined cycle power plants and incinerators.

1 Introduction

The advances in air quality modeling have been substantial in the last 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 and integrated and unique way. The first approaches – first and second generation – are related to the treatment of point emissions insolated of the surrounding atmosphere. The third generation of air quality modeling systems is representing the reality which 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 viceversa. 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 on this spectacular advance in air quality modeling systems. Because 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 on the atmospheric dynamics simulations. The atmospheric models have also reached high sophisticated levels which includes the simulation of the aerosol processes and cloud and aqueous chemistry. These models include sophisticated land use information and deposition /emission models [1]. The atmospheric models include traditionally two important modules: a) meteorological modelling 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 (70 – 80 %). This modelling system require 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 [2] and the ordinary differential equation system for the chemistry module [3], [4], [1]. 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.

The emission inventory is a model which 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 mentioned above. 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 modelling systems" – are: EURAD (University of Cologne, Germany), [5], EUROS (RIVM, The Netherlands), [6], EMEP Eulerian (DNMI, Oslo, Norway), MATCH (SMHI, Norrkoping, Sweden), [7], REM3 (Free University of Berlin, Germany), [8], CHIMERE (ISPL, Paris, France), [9], NILU-CTM (NILU, Kjeller, Norway), [10], LOTOS (TNO, Apeldoorn, The Netherlands). [11]. DEM (NERI. Roskilde. Denmark). [12]. STOCHEM (UK Met. Office. Bracknell. U.K.). [13]. In USA. CAMx Environ Inc., STEM-III (University of Iowa) and CMAQ (EPA. US) 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.

2 The MM5-CMAQ Modeling System

The CMAQ model (Community Multi-scale Air Quality Modelling System. EPA. US) is implemented in a consistent and balanced way with the MM5 model [12]. The CMAQ model is fixed "into" the MM5 model with the same grid resolution (6 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 showed in Figure 1. MM5 is linked to CMAQ by using the MCIP module which is providing the physical variables for running the dispersio/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 to produce every hour and every 1 km grid cell the emissions of total VOC's (including biogenic). SO2. NOx and CO. EMIMO is a emission model developed at our laboratory in 2001. 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 (EMIssion Model) 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 NOx. monoterpene and isoprene emissions in function of LAI (leaf Area Index) and PAR (photosintetic active radiation).

In Figure 2 we see a scheme of the computer platform needed to simulate different emission reduction scenarios in case of exceeding the pollution levels stated at the legislative directives (L282/69. 26.10.2001).

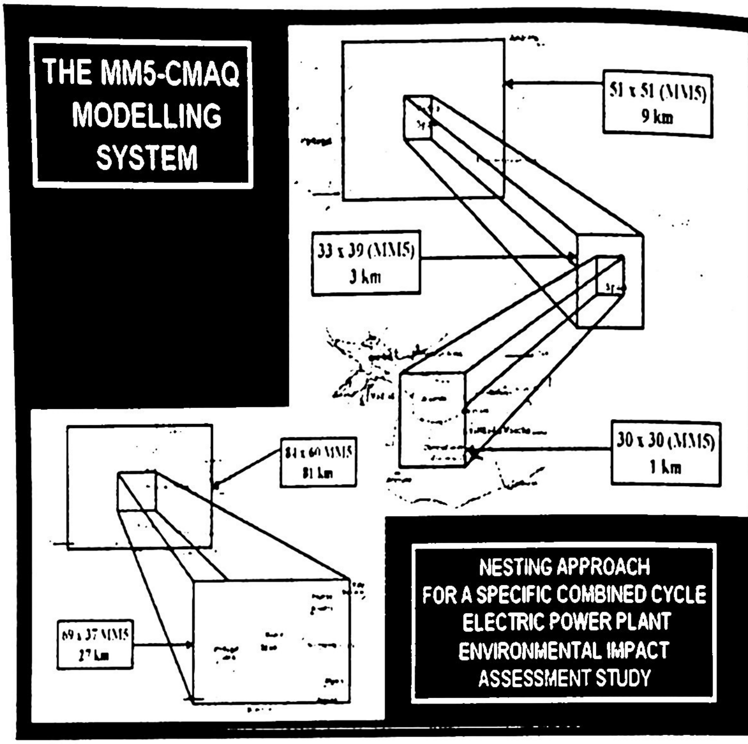

Fig. 1. MM5-CMAQ architecture for this experiment

Each emission scenario involves to run a complete version of the model which differs from others only on the tested emission reduction so that in the case of industrial plants, we have an OFF scenarios which represents to run the model with the complete emission set (provided by EMIMO) but "without" the emissions from the industrial plant and the so-called ON scenario represents to run the model with exactly the same emissions as in the OFF scenario but "with" the expected hourly emissions from the industrial plant. Obviously the differences between ON and OFF represent the impact of the industrial emissions in the pollutant concentrations. A similar approach can be applied for any emission source which we would like to analyze (traffic flow, domestic emissions, etc.).

