

Air Quality-forecasting Impacts from Industrial Sources with an Operational Atmospheric Modelling System. Spain Case Study

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The Asian Conference on Sustainability, Energy & the Environment 2019
Official Conference Proceedings

Abstract

Introducing an integrated software tool to help industrial plants assess the impact of their emissions on air quality in surrounding areas, based on air quality forecasts. It is a tool for mapping the expected exceedances of the EU Air Quality Directive over a large area centered on the industrial plants and the contribution of different emission sources. The system allows identifying in time and space the percentage of inmission concentrations due to industrial plants. The system uses the state-of-the-art of Eulerian models. The air quality forecasting system is highly automated, generating air quality prediction and impact results by each morning for the day following. The zero emission methodology (ON/OFF) has been used. To implement the numerical forecast system, scripts were developed in a Linux environment to automatically execute the various data preprocessor, postprocessors and model codes. Models results are converted to the visualization required format. We present the results of several simulations with 1 km of spatial resolution over Spain. The simulations demonstrate that differences (OFF-ON) show heterogeneity patterns at spatial and temporal scales due to significant topographic diversity and meteorological variations at short distances. The magnitude of these changes in concentration is potentially significant and illustrates the accuracy of the modelling tool and how it can be used in forecasting mode to provide meaningful and relevant information to stakeholders. The results show that the modeling system is capable of determining the impact of emission sources in real time and in forecast mode.

Keywords: Air quality, impact, operational, forecast

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Introduction

Accurately estimating the air quality impact of industrial plant is an important issue reflected in the EU Air Quality legislation. 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 short-term action plans at the appropriate administrative levels. In accordance with this legislation, industrial plants are required to have appropriate control systems in place so that air quality impact can be predicted in real-time and forecasting modes. 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

The ability to reduce emissions in real-time according to a forecast for a specific area and period of time is very challenging. In the past, the ability to forecast air quality in a timely manner was largely limited by computer power and the cost of vector parallel computers. Nowadays, a cluster system using a number of PC processors largely solves this problem in an economic way but it requires that the architecture of the air quality modelling system is carefully designed first. The new generations of air quality modelling systems are capable to simulate in detail atmospheric process which a few years ago was a quite difficult task. Nowadays, the advances in computer capabilities, 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. And the substantial increases in the knowledge in the atmospheric process have also conducted to new possibilities.

To develop cost-effective emission control strategies, methods for identifying the relative contribution of sources to air pollution are useful (Ribeiro et al., 2014). Air quality models have been shown to be useful in determining the spatio-temporal distribution of air pollutants, as they describe the transport and dispersion of air pollutants, as well as chemical and physical processes (Zhang, Bocquet, Mallet, Seigneur & Baklanov, 2012). A typical methodology for knowing the impact of emission sources on air quality is the well-known "brute force" (BF) method, in which the results of a "base" air quality simulation are compared with the results of a changed simulation using an altered parameter or data set (Samaali, Bouchet, Moran & Sassi, 2011). The traditional zero-out method (a case of BF) involves running the model twice: first with base scenario emissions (ON simulation) and then without emissions where the input of emissions from the sources to be studied is set to zero (OFFs simulations). The differences between the two simulations (OFF-ON) estimate the impacts or contributions of the sources. This approach has been used extensively in the past to isolate the response to changes in inputs from complex, non-linear systems such as air pollution (Thunis, Pernigotti & Gerboles, 2013).

The air quality modelling system is based on the below equation. It defines the fundamental relationship governing chemistry and transport in the atmosphere is the mass balance or continuity equation for minor species emitted and mixed into the air (primary pollutants) or generated by chemical transformation of such species (secondary pollutants). The equation describes the change of the concentration C_i of species i with time t .

$$\frac{\partial C_i}{\partial t} = P_i - L_i + E_i + \Delta(K\nabla C_i) - \nabla(vC_i)$$

where P_i and L_i are the chemical production and loss, respectively, and E_i the emission of the species. K represents the eddy diffusivity matrix and v three-dimensional wind vector.

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 (Dandou, 2005) and the ordinary differential equation system for the chemistry module (San José et al., 2005). The mathematical procedures to create an emission inventory are essentially two (José et al., 2002): 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. The system uses the EMIMO model to produce hourly 1 km x 1 km gridded emissions of total VOC's, SO₂, NO_x, CO and particles (PMs).

