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Abstract: A tool (TEAP) to evaluate in real-time and operational mode the air quality produced by industrial plants (power plants also) has been developed based on the third generation of air quality modelling systems. The system uses the non-hydrostatic mesoscale meteorological model MM5 (PSU/NCAR, USA) and the air quality modelling system (transport and chemistry) CMAQ (Community Multiscale Air Quality Modelling System) (EPA, USA) by using the so-called ON/OFF scenario which allows the user to have in advance (48 - 72 hours) a detailed information in time and space on what is the relative impact of the industrial emissions in an area up to 400 x 400 km (9 km spatial resolution) - between 24 x 24 km with 1 km spatial resolution, 100 x 100 km (9 km spatial resolution) and finally 400 x 400 km with 9 km spatial resolution - for those pollutants limited by EU Directives (SO2, NOx, CO, PM10 and Ozone). The system can be adapted to run in cluster platforms. Also, the system provides scenario analysis for different industrial plants at the same time and for different industrial loading capacities and provides the best scenario to avoid forecasted exceedances of the EU limits. The system is developed to provide the information in the Internet network. TEAP requires important hardware resources and intensive computer CPU demand but it can be implemented by using PC based platforms. The system can provide an important support for urban air quality since it can be easily adapted to traffic flow scenario analysis and another different emission reduction strategy. TEAP is and EUREKA project.

Keywords: Air Quality, Industrial plants, Modelling.

1. INTRODUCTION

Air Quality information has become an essential tool for industrial managements and citizens health. The air quality modelling systems have been improved substantially in the last decade. The simulation of the atmospheric process has had an important advance because of the improvement of the science knowledge and also because of the improvement of the capability of the computational platforms. The computer power has increased substantially in the last years and the PC based platforms have reached high performance levels. 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 (San José et al. [1997]). 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 (Grell et al. [1994] and the ordinary differential equation system for the chemistry module (San José et al. [1994, 1996, 1997]). 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), (Stockwell et al. [1997]), EUROS (RIVM, The Netherlands), (Langner et al. [1998]), EMEP Eulerian (DNMI, Oslo, Norway), MATCH (SMHI, Norrkoping, Sweden), (Derwent and Jenkin, [1991]), REM3 (Free University of Berlin, Germany), (Walcek, [2000]), CHIMERE (ISPL, Paris, France), (Schmidt et al. [2001]), NILU-CTM (NILU, Kjeller, Norway), (Gardner et al. [1997]), LOTOS (TNO, Apeldoorm, The Netherlands), (Roemer et al. [1996]), DEM (NERI, Roskilde, Denmark), (Gery et al. [1989]), STOCHEM (UK Met. Office, Bracknell, U.K.), (Collins et al. [1999]). 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 MODELLING 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 (Gery et al. [1989]). 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 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 Guenther et al. [1995] 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).

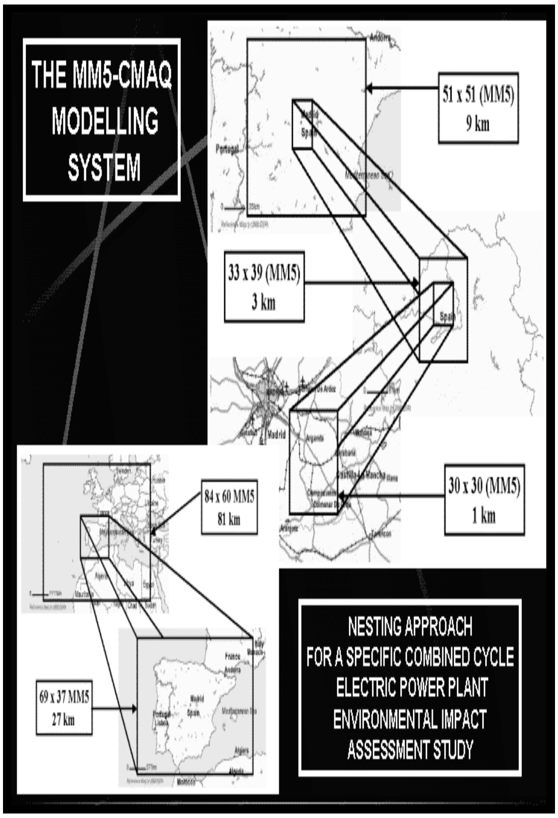

Figure 1.- MM5-CMAQ architecture for this experiment.

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.

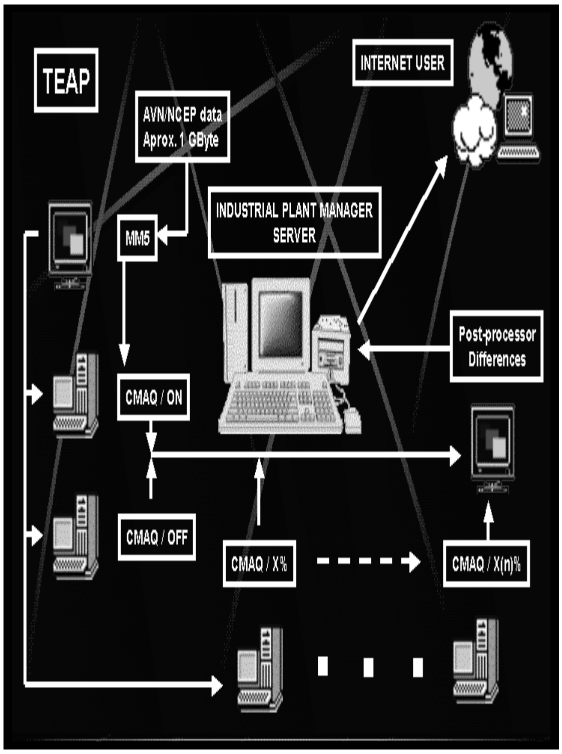

Figure 2.- TEAP Computer platform scheme.