In order to run these complex systems, a single PC seems to be quite limited because the required CPU time exceeds the available time for daily operational application. It is possible to use cluster platforms to reduce significantly the amount of computer time required for the different simulations. Figure 3 shows a scheme for the case of having a cluster with 6 nodes and how the model domain is divided. For running the MM5-CMAQ modeling system in the cluster platform, we use the cluster version of both modules. The only possible alternative is probably the cluster, with an acceptable cost/benefit relation to run such a complex systems. Particularly in the case shown in this contribution, where the modeling system should be run in ON and OFF scenario but additional scenarios (to be compared each other or with the base case, OFF) can be included but much more CPU time will be required. We are working under an architecture of daily operation so that the CPU limit time is formally 24 hours but in practice (because the CMAQ CPU time depends on the maximum wind speed – Courant Law-), 18-20 CPU hours is a realistic limit.

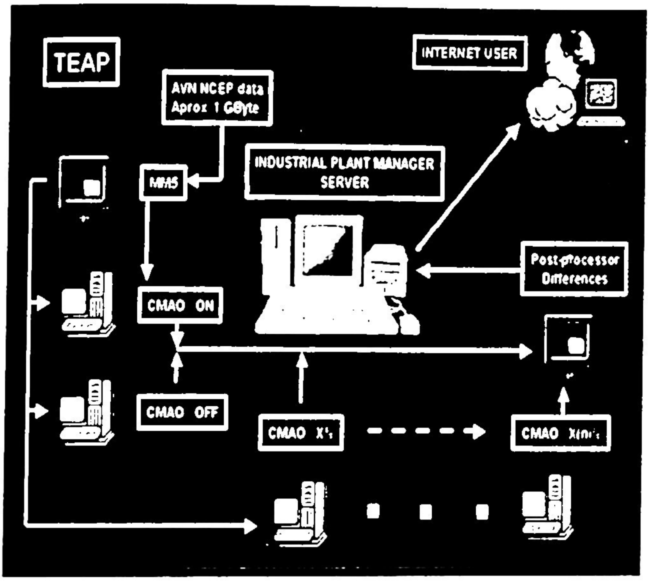

Fig. 2. TEAP Computer platform scheme

The results over platforms of about 20 nodes provide increases of time of about 10- 11 times for both modules (meteorological and chemical/transport). This rate is highly satisfactory but it may probably be increased by using faster connection architectures between PC's. The MM5-CMAQ modeling system constitutes a reliable and robust software tool which allows a historic and on-line operational simulation over any domain at global scale with several different nesting capabilities and approaches. MM5 is used by several states in USA for weather forecasts and in Europe it is used by several meteorological Institutes as a research code and also for operational applications. In our lab, MM5 has been used (http://artico.lma.fi.upm.es) for operational weather forecasts – provided in the Internet – since year 2000 with reliable results.

