

## 7.16 AIR QUALITY IMPACT ASSESSMENT TOOL FOR LARGE INDUSTRIAL AND POWER PLANTS FOR REAL-TIME AND FORECASTING OPERATIONAL OBJECTIVES

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### 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 to the transport/chemistry modules. CPU time is mainly used for transport/chemistry (70 – 80 %). These modelling system require of important initial and boundary data sets to simulate properly specific time periods and spatial domains, such as land use data, digital elevation model data, global meteorological data sets, vertical chemical profiles and emission inventory data sets. 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)*)).

The emission inventory is a model which provides in time and space the amount of a pollutant emitted to the atmosphere. 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. The emission inventory can also be source apportionment oriented which allows the user of the full system (atmospheric modelling system) to evaluate the impact in the concentrations of the different pollutants in the atmosphere in a relative perspective. Because of the high non-linearity of the atmospheric system, the only possibility to establish the impact of the part of the emissions (due to traffic or one specific industrial plant, for example) is to run the system several times – each time with a different emission scenario . It is also possible to modify the source code of the system to “follow-up” the importance of each part in the emissions but the CPU time is not substantially benefited with this approach.

## 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 system uses EMIMO model to produce every hour and every 1 km grid cell the emissions of total VOC’s (including biogenic), SO<sub>2</sub>, NO<sub>x</sub> and CO. Figure 1 shows an example of application of the MM5-CMAQ computer platform for an area located at the south-east of Madrid city. 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. Obviously each scenario suppose to run a simulation which differs from the OFF simulation only on a specific percentage or emission reduction pattern at the industrial plant (load reduction in combustion or any other specific decision to reduce the emissions). It is possible to use cluster platforms to reduce significantly the amount of computer time required for the different simulations. Figure 3 shows an scheme for the case of having a cluster with 6 nodes and how the model domain is divided. The cluster alternative is probably the only possible with an acceptable cost/benefit relation to run such a complex systems. 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 can probably be increased by using faster connection architectures between PC’s.

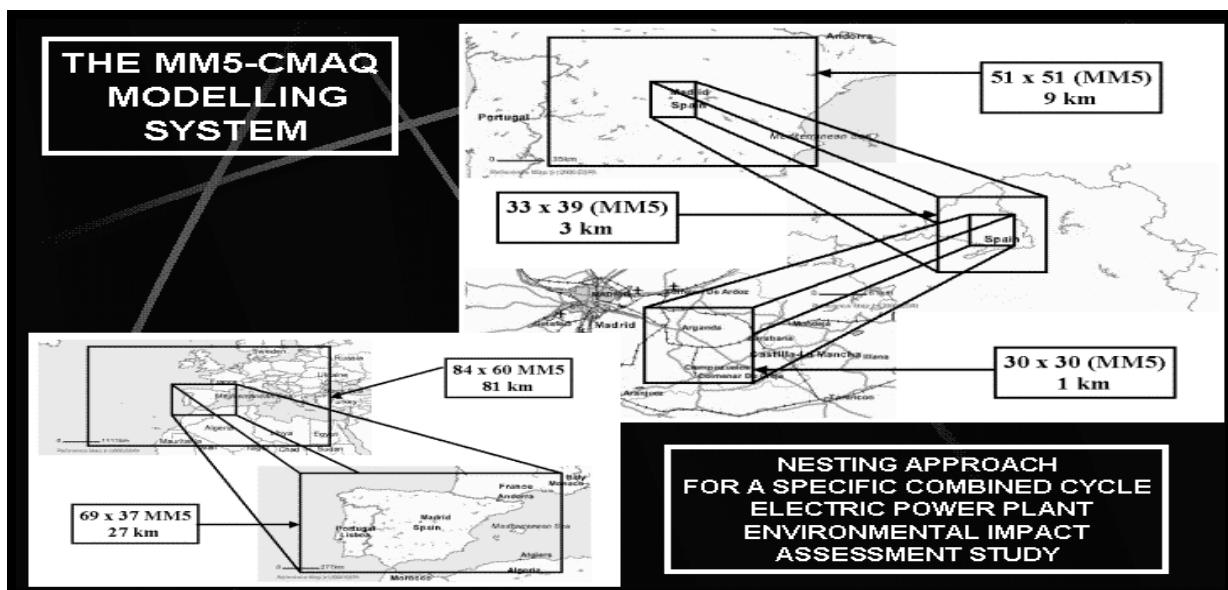


Figure 1. Example of application of TEAP at the South-East region of Madrid city.

