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KEYNOTE

Air quality impacts forecasting system for industrial air emissions running in operational mode

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Abstract: This paper shows how a predictive air quality system has been implemented in operational mode to predict the impact of emissions from industrial sources, in particular the implementation of this system in two industrial complexes near Madrid in Spain. Atmospheric emissions from point sources located around cities have a great influence on the concentrations of urban pollutants, since the transport of pollutants can bring them into the city depending on the meteorology at any given time.

The demand for electricity is growing worldwide and therefore more and more power plants are being built around cities, which can have an impact on urban air quality. This makes it necessary to know what impact the emissions of these power industries have on their environment, considering a wide area of tens or hundreds of kilometers, on the concentrations that city dwellers breathe. This is where modelling tools play a very important role. These tools make it possible to model and therefore predict the impact of emission sources in advance, enabling the authorities to take decisions on the operation of the industry to avoid pollution problems detected by the tool. The tool also allows the evaluation of different operating strategies of the industry in order to know in advance which is the most efficient to minimize or even avoid exceeding the values set in the air quality directive.

The air quality modelling system is based on the OPANA model, which consists of several modules. Its main modules are the meteorological model MM5, the transport and chemistry model CMAQ, and finally the EMIMO module for estimating emissions injected into the atmosphere.

The system is applied to model the impact of a power industry containing 4 combined cycle power plants. A base simulation is made to know the future impact of the groups and then several scenarios are simulated where each of the groups are disconnected, which allows us to see what impact each one has and if it is necessary to disconnect to avoid exceeding the directive, we have all the information to apply the most efficient strategy to avoid air quality problems and to have the least possible impact on the energy production of the industry.

The implementation of this system requires a cluster-type computational platform with several computational nodes that allow to have the prediction in time and from one day to the next. All the information produced by the system is updated daily in a web system that allows both system operators and policy makers to know if any pollution episode will occur and how it could be avoided if it can be avoided.

Before going into operational mode, the system is evaluated for its performance, i.e. the outputs of the modeling system are compared with the observed values of pollutants with monitoring stations. The performance of the simulation tool is good based on the correlation coefficients. The system is successfully operating in two industrial plants located in the surrounding area of Madrid. he confidence and accuracy of the atmospheric model is critical for the performance of the complex system.

In order to know the impacts of each of the emitting sources, it is based on the brute force or ON-OFF methodology, where the ON simulation includes all the emitting sources and in the OFF simulation some of the sources of which the impact is to be known are deactivated. New generations of the system are available, changing the meteorological and pollutant transport model to a single model, called WRF/Chem, which integrates meteorology and air quality in a single computational code. In any case, these types of tools are fundamental in helping stakeholders to make decisions.

Keywords: *Emissions industrial impact, mesoscale modeling, forecasting, air quality*

1. INTRODUCTION

The concept of real-time is based on being able to take actions in advance and that have been previously evaluated for their effectiveness in order to avoid exceeding the limit values set by air quality directives. The system may also conclude that the expected exceedance cannot be avoided because emissions from its industry are not the main contributor to the exceedance. 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 inadequate computer power and the cost of vector parallel computers. Nowadays, cluster system composed of PC processors provide an acceptable capability—once we have designed a proper architecture of the air quality modelling systems—to run these complex systems in real-time and forecasting mode (Pospisil et al., 2004). 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 and 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.

Dispersion models are commonly used tools in atmospheric science for estimating the dispersion and transport of pollutants emitted from various sources. These models use mathematical algorithms to simulate the behavior of pollutants in the atmosphere based on meteorological data, emission rates, and other environmental factors. Dispersion models have been widely utilized to assess the air quality from different sources as traffic (Venkatram et al. 2007) and industry (Lopez et al, 2005). By isolating individual sources, these models can provide valuable information for source management and relevant policymaking. The effectiveness of dispersion models in estimating pollutant concentrations has been extensively studied and validated through comparisons with field measurements (Brown et al, 2015). Gaussian dispersion models are widely used in atmospheric science for estimating the dispersion and transport of pollutants emitted from various sources. These models use a Gaussian distribution to describe the concentration of pollutants as a function of distance from the source, and they typically use measured upwind rural concentrations to represent long-range transport. This approach has been successful in modeling historic periods, but it has limited applicability for assessing future scenarios, including those related to climate change or the local effects of regional emissions changes. Additionally, the use of a limited number of upwind monitoring sites can make the upwind concentration data less representative and does not allow for variations over a large area. To overcome these limitations, Eulerian coupled air quality models can be used. These models use a grid-based approach to simulate the behavior of pollutants in the atmosphere. This approach allows for the modeling of future scenarios and the assessment of the local effects of regional emissions changes. Eulerian models also allow for the simulation of pollutant concentrations over a large area, capturing variations that may exist.