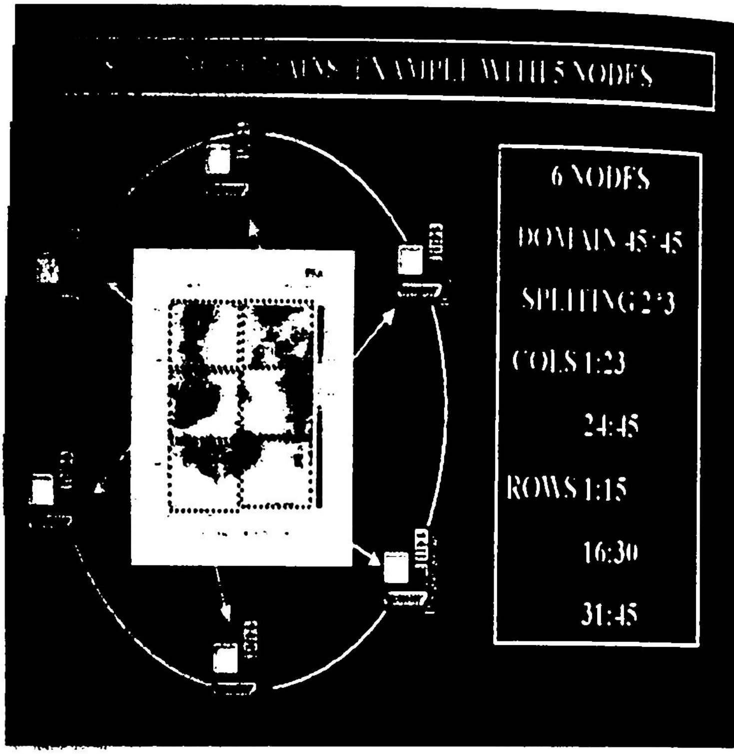

Fig. 3. Cluster platform with 6 nodes for TEAP application

The code has shown an extraordinary performance without any problems along these years. We have been using CMAQ since 2001 and – although this model was originally more unstable -, nowadays, the last version are very stable and robust. We have used the CMAQ model (and MM5) for carrying out several air quality assessment studies for incinerators (Basque Country (Spain, 2003)) and future combined cycle power plant installations with excellent performance. Also the system is being used in operational and forecasting mode in Canary Islands (Las Palmas de Gran Canaria, Spain) for the city authorities (http://ambiente.lma.fi.upm.es/lpgc_v2). The modular architecture allows to use several different numerical schemes for different atmospheric processes. This modularity allows to evaluate the different physical and chemical schemes and how they are simulated by the modelling tools.

The MM5-CMAQ modelling system allows to evaluate the impact on the air quality for different pollutant concentrations at different levels (surface and up to several layers in height, typically and in this experiment 23 layers, up to 100 mb) and for different physical and chemical processes such as: a) XYADV: Advection in the E-W and N-S direction; b) ZADV: vertical advection; c) ADJC: mass adjustment for advection; d) HDIF: horizontal diffusion; e) VDIF: vertical diffusion; f) EMIS: emissions: g) DDEP: dry deposition: h) CHEM: chemistry: i) CLDS: cloud processes in aqueous chemistry. The system can provide a detailed information of the impact on the production or loss of several criteria pollutants for the different physical and chemical processes described. This information can be provided for every grid cell and for every specific time step for the simulation period.

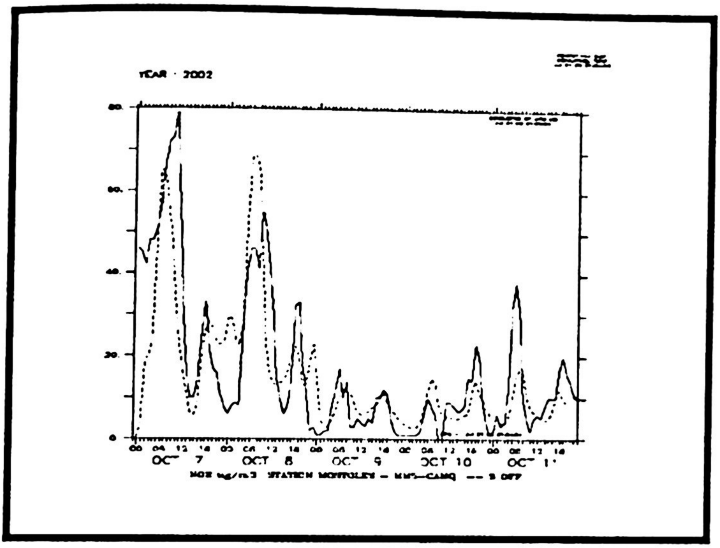

Fig. 4. Comparison between observed NO2 concentrations at the monitoring station in Móstoles (Madrid, Spain) and modelled NO2 concentrations by MM5-CMAQ at the grid cell where the monitoring station is located (MM5-CMAQ with 3 km spatial resolution)

The MM5 – CMAQ, in this application, has been configured to use CBM-IV [12] chemical scheme for organic reactions, and the SMVGEAR [14] numerical scheme for solving the chemistry. More than 75 % of the computer time is devoted to solve the chemical scheme (more then 90 chemical reaction and 40 species).

