

## AIR QUALITY MODELLING AS A TOOL TO EVALUATE THE AIR QUALITY INDUSTRIAL PLANT IMPACT

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### INTRODUCTION

The air quality impact of industrial plants has been a key issue on air quality assessment and modelling since the 70's. Nowadays, the increased capacity on computer power and progress on air pollution science provide a powerful and reliable tool to measure the air quality impact on industrial emissions. In the last decade a considerable effort to incorporate the industrial production processes in an integrated environmental evaluation in on-line mode has been done. In a parallel way, a considerable increase of citizen concern has been detected particularly in those areas where important industrial point sources are present together with highly populated areas (urban areas). This case is particularly sensitive for refineries, waste city incinerators, etc. In this contribution we will show the results of a preliminary modelling experiment to build a so-called TEAP tool (A tool to evaluate the air quality impact of industrial emissions).

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 center of the model domain. The model domain can be as extensive as wished but a specific nesting architecture should be designed for each case together with a 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 the system with the so-called OPANA model. OPANA model stands for Operational Atmospheric Numerical pollution model for urban and regional areas and was developed at the middle of the 90's by the Environmental Software and modeling Group at the Computer Science School of the Technical University of Madrid (UPM) based on the MEMO model developed in the University of Karlsruhe (Germany) in 1989 and updated on 1995, for non-hydrostatic three dimensional mesoscale meteorological modeling 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).

In this contribution we will use the MM5-CMAQ modeling system. MM5-CMAQ is a representative of the last generation of AQMS (third generation) developed by EPA (USA) in 2000. The model uses a full modular structure with the last advances on computer

programming (FORTRAN-95). In essence many of the features of MM5-CMAQ are similar to OPANA but the programming and modularity is more advanced. MM5-CMAQ is not a limited area model and it can run over large domains (even at global level although a CMAQ global version is not existing yet). The model domains are obviously closely related to model forecast horizon so that the nesting capability (in a similar way that it was done in OPANA) plays an essential role to have reliable simulations over city and regional domains. Another representatives of third generation of AQMS are CAMx (Environ Co., USA) and EURAD (European Ford Research Group and university of Cologne (Germany)). MM5 is the well known Non-hydrostatic Mesoscale Meteorological Model developed in the Pennsylvania State University and NCAR starting on 1983.

The MM5 model is today one of the most robust and reliable meteorological models. In both cases and in all Eulerian models, the input datasets are key elements to work down to have reliable and accurate simulations. These datasets are: DEM (Digital elevation model), Land use data (usually satellite data, AVHRR/NOAA, Landsat, Spot, etc.), Initial and boundary meteorological conditions, initial and boundary air concentration profiles and finally, emission data sets. The emission datasets are usually the bottle neck on this type of applications since the uncertainty involved is important. In spite of this limitation, the TEAP tool extract the most important benefits from the relative difference between a simulation with full emission inventory and a second simulation with an emission inventory *without* the industrial plant to be studied.

#### **EXPERIMENT**

We have implemented the MM5-CMAQ modeling system in a nesting architecture. The MM5 Mesoscale Meteorological Model (PSU/NCAR) and the Community Multiscale Air Quality Model (CMAQ) [1] from EPA (USA) (third generation of air quality modelling systems) are used as mainframe platform. The MM5 is built over a mother domain with 36 x 36 grid cells (81 km spatial resolution) and 23 vertical levels. This makes a domain of 2916 x 2916 km. The nesting MM5 level 1 model domain is built over a 69 x 66 grid cells (27 km spatial resolution) and 23 vertical levels, which makes a model domain of 1863 x 1782 km centered over the Iberian Peninsula. CMAQ model domains are 30 x 30 grid cells for mother domain and 63 x 60 over the nesting level 1 model domain. CMAQ mother domain lower left corner is located at (-1215000 m, -1215000 m) at the reference locations (-3.5W, 40N) and the first and second standard parallels (30N, 60N). The CMAQ nesting level 1 lower left corner is located at (-891000, -810000) with the same reference locations. The 9 km MM5 spatial resolution model domain has 54 x 54 grid cells, the 3 km MM5 spatial resolution model domain has 33 x 39 grid cells and finally the 1 km MM5 spatial resolution model domain has 30 x 30 grid cells. The corresponding CMAQ model domains are: 48 x 48 km, reference (-216000, -216000) in Lambert Conformal projection with 9 km spatial resolution; 27 x 33 grid cells, reference (-54000, -9000) with 3 km spatial resolution and finally, 24 x 24 grid cells, reference (-27000, 33000) with 1 km spatial resolution. In this contribution we will show results for the 3 km spatial resolution or nesting level 3 only.

The industrial plant is located at (.6727.0, 62909.65) in Lambert Conformal Coordinates. This industrial plant emits 340 Tn/year of SO<sub>2</sub>, 155 Tn/year NO<sub>x</sub> and 2.9 Tn/year VOC's. We have selected – as a preliminary test – the period of February, 4-8, 2002. The emission database is obtained from the EMIMA model [2] and EMIMO model – a new emission model for large domains based on global emission inventories such as GEIA, EMEP, EDGAR and the Digital Chart of the World.