The MM5-CMAQ modelling 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. 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.

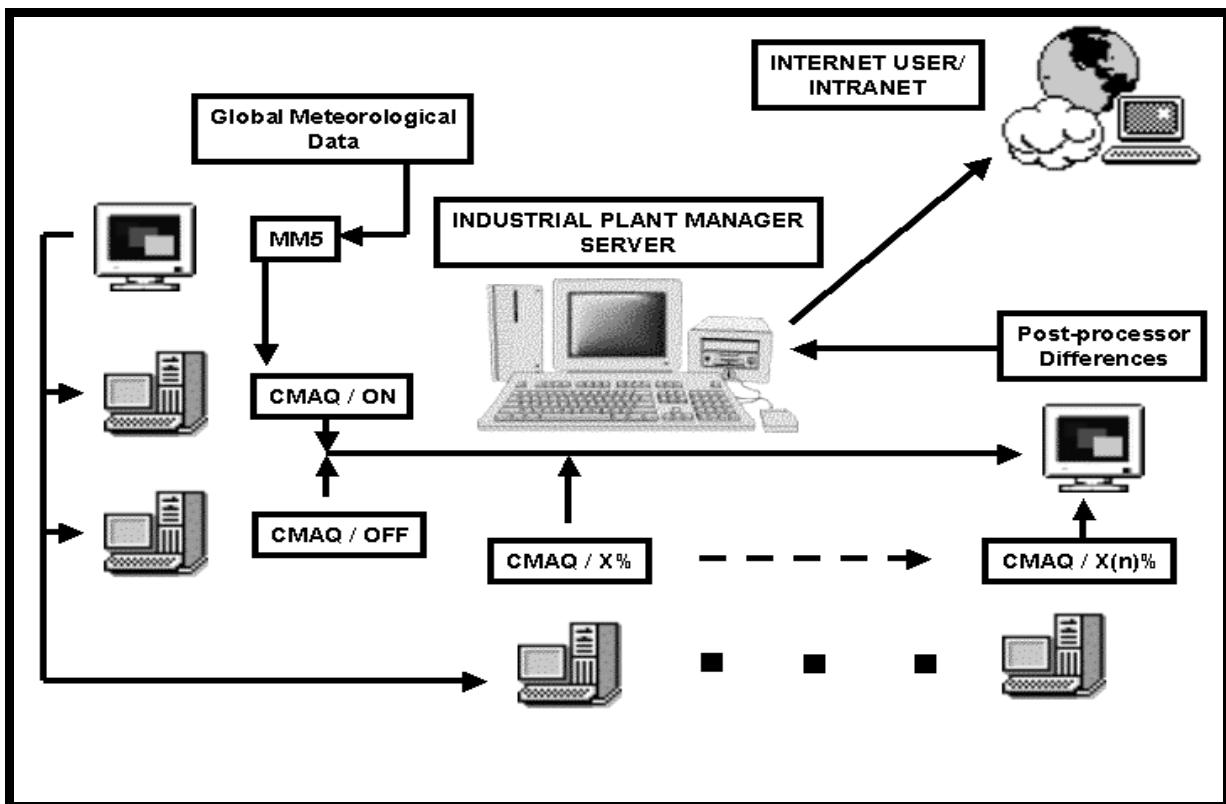


Figure 2. Computer platform (TEAP) used to simulate different emission reduction scenarios for different large industrial plants.