3 Results and Discussion

Different applications have been carried out over different domains and emission sources. In this contribution we will show particularly some examples over combined cycle power plants which required an air quality impact assessment before starting to operate and also the case of several incinerators in the Basque Country area in the north of Spain.

3.1 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. 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. In Figure 4 we observe the comparison between observed NO2 concentrations at the monitoring station in Móstoles (Madrid, Spain) and modelled NO2 concentrations by MM5-CMAQ at the grid cell where the monitoring station is located (MM5-CMAQ with 3 km spatial resolution). Figure 5 shows the surface ozone concentration differences over a domain of 27 x 33 grid cells (3 km) centered at the planned power plant. The planned power plat emissions are incorporated to the system in ON scenario under the maximum impact mode i.e. the expected maximum hourly emissions produced by the power plant (worst scenario).

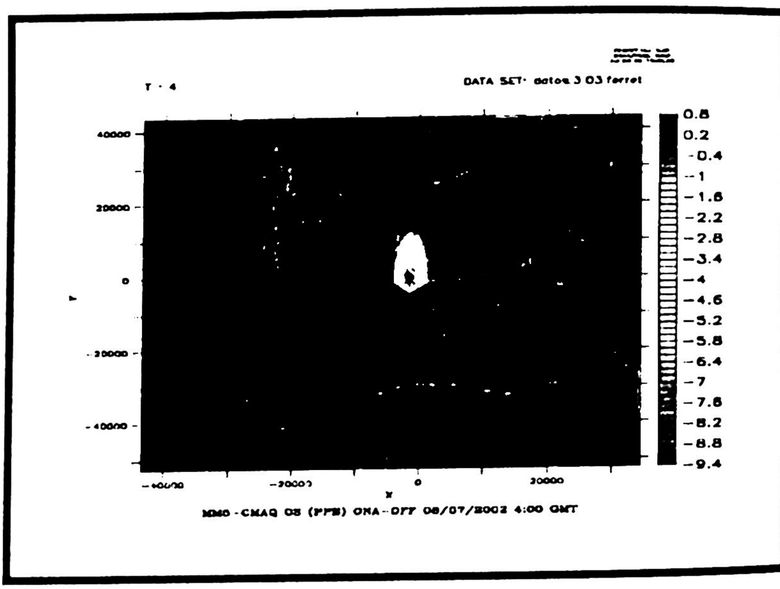

Fig. 5. Surface concentration differences over a domain of 27 x 33 grid cells (3 km) centered at the planned power plant. Differences between ozone concentrations (ppb) in OFF mode and with the planned power plant emissions at 4h00 (GMT) on July, 8, 2002

These results show an excellent agreement between observations and modelling 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 on 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 under daily basis for 120 hours period 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 an increase on the speed of about 10 –11 times. This test was performed at a cluster in the University of Iowa (USA).

3.2 Combined Cycle Power Plant in Andalusia (South of Spain)

In this section we will show results of an application over an existing combined cycle power plant in the Andalusia area (South of Spain). The domain is defined as shown in Figure 6. In Figure 7 we show a 3D image of the 9 km spatial resolution model domain. In Figure 8 we show an example of the calibration process which compares modeling results with measured values from the different air quality monitoring stations located in the model domain.

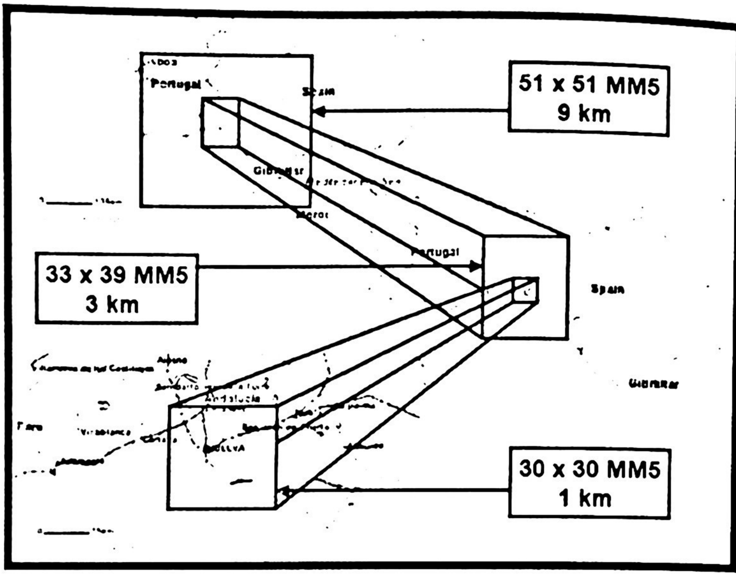

Fig. 6. Domain architecture for the study carried out over the combined cycle power plant in the Andalusia area (South of Spain)

