

## TEAP: AN OPERATIONAL REAL-TIME AIR QUALITY DECISION SUPPORT SYSTEM FOR INDUSTRIAL PLANTS

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### INTRODUCTION

The air quality impact of industrial plants is an essential issue in air quality assessment and modelling which is becoming more important due to the more strict EU legislation in air quality standards. The 2002/3/EC Directive of the European Parliament and of the Council of 12 February 2002 related to ozone in ambient air provides information related to shirt-term action plans at the appropriate administrative levels. In accordance with this legislation, industrial plants are being requested by environmental authorities to have appropriate control systems to provide in real-time and forecasting mode information related to the relative impact of their industrial plants in the forecasted pollution levels – in particular on the O3, SO2, NOx, CO and PM10 levels which are limited by different EU Directives -. The capability to reduce specific emissions in real-time according to a forecast for a specific area and period of time is actually a challenging issue. In the past years, this objective was limited due to the limited computer power and the cost of vector parallel computers. Nowadays, cluster system composed by PC processors (3,4 Ghz or 3,6 Ghz) provide an acceptable capability – once we have designed a proper architecture of the air quality modelling systems – to run this complex systems in real-time and forecasting mode.

The concept of real-time in our case is related to the fact of taking appropriate decisions in advance to avoid specific exceeds of the EU Directive limits. Following above Directive the responsibility to design of short-term action plans, including trigger levels for specific actions, is the responsibility of Member States. Depending of the individual case, the plans may provide for graduated, cost-effective measures to control and, where necessary, reduce or suspend certain activities, including motor vehicle traffic, which contribute to emissions which result in the alert threshold being exceeded. These may also include effective measures in relation to the use of industrial plants or products. In this application we focus on the possible reduction of industrial activities – in our case, a combined cycle power plant -.

The complete tool designed for this application is called TEAP (a Tool to Evaluate the Air quality impact of industrial Plants) (San José et al., 1994, 1996). This tool is designed to be used by the environmental impact department at the industrial site. The tool provides a response to air quality impact to industrial emissions in the form of surface patterns and lineal time series for specific geographical locations into the model domain. The model domain is designed in a way that the industrial source point is located approximately in the centre of the model domain. The model domain can be as large as wished but a specific nesting architecture should be designed for each case together with balanced computer architecture.

The TEAP tool (an EUREKA-EU project) has the capability to incorporate different modelling systems. In a preliminary stage we have tested thee system with the so-called OPANA model (ETC/ACC03). OPANA model (San José et al, 1996) stands for Operational Atmospheric Numerical pollution model for urban and regional areas and was developed at



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the middle of the 90's by the Environmental Software and modelling Group at the Computer Science School of the Technical University of Madrid (UPM) based on the MEMO model (ETC/ACC03) developed in the University of Karlsruhe (Germany) in 1989 and updated on 1995, for non-hydrostatic three dimensional mesoscale meteorological modelling and SMVGEAR model for chemistry transformations based on the CBM-IV mechanism and the GEAR implicit numerical technique developed at University of Los Angeles (USA) in 1994. The OPANA model has been used (different versions) for simulating the atmospheric flow – and the pollutant concentrations – over cities and regions in different EU funded projects such as EMMA (1996-1998), EQUAL (1998 - 2001), APNEE (2000-2001). In these cases and others the model has become an operational tool for several cities such as Leicester (United Kingdom), Bilbao (Spain), Madrid (Spain), Asturias region (North of Spain) and Quito (Ecuador, BID, 2000). In all these cases the model continue to operate under daily basis and simulates the atmospheric flow in a three dimensional framework. The OPANA model, however, is a limited area model – which means that the model domain is **limited** by the earth curvature – and the cloud chemistry and particulate matter is not included (aerosol and aqueous chemistry).

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.*, (1977), EUROS (RIVM, The Netherlands), *Lagner et al.* (1998), EMEP Eulerian (DNMI, Oslo, Norway), MATCH (SMHI, Norrkoping, Sweden), *Dervent R. and Jenkin M.* (1991), REM3 (Free University of Berlin, Germany), (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.* (1997). 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.