Air quality modelling system

An air quality modelling system has three fundamental modules, as can be seen in figure 1.

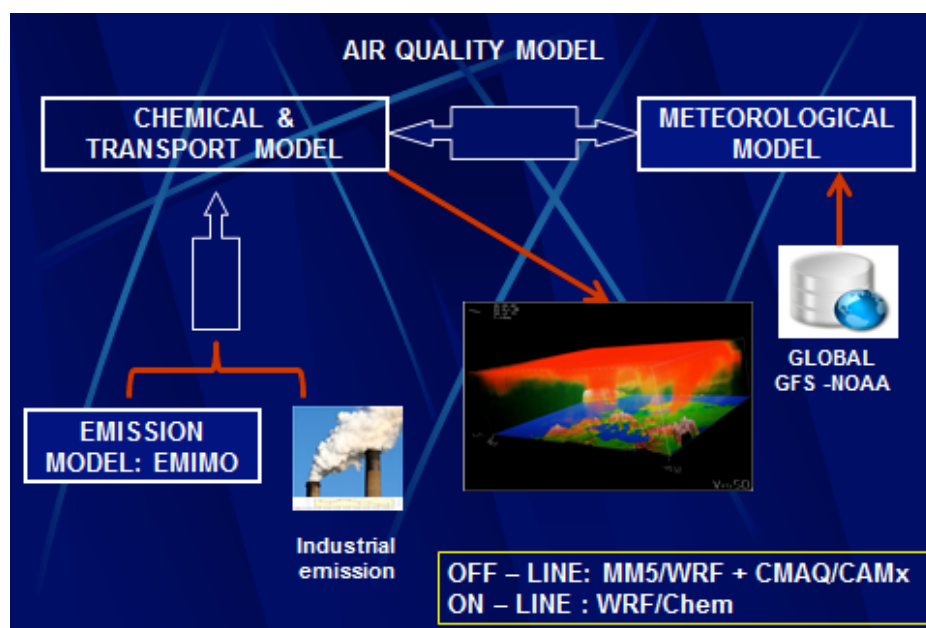


Figure 1: Modules and links for an air quality modelling system.

The chemical and transport module for pollutants, which receives meteorological data and emission data as inputs. The meteorological data are generated by an independent meteorological model or connecting to the chemical module. The meteorological module requires boundary conditions that can be extracted from any global model. Emissions from all sources, including point sources, must be estimated for injection into the atmosphere.

The third generation of air quality models is based on the so-called “one atmosphere” concept. The “One atmosphere” considers the entire atmosphere as a research object, simulating all atmospheric physics and chemical processes at various spatial scales. A commonly used numerical model is the Community Multi-scale Air Quality (CMAQ) modeling system (Byun & Schere, 2006). The meteorological field needed by the numerical calculation of CMAQ is provided by the meteorological models, such as the Mesoscale Meteorological Model 5 (MM5) and the Weather Research and Forecasting (WRF) Model. MM5 is the fifth generation of the National Center of Atmospheric Research/Penn State mesoscale model and WRF is the Weather Research and Forecasting model. MM5 and WRF provide the meteorological input fields for vary air quality models (Appel, Roselle, Gilliam & Pleim, 2010).

In the real atmosphere, chemical and physical processes affect each other. For example, aerosols can affect the balance of atmospheric radiation. Cloud condensation nuclei can also be formed in the cloud, further affecting precipitation. Weather phenomena such as precipitation, wind, or turbulence can affect the Chemical transport and sedimentation process. So, the chemical model is often used in couple with other models. The most popular chemistry coupling model is the WRF/Chem. In the coupled model, the air quality component of the model is fully consistent with the meteorological component; such as, the same transport scheme (mass and scalar preserving), the same grid (horizontal and vertical components), and the same physics schemes for subgrid-scale transport (Grell et al., 2005). WRF-Chem is the Weather Research and Forecasting (WRF) model coupled with Chemistry. WRF is 3-D non-hydrostatic prognostic model that simulates mesoscale atmospheric circulations. Chem model simulates the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology.