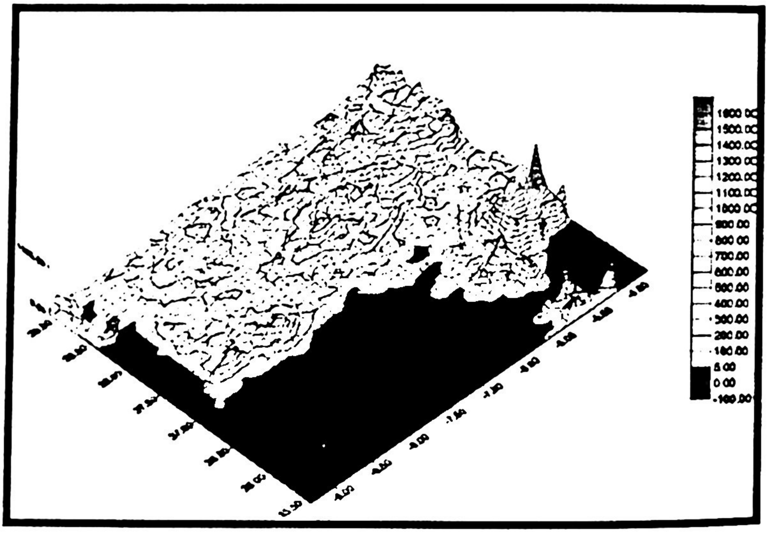

Fig. 7. 3D topography corresponding to the 9 km spatial resolution model domain

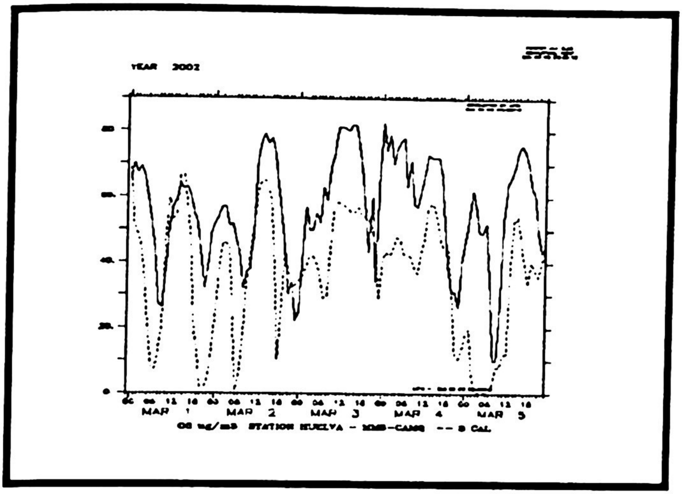

Fig. 8. Comparison between ozone concentrations measured at station Manuel Lois and the modelling concentrations in the 3 km spation resolution domain in OFF mode and for the period March, 1-5, 2002

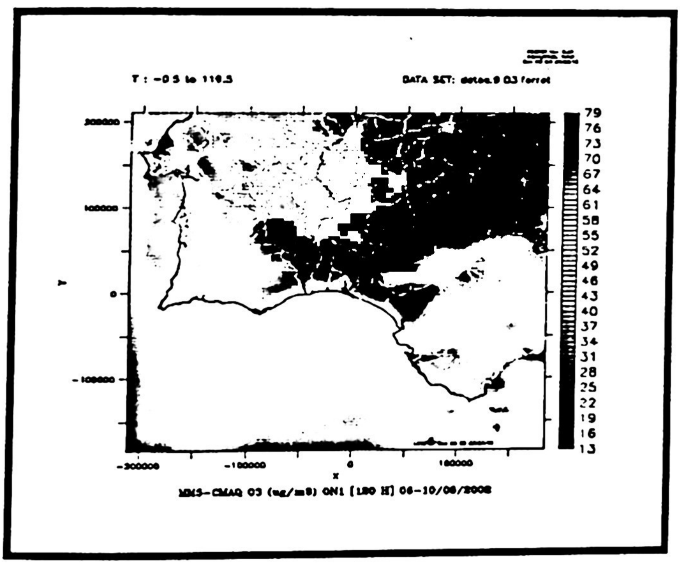

Fig. 9. Total O3 concentrations when operating one combined cycle power plant group, averaged over 120 hours for 6-10, August, 2002