### THE MM5-CMAQ MODELING SYSTEM

The CMAQ model (Community Multi-scale Air Quality Modeling System, EPA, US) is implemented in a consistent and balanced way with the MM5 model. 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). As an example a domain architecture is showed in Figure 1 for an application in a combined cycle power plant in the south area of Madrid Community. 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) which can be substituted for any more accurate high spatial resolution landuse information in the implementation of the input data.

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



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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 (photosynthetic active radiation). 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.



Figure 1. Comparison between NO observations and simulated data by using TEAP tool for analyzing the impact of emissions from combined cycle plants.

In this application we have applied the MM5-CMAQ modelling system over a power plat with 4 400 MW combined cycle power groups which are expected to operate simultaneously. The simultaneous simulations of the so-called ON run (the four groups running) and OFF1, OFF2, OFF3 and OFF4 runs – which are representing the air concentrations when switching off the first combined cycle power group, the second one and so on successively – is analyzed by generating the corresponding differences between ON-OFF1, ON-OFF2 and so on. These differences represent the respective impact of each of the successive switching off process until the OFF4 scenario which represent the complete disconnection of the 4 400 MW combined cycle power plant groups and the subsequent zero emissions from the power plant.



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The system was calibrated for 60 day selected periods by using 5 day periods per month along the 2004 year. Figure 1 shows an example of the comparison between NO air concentration in Leganes monitoring station (located in the surrounding area of Madrid city) and the simulated NO concentrations.

The impacts – due to the high chemical non linearity involved – are analyzed respecting on the absolute concentration pollution values and these values respecting the EU Directive limits. The post-processing is done automatically and presented in the specifically designed Web site.

### RESULTS

The system is operating since July, 1, 2005 with full success. The developed system provides 72 hours forecasts for the impact of the 4 independent 400 MW combined cycle power groups. The access to the web site is restricted to environmental authorities and company authorized personnel. The system is operating from the Computer Center at Computer Science School at Technical University of Madrid (UPM) managed by the Environmental Software and Modelling Group (ESMG). The system has been mounted over an 8-node 3,4 Ghz cluster platform. Figure 2 shows an example of the TEAP prototype mounted over a Petrochemical plant also in the South of Madrid Area (150 km away).



Figure 2. TEAP web site to analyze the impact of a petrochemical plant located 150 km at the south of Madrid area.

The system is the first operating in Spain by using such a sophisticated 3<sup>rd</sup> Generation Air Quality Modelling System and it is expected to be installed in several other combined cycle power plants and in general in different industrial plants to help the local and regional authorities to identify the relative impact of the different industrial plants located in the



surrounding area. The system can be adapted to identify the impact of traffic sources and also different scenarios.

#### 1.5. Acknowledgements

We would like to thank PSU/NCAR and EPA (US) for the MM5 and CMAQ codes. The Spanish Industrial Funding Agency (CDTI) and the SOLUZIONA S.A. company.

#### 1.6. References

- Collins W.J., Stevenson D.S., Johnson C.E. and Derwent R.G. (1997). Tropospheric ozone in a global scale3D Lagrangian model and its response to NOx emission controls. J. Atmos. Chem., 86, 223-274.
- Gardner R.K., Adams K., Cook T., Deidewig F., Ernedal S., Falk R., Fleuti E., Herms E., Johnson C., Lecht M., Lee D., Leech M., Lister D., Masse B., Metcalfe M., Newton P., Schmidt A., Vandenberg C. and van Drimmelen R. (1997). The ANCAT/EC global inventory of NOx emissions from aircraft. Atmospheric Environment 31, 1751-1766.
- 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.
- Langner J., Bergstrom R. and Pleijel K. (1998), 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.
- Roemer M., Boersen G., Builtjes P. and Esser P. (1996). The budget of ozone and precursors over Europe calculated with the LOTOS model. TNO publication P96/004, Apeldoorn, The Netherlands.
- 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.
- Schmidt H., Derognat C., Vautard R. and Beekmann M. (2001). A comparison of simulated and observed ozone mixing ratios for the summer 1998 in Western Europe. Atmospheric Environment, 35, 6277-6297.
- Stockwell W., Kirchner F., Kuhn M. and Seefeld S. (1977). A new mechanism for regional atmospheric chemistry modeling. J. Geophys. Res., 102, 25847-25879.