EMIMO emission model provides accurate hourly and high spatial resolution (1 km) pollution emission data at global level. Uses data from global emission inventories (TNO-EMEP, EDGAR) and surrogates (Roads, population, land-use) Includes a biogenic module (BIOEMI) for natural emissions European temporal profiles and VOC speciation (Speciate).

To study the impact of a source's emissions on air quality, it is necessary to run several simulations. The flow chart in Figure 2 shows the steps to be performed and the order of their implementation. The first step is to run a meteorology simulation, then the emissions of the base case are estimated, in this case with the active sources, ON and finally the air quality simulation is performed and the reference simulation would be complete. Then, based on the scenarios, the emissions of the source to be studied are adjusted and the air quality simulations are completed with the modified

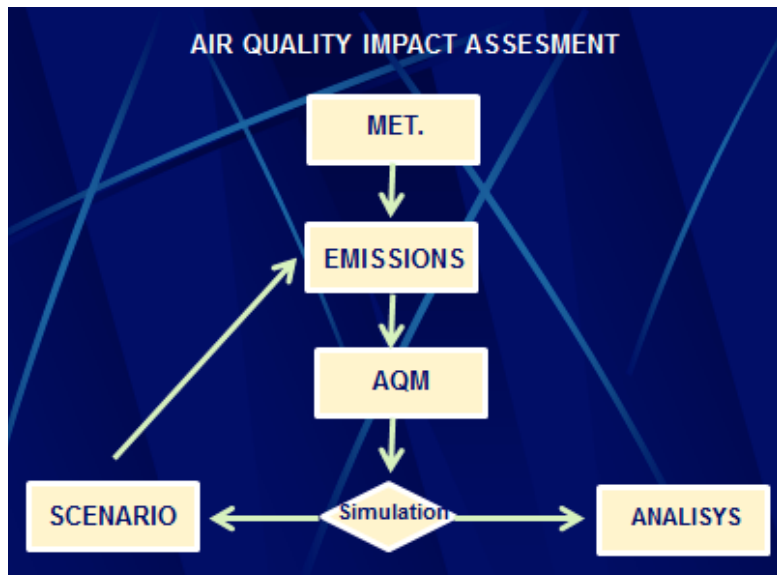


Figure 2: Flow chart of an air quality impact assessment.

The air quality forecasting system is highly automated, generating air quality prediction and impact results by each morning for the day. To implement the numerical forecast system, scripts were developed in a Linux environment to automatically execute the various data preprocessor, postprocessors and model codes. Models results are converted to the visualization required format. Visualization post-processing is done using the Ferret software. The automation of the system is accomplished using TCL and shell scripts.

The web system is based on a combination of data processing programs and visualization tools for the manipulation and visualization of the data produced by the modeling system. The web interface is designed to provide easy access to a wide variety of air quality data produced by the modelling system. The design enables users to explore and analyze datasets in a consistent manner through web services. The tool has a client-server integrated system with a friendly web interface and a modular design which allows optimizing the system to the user requirements. Access is through any standard web browser and HTTP protocol. The user interface and communication dialog is bases on standard HTML, Javascript and PHP, on client side so software requirements are limited to a web browser. The client uses a web browser and the server is running over Linux operating system with the Apache web server. Output maps are dynamically generated that can be interactively controlled and configured by the user. Options include zooming, interactive color scales, animation of dynamic model runs

Results

Before the air quality system starts to predict it is necessary to conduct a process of evaluation and calibration of emissions, to ensure that the system is as accurate as possible. To implement this step, a simulation of at least one year of the past is run, and the results of the model are compared with the results measured by the stations. From this comparison we obtain a series of statistical parameters (bias, root mean square error, correlation coefficient, ...) that allow us to assess the performance of our modelling system. When performing the comparison we must take into account that the data measured by the station are very local and only have validity in a short radius

of influence, while the concentrations predicted by the modeling system correspond to average values of the grid cell that usually have a maximum spatial resolution of 1 km in these systems (San José et al., 2015).

Figure 3 shows a regression analysis between observed data and simulated data corresponding to a Spain case study. It is part of the comparison between ozone observed concentrations at Coslada air quality monitoring station (in the east area of Madrid city, Spain) and modelled with MM5-CMAQ-EMIMO modelling system. The correlation coefficient is 0.854, which is an excellent value that demonstrates a good performance of the air quality modelling system.