The MM5-CMAQ modeling system is initiated by using global data sets from MRF (NOAA/NCEP, USA) and mother, nesting levels 1 and 2 provide the boundary conditions for

running MM5-CMAQ for nesting level 3 over the Madrid Community Area with 27 x 33 grid cells (3 km) which makes 81 x 99 km. The OPANA model runs over a domain of 80 x 100 km with UTM coordinates and using only EMIMA data sets. EMIMA datasets are also used for MM5-CMAQ over nesting level 3. EMIMO data set is used for mother and nesting levels 1 and 2 for MM5-CMAQ. We have performed two simulations (MM5-CMAQ), one simulation with the industrial plant emissions and the second one *without* the industrial plant emissions.

## RESULTS

The results show important differences in relative values for ozone concentrations over the model domain. The impact of industrial emissions on ozone concentrations are distributed along the North-East wind direction on average for the 120 hours simulation period. In the immediate surrounding areas of the industrial plant the impact of NO<sub>x</sub> and VOC's emissions are capable to reduce up to 40-50 % of ozone concentrations on "average" over the 120 hours. A depth analysis on the impact of industrial emissions by using process analysis techniques is shown in Figures 1 and 2. These plots illustrate the variations in process contributing during the simulation period. Figure 1 shows the contributions to ozone concentrations at industrial grid cell (16,23) over the simulation period (0- 120 hours) for advection in E-W and N-S direction (XYADV), vertical advection (ZADV), mass adjustment for advection (ADJC), chemistry (CHEM) and finally the simulated ozone concentrations (with industrial emissions). Horizontal advection and chemistry seem to play an important role at the industrial grid cell in accordance with the simulated ozone concentrations during the days 3-4 of the 120 hour simulation period. In Figure 2, the process analysis is shown for vertical diffusion (VDIF), horizontal diffusion (HDIF) and dry deposition (DDEP) – together with the ozone simulated concentrations.

Vertical diffusion is clearly the most important mechanical process affecting the simulated ozone concentrations for the 3-5 days of the simulation period. The above time series show that TEAP can be a relevant software tool to help industrial plant managers to integrate friendly environmental practices into the industrial production process and help to fulfill to the city and regional authorities with the environmental regulations particularly when pollution episodes are forecasted and the industrial plant plays an important role on those episodes. TEAP can identify in a clear and systematic way the impact of the industrial plant emissions (the industrial plant implemented in each specific case) over the spatial domain and under temporal basis. The spatial and temporal location is immediately identified by using the software expert system designed in TEAP just after ending both simulations (ON and OFF).

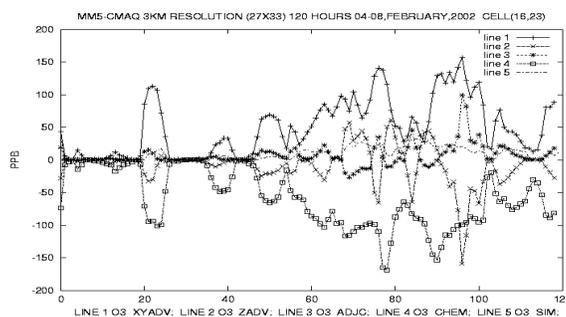


Figure 1. Process analysis (I) at industrial grid cell.

The results of this modeling experiment show that TEAP can constitute an important tool for industrial managers in order to fulfill with the environmental regulations present at different countries. The tool has been implemented over three PC-LINUX-Red Hat machines with 1 GB

RAM memory and 120 Gb hard disk each. The three PC's have been connected in an Internet network to run in operational mode to produce real-time industrial air quality impacts under daily basis. The software is still under further developments and adaptation since several additional features will be implemented focusing on the features required to avoid pollution episodes being partially due to industrial emissions particularly on those areas in the near by of industrial plants. The second phase is planned to integrate the industrial production process under an optimized cost-benefit analysis into the environmental conscious industrial management.

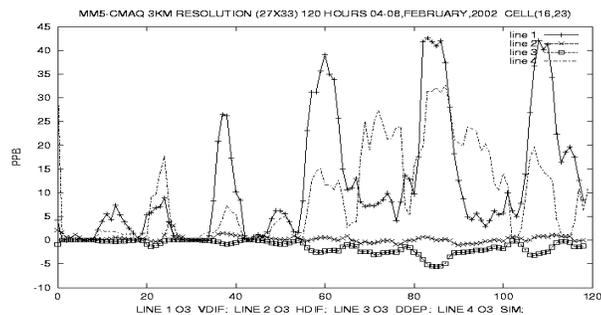


Figure 2. Process analysis (II) at industrial grid cell.

The surface patterns illustrated here show that differences between 10 to 50 % - depending of the air pollution model - can be found in the surrounding area of the industrial plant. These differences are important since they generate increases in ozone concentrations up to 40 % in the surroundings of the industrial plant in MM5-CMAQ model. Further analysis and more simulation periods are required to establish more solid consequences than those obtained in this preliminary analysis. The TEAP-EUREKA project is intended to develop an expert system tool to analyze a large amount of simulation periods to establish the calibration between monitoring data and simulated data. The results will be used to interpret the relative differences between ON and OFF scenarios with the corresponding error margins. The results in real-time will be used by the industrial plant managers to optimize the cost-performance-pollution impact relation in order to quantify the impact on the area of the different emissions.

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