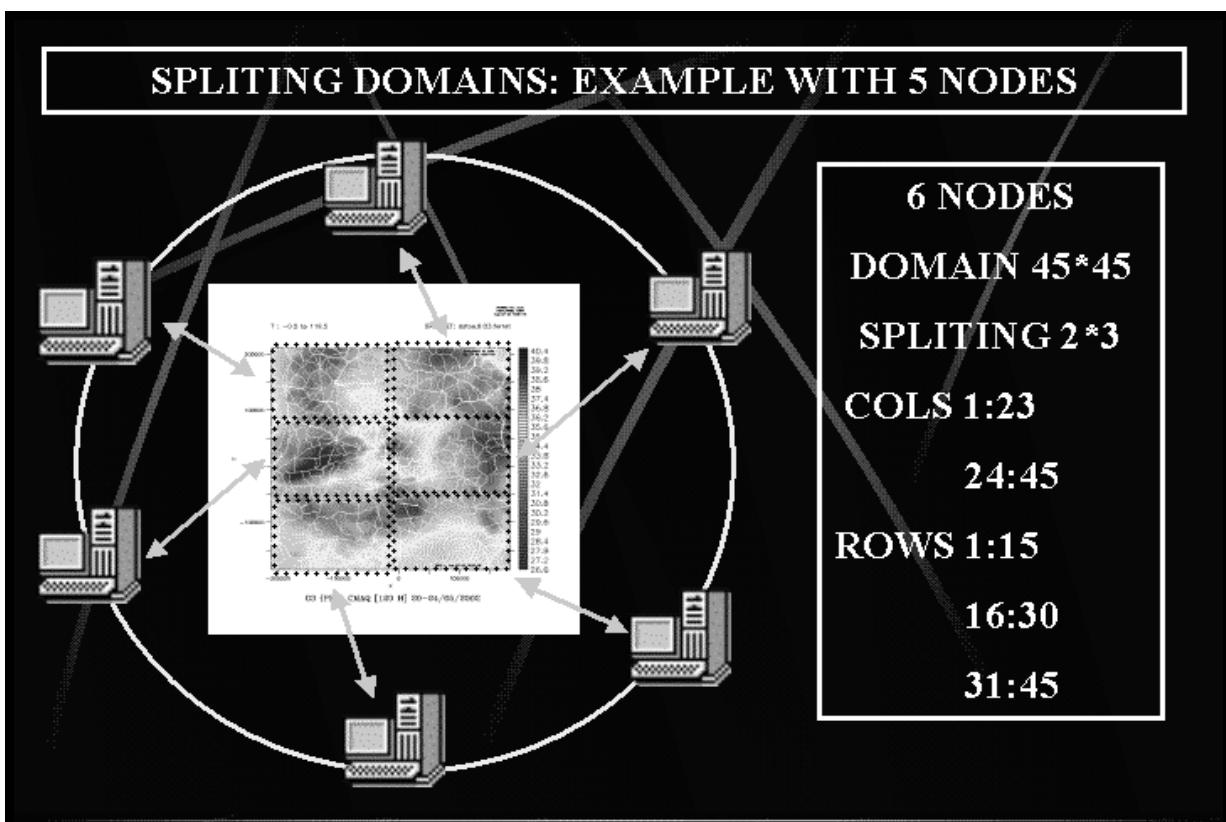
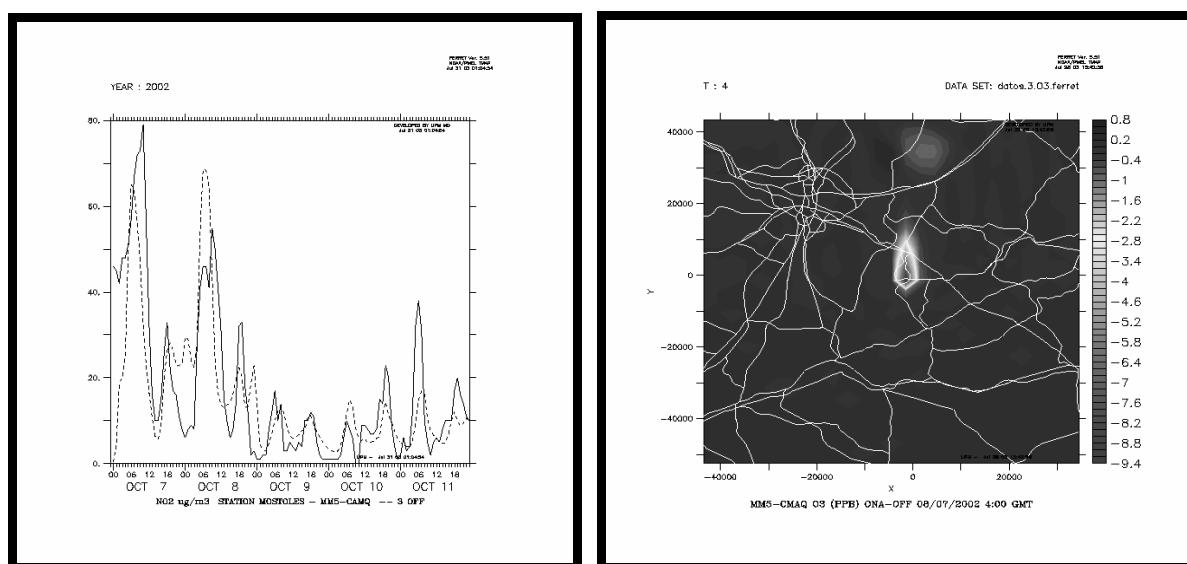