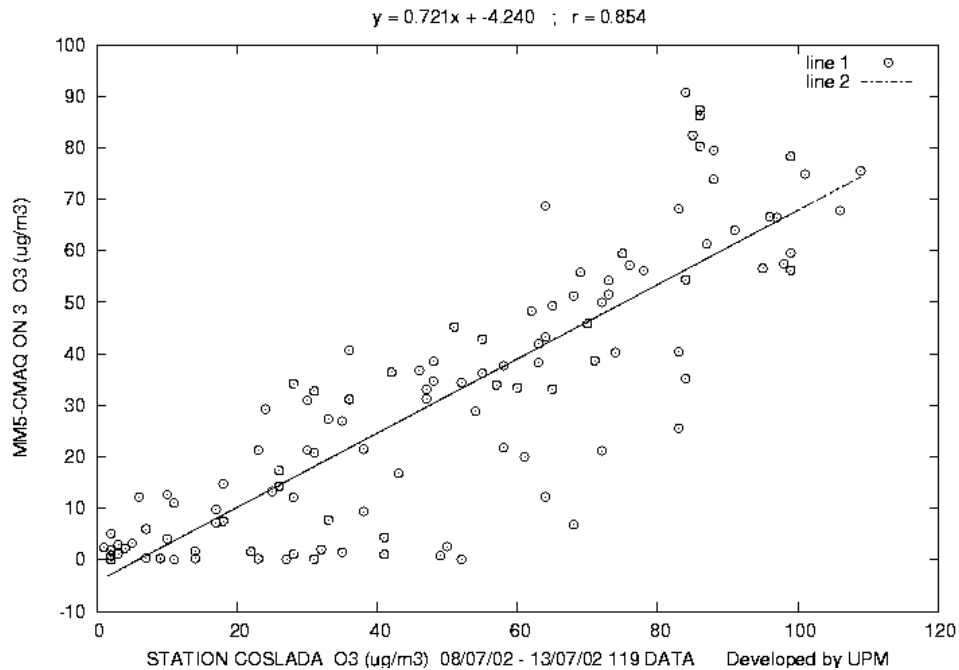


Figure 3: Scatter plot of the modelled and observed O₃ concentrations in Coslada monitoring station (Spain) using MM5-CMAQ-EMIMO modelling system.

In Figure 4 we observe how the NO₂ impact on the surrounding area for the 24 km domain with 1 km spatial resolution. We observe that there are areas with increases of 10 % and decreases up to 2 %. These nonlinear processes change substantially hour by hour. In this case the forecast is done for May, 21th, at 6:00 GMT over the area. The impacts correspond to a emissions from power plant with 400 MW in an area located at the South East of Madrid Metropolitan Area, Spain. The impacts are calculated using the ON-OFF mode which means that it will simulate the scenario representing the full operation (ON) and the emission reduction scenario without operation (OFF).

