Real-Time Air Quality Operational Forecasting Systems in Spain: an Application of the MM5-CMAQ-EMIMO Modelling System

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ABSTRACT:

In this contribution we show the description, implementation and operation of an Operational Air Quality Forecasting System for industrial plants, urban and regional areas. The system is called OPANA (OPerational Atmospheric Numerical model for urban and regional Areas) and is the evolution and result of more than 10 years of research on sophisticated state-of-the-art numerical air quality modelling systems and the implementation on state-of-the-art computer platforms. The system is in operation since 2005 although older versions started to operate at the end of the 90's. The OPANA tool is operating on different industrial plants in the south of Madrid area and also over urban areas such as Madrid (Spain), Leicester City (U.K.), Las Palmas de Gran Canaria (Canary Islands, Spain). OPANA modelling tool is actually operating with MM5 mesoscale meteorological model (PSU/NCAR, US) and the CMAQ (Community Multiscale Air Quality Modelling System) model developed by EPA (US). Additionally, a complex emission model (EMIMO) developed by our group in UPM (Spain) in 2001 is also described and needed to provide accurate hourly and high spatial resolution (1 km) pollution emission data at global level. Results show that these tools can provide reliable and robust information to authorities and industrial managers to control – in forecasting mode – the air quality in the surrounding areas of the industrial plant or to forecast the air quality in the whole city or region.

Key words: air quality modelling, industrial plants, urban air quality, mesoscale models, numerical meteorological models, ozone modelling.

Sistemas de Predicción de la Calidad del Aire en Tiempo Real en España: una aplicación del sistema MM5-CMAQ-EMIMO

RESUMEN:

En esta contribución mostramos la descripción, la implementación y la operativa de un Sistema de Predicción Operacional de la Calidad del Aire para plantas industriales, áreas urbanas y regionales. El sistema se denomina OPANA (acrónimo de *Operational Atmospheric Numerical model for urban and regional Areas*) y es un producto consecuencia de la investigación en el área durante más de 10 años de nuestro laboratorio, sobre sistemas numéricos sofisticados de calidad del aire que reflejan el estado-del-arte en este área y su implementación en plataformas computacionales actuales. El sistema se encuentra operando desde el año 2005 aunque hubo versiones anteriores que inician su desarrollo al final de los años 90. Esta herramienta - OPANA - opera sobre diferentes plataformas industriales en el área del sur de la comunidad de Madrid

y también sobre áreas urbanas como la ciudad de Madrid (España), la ciudad de Leicester (Reino Unido), Las Palmas de Gran Canaria (Islas Canarias, España). La herramienta OPANA opera en la actualidad con el modelo meteorológico de mesoescala MM5 (PSU/NCAR, US) y el modelo CMAQ (Sistema de Modelización de la Calidad del Aire de Multi-escala y comunitario) desarrollo por USEPA. Además, un modelo de emisiones denominado EMIMO, desarrollado por nuestro laboratorio en el año 2001, es necesario para proporcionar las estimaciones de las emisiones horarias con alta resolución espacial (1 km) de los diferentes contaminantes atmosféricos en cualquier parte del globo. Los resultados muestran que este tipo de herramientas pueden proporcionar una información robusta y confiable a las autoridades ambientales y a los responsables industriales para controlar –en modo predictivo– la calidad del aire en aquellas áreas que rodean las áreas industriales o para predecir la calidad del aire en la ciudad o en toda la región.

Palabras clave: calidad del aire, modelización, plantas industriales, calidad del aire urbana, modelos de mesoescala, modelos numéricos meteorológicos, modelización del ozono.

1. INTRODUCTION

The interest of understanding and knowing the air quality over large domains and with high temporal and spatial resolution is growing rapidly together with the interest of knowing the relative quantitative and qualitative impact on a specific area (grid) and time (Jacobson and Turco, 1994). The micrometeorological process are fully included into the modern mesoscale air quality modelling systems by using different parameterizations, particularly for the deposition processes which include several resistances which are parameterized according to several turbulence stratification schemes. The advances in air quality modelling have been substantial in the last decade. The third generation of air quality modelling systems use the so-called "oneatmosphere" approach which means that the dispersion and chemical transformation of the different pollutants emitted to the atmosphere is treated in an 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 problem of model the air concentrations is an interdisciplinary problem which has been investigated very much during the last decade in parallel with the computer power increase. These type of tools are used for air quality impact assessments, urban simulations and air quality forecasts and operational industrial air quality industrial forecasting systems. The complex interactions between the chemistry, sub-grid parameterizations, physics, surface characterization, solar modelling, advection, diffusion, numerical properties and computer platform capabilities advise to integrate all this processes and elements in one integrated tool which when running produces a results which accounts for all these aspects. So that, these models are progressively substituting the old and classic approaches based on specific approaches such as synoptic meteorology, atmospheric chemistry, etc. The integrated solution seems to be the only reliable approach to account for all possible aspects involved in the air pollution process.

The cluster approaches open new scenarios for many applications and particularly on the atmospheric dynamics simulations. These models include sophisticated land use information and deposition/emission models (San José R. 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 (75 %). 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 G.A. et al. (1994)) and the ordinary differential equation system for the chemistry module (San José R. et al. (1994) ; 1996 and 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 due to the emission uncertainty.