Figure 3. Example of a TEAP cluster computer platform.

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 layer in height – typically and in this experiment 23 layers –) 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. The MM5 – CMAQ in this application has been configured to use CBM-IV chemical scheme for organic reactions, and the SMVGEAR numerical scheme for solving the chemistry.

## 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 area in the Iberian Peninsula for different industrial type plants. 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 4A we observe the comparison between observed NO<sub>2</sub> concentrations at the monitoring station in Móstoles (Madrid, Spain) and modelled NO<sub>2</sub> concentrations by MM5-CMAQ at the grid cell where the monitoring station is located (MM5-CMAQ with 3 km spatial resolution). Figure 4B shows the surface ozone concentration differences over a domain of 27 x 33 grid cells (3 km ) centered at the planned power plant.



*Figure 4. A) Comparison between observed and modelled (MM5-CMAQ) NO<sub>2</sub> concentrations at the monitoring station in Móstoles (Madrid, Spain).B) Surface ozone concentration differences over a domain of 27 x 33 grid cells (3 km) centered at the planned power plant..*

All 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 or 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). All this 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 these 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). An increase on the speed of about 10 – 11 times is obtained in this platform (Iowa University cluster).

## ACKNOWLEDGEMENTS

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## REFERENCES

- Gery M.W., Whitten G.Z., Killus J.P. and Dodge M.C (1989), A photochemical kinetics mechanism for urban and regional scale computer modelling, *Journal of Geophysical Research*, 94, D10, pp. 12925-12956.
- Grell G.A. (1994), Dudhia J. And Stauffer D.R. A description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5). NCAR/TN- 398+ STR. NCAR Technical Note.
- San José R., Rodriguez L., Moreno J., Palacios M., Sanz M.A. and Delgado M. (1994) Eulerian and photochemical modelling over Madrid area in a mesoscale context, *Air Pollution II, Vol. 1 Computer Simulation, Computational Mechanics Publications, Ed. Baldasano, Brebbia, Power and Zannetti.*, pp. 209-217.
- San José R., Cortés J., Moreno J., Prieto J.F. and González R.M. (1996) 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*, pp. 309-319.
- San José R., Prieto J.F., Castellanos N. and Arranz J.M. (1997) 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*, pp. 119-130.