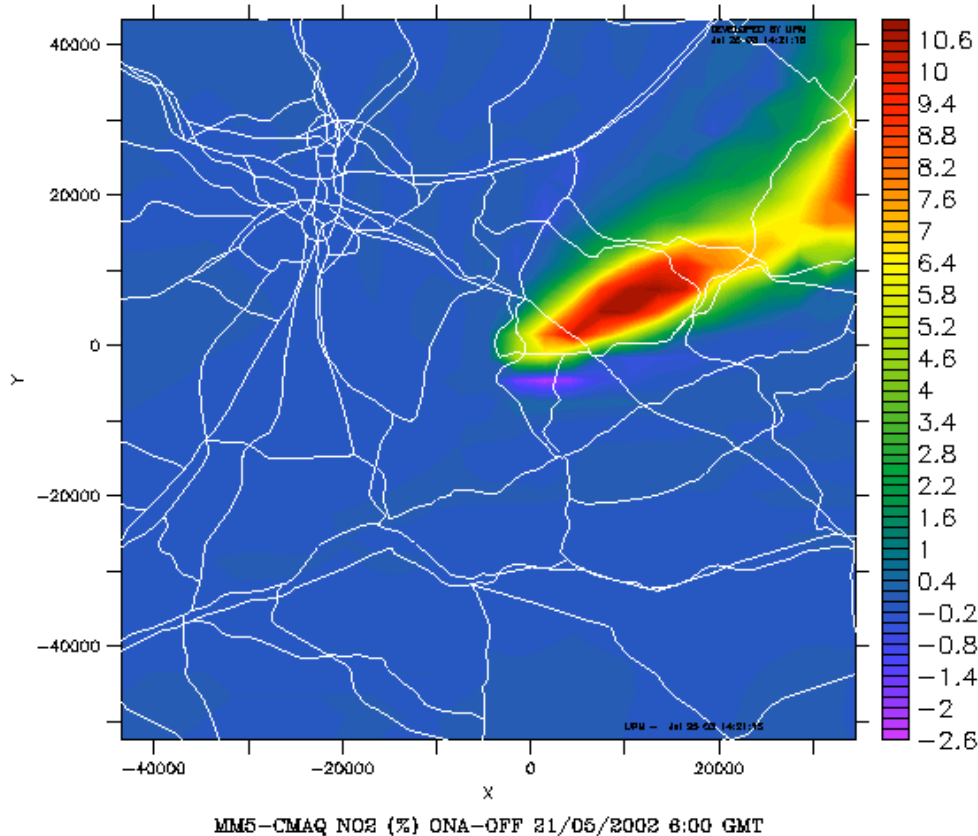


Figure 4: Contribution (ON-OFF) to NO₂ concentrations (%) due to emissions of the power plant.

Figure 5 is an example of a Spain case study. The objective was to analyze the contribution of two elevated point sources (plants for waste or residual treatment) to the Madrid air quality. Identifying in time and space the percentage of inmission concentrations due to the industrial plants. The model has been configured with three unidirectional domains of 25, 5 and 1 km of network separation representing Spain, the Community of Madrid and the city of Madrid with its surroundings. Two elevated point sources have been analysed in this study. Both sources are companies whose activity is focused on waste treatment. The base case or simulations ON, all sources emit. The WRF/Chem modeling system, which is commonly used in air quality prediction studies, was implemented to simulate meteorology as well as the dispersion and transport of pollutants. The next is the OFF simulation, whose emissions from sources 1 and 2 are set to zero. Differences between OFF and ON (OFF-ON) simulations report impacts of the two sources when working together. A year of simulation of the designed architecture spent 32,000 CPU hours. For the entire experiment, 300,000 CPU hours have been spent including calibration processes using 1800 cores.