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. 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 W. et al. (1977)), EUROS (RIVM, The Netherlands), (Lagner J. et al. (1998)), EMEP Eulerian (DNMI, Oslo, Norway), MATCH (SMHI, Norrkoping, Sweden), (Derwent R. and M. Jenkin (1991)), REM3 (Free University of Berlin, Germany), (Walcek C. (2000)), CHIMERE (ISPL, Paris, France), (Schmidt H. et al. (2001)), NILU-CTM (NILU, Kjeller, Norway), (Gardner R.K. et al. (1997)), LOTOS (TNO, Apeldoorm, The Netherlands), (Roemer M. et al. (1996)), DEM (NERI, Roskilde, Denmark), (Gery M.W. et al. (1989)), STOCHEM (UK Met. Office, Bracknell, U.K.), (Collins W.J. et al. (1997)). In USA, CAMx Environ Inc., STEM-III (University of Iowa) and CMAQ model are the most up-to-date air quality dispersion chemical models. In this application we have used the CMAQ model (EPA, Environmental Protection Agency, 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 is implemented in a consistent and balanced way with the MM5 model (Gery M.W. et al. (1989)). The CMAQ model is fixed "into" the MM5

model with the same grid resolution (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 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 modelling system (MM5-CMAQ) with USGS 1 km land use data and GTOPO 30" for the Digital Elevation Model (DEM).

The system uses EMIMO model (EMIssion Model) to produce every hour and every 1 km grid cell the emissions of total VOC's (including biogenic), SO2, NOx and CO. 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 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).



Figure 1.- MM5-CMAQ architecture for an application.



Figure 2.- TEAP Computer platform scheme.

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). Each emission scenario involves running 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) "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 "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. Figure 3 shows a scheme for the case of having a cluster with 6 nodes and how the model domain is divided.

The results over platforms of about 20 nodes provide increases of time of about 10 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. MM5 is used by several states in USA for weather forecasts and in Europe it is used by several meteorological Institutes as a research



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

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.

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 - now the last version is 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.

The MM5 – CMAQ, in this application, has been configured to use CBM-IV (Gery M.W. et al. (1989)) chemical scheme for organic reactions, and the SMVGEAR (Jacobson M.Z. and R.P. Turco, (1994)) numerical scheme for solving the chemistry. More than 75 % of the computer time is devoted to solve the chemical scheme (more than 90 chemical reaction and 40 species).

3. RESULTS AND DISCUSSION

Different applications have been carried out over different domains and emission sources. We show different applications: (1) Different simulations to know the air quality impact of a combined cycle power plant in Madrid area; (2) Similar application than in Madrid (Spain) area but in Andalusia (Spain); (3) A study of the impact of the emissions of an incinerator in the Basque Country (Spain) and (4) A real-time air quality forecasting system for Las Palmas de Gran Canaria (Canary Islands, 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 for different years. 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 modeled NO₂ concentrations by MM5-CMAQ at the grid cell where the monitoring station is located (MM5-CMAQ with 3 km spatial resolution). The results show that the MM5-CMAQ air quality modelling system reproduces the observed data satisfactory, however, due to the uncertainity of the emission data, there are some deviations between observed and modelled data. The model follows the trend (decreasing) for the 9-11 October, 2002 period and the maximum peaks for 7-8 October, 2002 are followed by the model in a consistent and satisfactory way.

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. We observe that activation of the power plant produces substantial decreases in the ozone concentrations (up to 9,1 ppb, - 18,2). The maximum impact is focused in the surrounding area of the power plant. Figure 5 shows the map of the differences between ON and OFF scenarios at



Figure 4.- Comparison between observed NO2 concentrations at Móstoles the monitoring station (solid line) and modeled NO2 concentrations by MM5-CMAQ (dotted line) at the grid cell where the monitoring station is located. Period time October, 7-11, 2002



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.

04:00 GMT, July, 8, 2002. The planned power plant 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 shows that the impact is concentrated in the surrounded area of the power plant.

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.

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). In Figure 6 we show a 3D image of the 9 km spatial resolution model domain.

Figure 7 shows the average ozone surface concentrations when the power plant is activated. The averaged period of time is 6-10, August, 2002 and the values show a strong gradient over the model domain (405 x 405 km with 9 km spatial resolution).

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 13 shows the comparison between observed and



Figure 6.- 3D topography corresponding to the 9 km spatial resolution model domain.



Figure 7.- Total O_3 concentrations when operating one combined cycle power plant group, averaged over 120 hours for 6-10, August, 2002.



Figure 8.- Comparison between observed O_3 concentrations (solid line) at the Agurain monitoring station and modeled O_3 concentrations (dotted line) at the grid cell where the monitoring station is located for December, 9-13, 2003.

modeled ozone data for Agurain (Basque Country, Spain) air quality monitoring station. We observe that the comparison is very good, however there is a peak on December, 12, 2003 which is not captured by the model. The remaining pattern of the five days simulation is captured in an excellent way by the MM5-CMAQ air quality modelling system.

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 9 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).

Figure 10 shows an example of the predicted surface concentrations over the Las Palmas de Gran Canaria Municipality area (a domain of 16 x 16 km, with 1 km spatial resolution) for August, 18, 2004 at 08:00 GMT and for ozone concentrations (). All the air quality forecasting systems produced by our laboratory over cities and industrial plants operate under daily basis operational mode which means that the



Figure 9.- Air Quality forecasts in Las Palmas de Gran Canaria provided by the MM5-CMAQ modelling system under daily basis through the web.

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Figure 10.- Example of surface ozone concentrations at 08h00 GMT on August, 18, 2004 as provided through the web.

model simulates 5-6 days in 12 - 20 CPU hours over different cluster platforms starting around 01:00 GMT and ending on the late evening of the same day. The web sites are updated under daily basis operational scheme.

4. CONCLUSIONS

In this contribution we have shown several applications and studies by using the sophisticated MM5-CMAQ modelling system. The system has been proved to be very robust and reliable. The results assure that it is possible to have in realtime 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.

Further work should be done to improve the quality of the emission inventory to optimize the agreement between observations and simulations.

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