3.3 Incinerator in Basque Country (North of Spain)

Another application has been carried out over an incinerator project in the Basque Country in Spain. Figure 10 shows the architecture model domain.

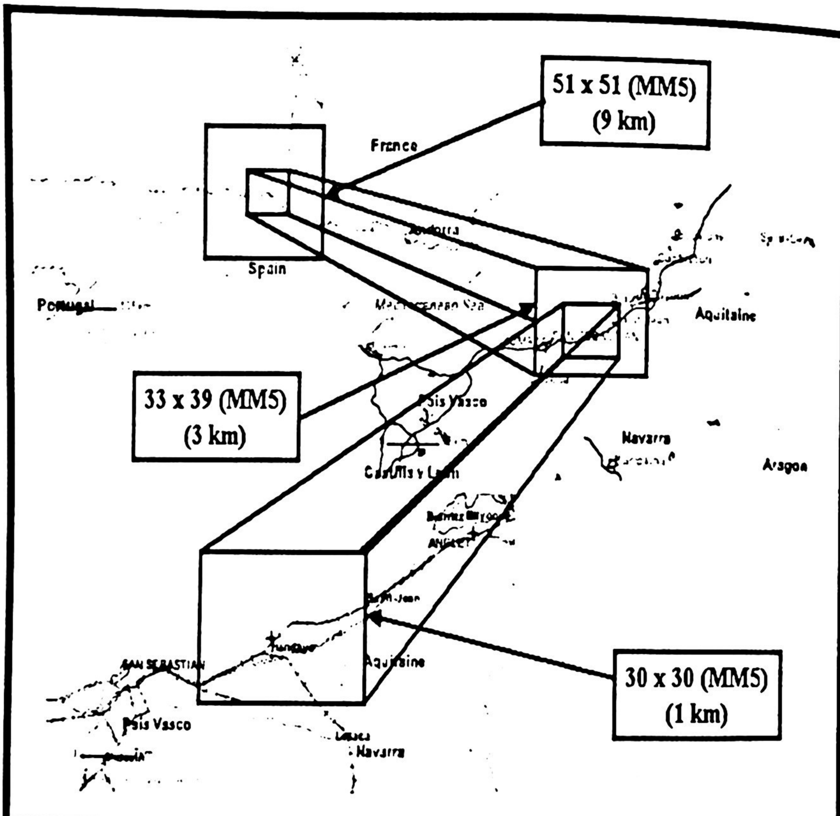

Fig. 10. Architecture model domain for the application of the MM5-CMAQ modeling system for air quality impact assessment of an planned incinerator

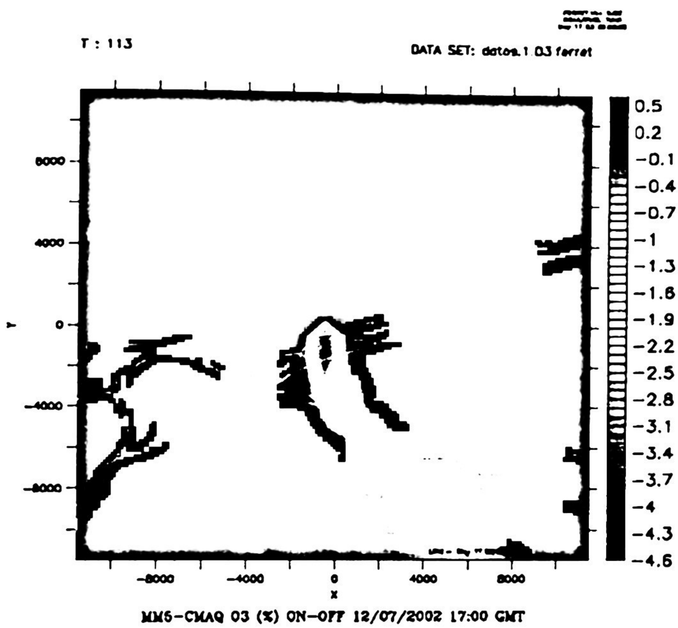

Fig. 11. Percentage of reduction in ozone concentrations due to the expected emissions (maximum mode) of the planned incinerator over the 1k spatial resolution model domain (24 x 24 km) at 17h00 GMT on July. 12, 2002

3.4 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 12 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).