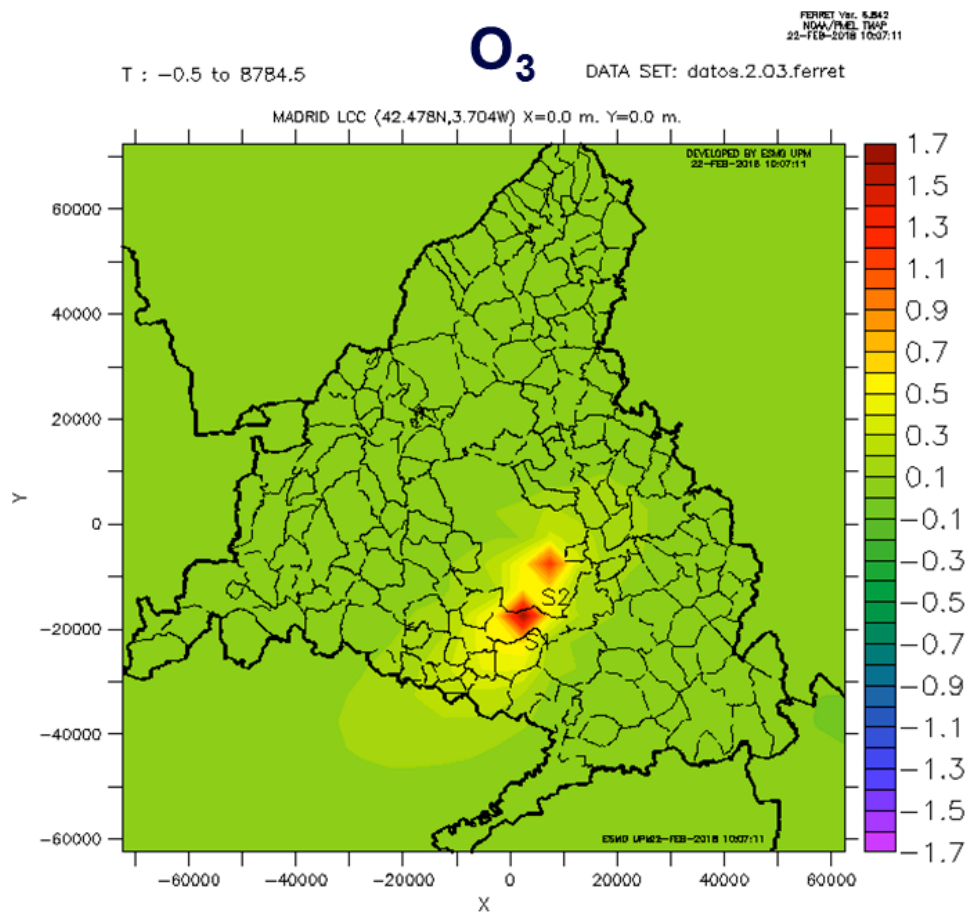


Figure 5: Surface impacts (%) in O₃ yearly average concentration of two elevated point sources (OFF-ON).

Fig. 5 shows the impact (%) of the two emission sources on the yearly average concentration of O₃. S1 is the source with the largest impact, as its emissions are responsible for decreases in O₃ concentrations of up to 1.7 % over an annual average. In areas with NO_x emissions, O₃ is often decreased locally. Areas close to NO_x sources often become O₃ sinks. However, the cycle between NO and NO₂ is fast and NO₂ could be lost through dry deposition and chemistry, and these non-linear processes make it difficult to model NO_x and O₃ concentrations (San José, Pérez, Morant & González, 2008). The efficiency of emission control depends on the relationship between primary and secondary pollutants, as well as environmental weather conditions. Due to the chemical coupling of O₃ and NO_x, the levels of O₃ and NO₂ are closely linked (San José, Pérez, Morant & González Barras, 2009). Therefore, the response to NO_x emission reduction is significantly non-linear and any resulting reduction in NO₂ level is invariably accompanied by an increase in O₃ level (Jose, Perez & Gonzalez, 2008). In addition, changes in the local level of O₃ and NO₂ will lead to an increase in the background level, so it is necessary to obtain a thorough understanding of the relationships between O₃, NO and NO₂ under various atmospheric conditions (San José, Pérez & González, 2008).

Conclusions

An integrated software tool to help industrial plants assess the impact of their emissions on air quality, based on air quality forecasts has been presented. The air quality modelling system includes an emission model (EMIMO) and a pollutant transport and meteorological-chemistry models. The air quality forecasting system is highly automated, generating air quality prediction and impact results by each morning for the day. Scripts were developed in a Linux environment to automatically execute the various data preprocessor, postprocessors and model codes.

The modelling system has been used to analyze the contribution of different elevated point sources with high spatial resolution (1 Km) using a ON-OFF methodology. The system allows identifying in time and space the percentage of inmission concentrations due to industrial plants. The system uses the state-of-the-art of Eulerian models. During the last years the system has been installed in a few more industrial plants running operationally in real-time to provide air quality impact services to industrial plant owners and environmental authorities in Spain with full success.

The system has been evaluated using developed scripts for the diagnostics and assessment of air quality model performances. It fulfils all criteria for correlation, bias, standard deviation and, so it can be used for applications. The evaluation of the performance has been very satisfactory. The simulations showed that point source emissions were contributors to exceedances in the nonattainment areas. Also the sources can reduce the number of O₃ exceedances.

The differences (OFF-ON) distributions show heterogeneity patterns in spatial and temporal scales due to significant topographic diversity and meteorological variations over short distances. The magnitude of these concentration changes is potentially significant and illustrates that accurate of the tool and how it can be used in forecasting mode to provide meaningful and policy-relevant information for the stakeholders

Acknowledgment

The UPM authors acknowledge the computer resources and technical assistance provided by the Centro de Supercomputación y Visualización de Madrid (CeSViMa). The UPM authors thankfully acknowledge the computer resources, technical expertise and assistance provided by the Red Española de Supercomputación.