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.

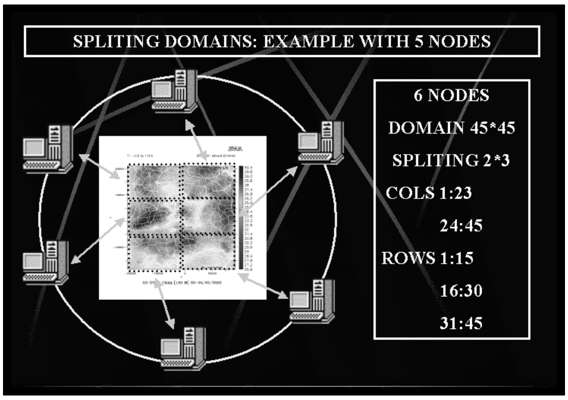

Figure 3. Cluster platform with 6 nodes for TEAP application.

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.

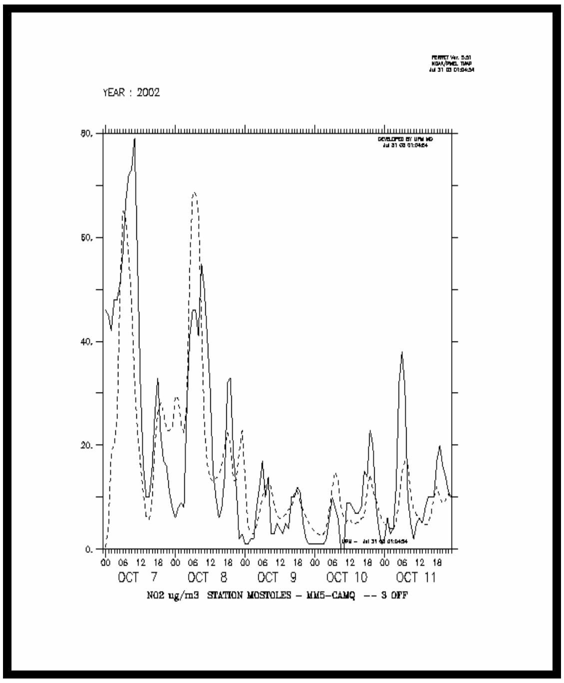

Figure 4. Comparison between observed NO2 concentrations at the monitoring station in Móstoles (Madrid, Spain) and modelled NO2 concentrations by MM5-CMAQ at the grid cell where the monitoring station is located (MM5-CMAQ with 3 km spatial resolution).

The MM5 – CMAQ, in this application, has been configured to use CBM-IV (Gery et al. [1989]) chemical scheme for organic reactions, and the SMVGEAR (Jacobson et al. [1994]) 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

In this contribution 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).

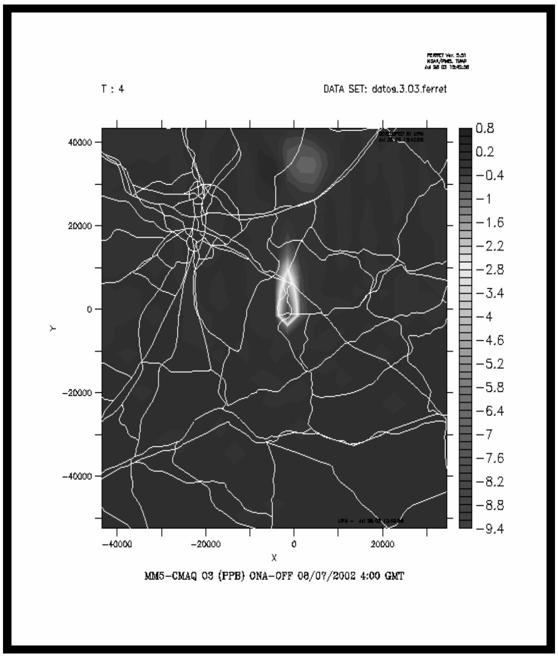

Figure 5. Surface concentration differences over a domain of 27 x 33 grid cells (3 km) centered at the planned power plant. Differences between ozone concentrations (ppb) in OFF mode and with the planned power plant emissions at 4h00 (GMT) on July, 8, 2002.

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).

4. CONCLUSIONS

The MM5-CMAQ air quality modeling system has been implemented with several architectures for several cases of industrial and power plants in different geographical locations in the Iberian Peninsula with excellent results. The system constitutes a reliable 3rd generation of air quality modelling tool for analysis of city and regions and also for the analysis of impact of emissions of different industrial and power plants. Also, the system can be used to analyze the impact of different emission scenarios even from different emission sources such as traffic, biogenic, domestic, etc. We have used the EMIMO model, which uses a Top-Down approach (an partially a Bottom-up approach) for evaluating the high spatial and temporal emissions adapted to the different model domains. We have shown that the comparison between observed monitoring data and modelled data agrees sufficiently – having in mind that the modelled data is an averaged for the grid cell (9 km, 3 km or 1 km spatial resolution) and observed data is a value with a limited representation since in most of the cases is located in urban or suburban areas -.

The results provides a full analysis of every physical and chemical process and the relative increases and decreases (in ozone concentrations for example around the industrial or power plant). Future developments should focus on implementing the system in operational mode for real cases and cluster platforms running over long periods.

5. ACKNOWLEDGEMENTS

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