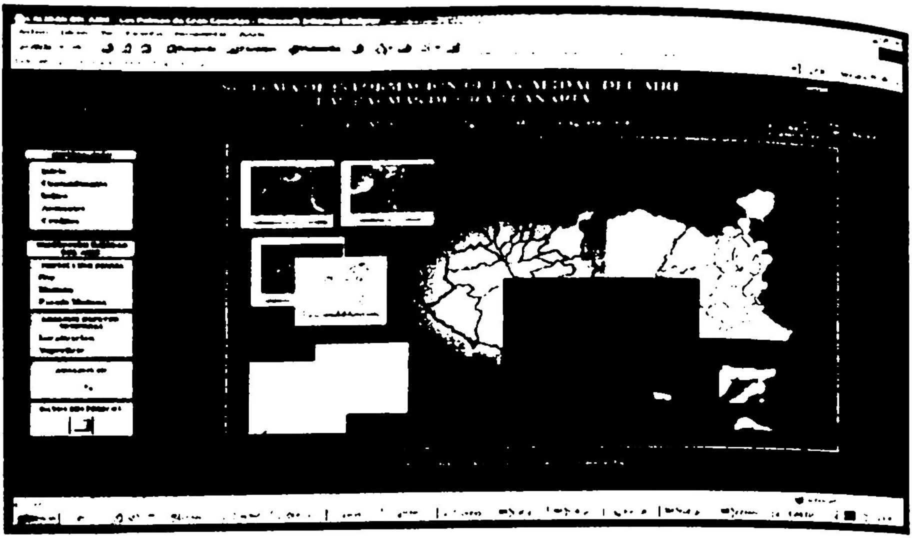

Fig. 12. Air Quality forecasts in Las Palmas de Gran Canaria provided by the MM5-CMAQ modeling system under daily basis through the web

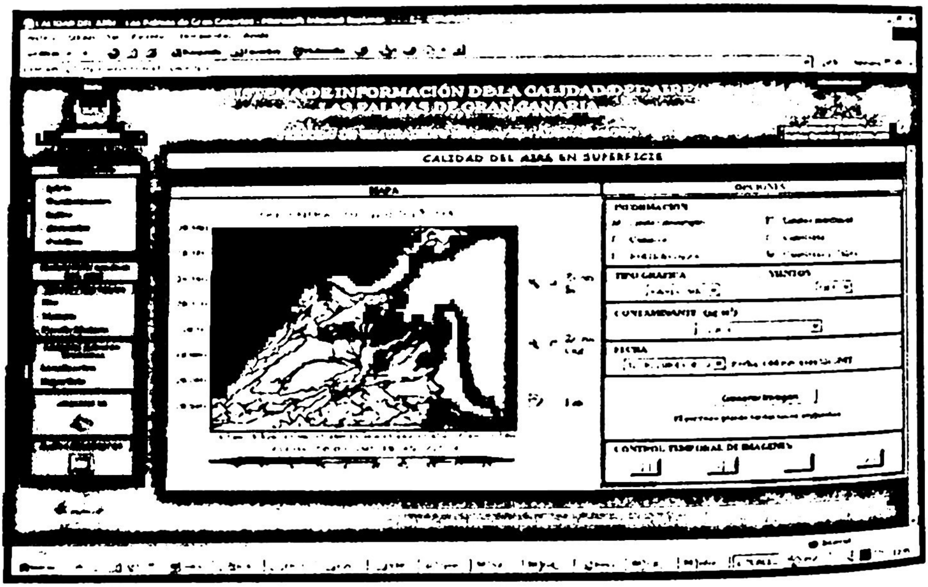

Fig. 13. Example of surface O3 concentrations at 08h00 GMT on August, 18, 2004 as provided through the web

4 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 that it is possible to have in real-time and forecasting mode tools over the Internet which provides 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.

Acknowledgements

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