References

- Appel, K., Roselle, S., Gilliam, R., & Pleim, J. (2010). Sensitivity of the Community Multiscale Air Quality (CMAQ) model v4.7 results for the eastern United States to MM5 and WRF meteorological drivers. *Geoscientific Model Development*, 3(1), 169-188. doi: 10.5194/gmd-3-169-2010
- Byun, D., & Schere, K. (2006). Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. *Applied Mechanics Reviews*, 59(2), 51. doi: 10.1115/1.2128636
- Dandou, A. (2005). Development and evaluation of an urban parameterization scheme in the Penn State/NCAR Mesoscale Model (MM5). *Journal Of Geophysical Research*, 110(D10). doi: 10.1029/2004jd005192
- Grell, G., Peckham, S., Schmitz, R., McKeen, S., Frost, G., Skamarock, W., & Eder, B. (2005). Fully coupled "online" chemistry within the WRF model. *Atmospheric Environment*, 39(37), 6957-6975. doi: 10.1016/j.atmosenv.2005.04.027
- Jose, R., Perez, J., & Gonzalez, R. (2008). An incinerator air quality impact assessment for metals, PAH, dioxins and furans by using the MM5-CMAQ-EMIMO atmospheric modelling system: Spain case study. *International Journal Of Environment And Pollution*, 32(2), 250. doi: 10.1504/ijep.2008.017105
- José, R., Salas, I., Martín, A., Pérez, J., Carpintero, A., & Ramos, M. et al. (2002). Development of A Global-Through-Urban Scale Nested Air Quality Forecast Model (RSM-ANA): Application Over the Madrid Domain. *Systems Analysis Modelling Simulation*, 42(11), 1551-1560. doi: 10.1080/716067177
- Ribeiro, I., Monteiro, A., Fernandes, A., Monteiro, A., Lopes, M., Borrego, C., & Miranda, A. (2014). Air quality modelling as a supplementary assessment method in the framework of the European Air Quality Directive. *International Journal Of Environment And Pollution*, 54(2/3/4), 262. doi: 10.1504/ijep.2014.065127
- Samaali, M., Bouchet, V., Moran, M., & Sassi, M. (2011). Application of a tagged-species method to source apportionment of primary PM_{2.5} components in a regional air quality model. *Atmospheric Environment*, 45(23), 3835-3847. doi: 10.1016/j.atmosenv.2011.04.007
- San José, R., Pérez, J., & González, R. (2008). The evaluation of the air quality impact of an incinerator by using MM5-CMAQ-EMIMO modeling system: North of Spain case study. *Environment International*, 34(5), 714-719. doi: 10.1016/j.envint.2007.12.010
- San José, R., Pérez, J., Morant, J., & González Barras, R. (2009). The Use of Modern Third-Generation Air Quality Models (MM5-EMIMO-CMAQ) for Real-Time Operational Air Quality Impact Assessment of Industrial Plants. *Water, Air, & Soil Pollution: Focus*, 9(1-2), 27-37. doi: 10.1007/s11267-008-9196-4

San José, R., Pérez, J., Morant, J., & González, R. (2008). European operational air quality forecasting system by using MM5–CMAQ–EMIMO tool. *Simulation Modelling Practice And Theory*, 16(10), 1534-1540. doi: 10.1016/j.simpat.2007.11.021

San José, R., Pérez, J., Balzarini, A., Baró, R., Curci, G., & Forkel, R. et al. (2015). Sensitivity of feedback effects in CBMZ/MOSAIC chemical mechanism. *Atmospheric Environment*, 115, 646-656. doi: 10.1016/j.atmosenv.2015.04.030

San José, R., Stohl, A., Karatzas, K., Bohler, T., James, P., & Pérez, J. (2005). A modelling study of an extraordinary night time ozone episode over Madrid domain. *Environmental Modelling & Software*, 20(5), 587-593. doi: 10.1016/j.envsoft.2004.03.009

Thunis, P., Pernigotti, D., & Gerboles, M. (2013). Model quality objectives based on measurement uncertainty. Part I: Ozone. *Atmospheric Environment*, 79, 861-868. doi: 10.1016/j.atmosenv.2013.05.018

Zhang, Y., Bocquet, M., Mallet, V., Seigneur, C., & Baklanov, A. (2012). Real-time air quality forecasting, part I: History, techniques, and current status. *Atmospheric Environment*, 60, 632-655. doi: 10.1016/j.atmosenv.2012.06.031

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