The complete tool designed for this application is called TEAP (a Tool to Evaluate the Air quality impact of industrial Plants) (San Jose et al., 2003). 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 the system with the so-called OPANA model. 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 are not included (aerosol and aqueous chemistry). Since OPANA includes many scripts to communicate the different modules, the name "OPANA" has been maintained to include different meteorological and dispersion models but keeping all the software framework to operate in historical and forecasting models. When the OPANA system is applied for operational forecasting air quality impact analysis, the system is called TEAP.

2. AIR QUALITY MODELLING SYSTEM

Further versions of the model included MM5 and CMAQ (Byun et al., 1998) as part of the meteorological module and chemistry transport module. The system includes and emission model, EMIMO, which has also different version which includes biogenic and anthropogenic emissions with different updated version of the global or European emission data base. Actually, OPANA V4 includes a sophisticated CFD (Computational Fluid Dynamics) code (Moussiopoulos et al., 2005) which runs in diagnostic mode over a 1 km x 1 km model domain over highly dense populated areas in cities (Madrid, Las Palmas de Gran Canaria, etc.). The CFD code

(Ehrhard, et la., 200) is called MICROSYS and has a resolution 1-10 m (Pullen et al., 2005) receiving traffic emission data from a sophisticated cellular automaton model (CAMO) – developed also by the ESMG-FI-UPM. This CFD code receives the initial and boundary conditions from the mesoscale part of the model (typically MM5-CMAQ-EMIMO). OPANA V3 is used in several forecasting applications for urban and industrial sites but it does not include the CFD part. The CMAQ model is implemented in a consistent and balanced way with the MM5 model (Grell et al. 1997).

The CMAQ tool is a transport and chemical model based on the atmospheric diffusion and advection equation and the gas-phase chemistry. The species continuity equation in generalized coordinates is given as:

$$\frac{\partial(\varphi_i J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\varphi_i J_s V_s}{m^2} \right) + \frac{\partial(\varphi_i J_s \dot{s})}{\partial s} = J_s Q_\varphi \tag{1}$$

where φ_i is the trace species concentration in density units (e.g., kg m $^{-3}$), J_s is the vertical Jacobian of the terrain-influenced coordinate s, m is the map scale factor, V_s and $\dot{s}$ are the horizontal and vertical wind components in the generalized coordinates, and Q_φ is the source or sink term. To make the instantaneous species continuity equation useful for air quality simulation, we need to derive the governing diffusion equations. This is done by decomposing the variables in equation 2.1, except for the Jacobian and map scale factor, in terms of mean and turbulent components. The Reynolds decompositions of species concentration and mixing ratio are expressed as: $\varphi_i = \overline{\varphi_i} + \varphi_i^{''}$; $q_i = \overline{q_i} + q_i^{''}$ and $\overline{\varphi_i} + \varphi_i^{''} = q_i^{''}\overline{\rho} + \overline{q_i}\rho^{''} + q_i^{''}\rho^{''}$, where $q_i = \frac{\varphi_i}{\rho}$ is the species mass mixing ratio and a stochastic quantity is decomposed into mean.

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. 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 landuse 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 (photosynthetic active radiation).

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3. EXPERIMENT

In this application we have applied the MM5-CMAQ modelling system over a power plant 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—are 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 represents the complete disconnection of the 4 400 MW combined cycle power plant groups and the subsequent zero emissions from the power plant.

4. RESULTS

The system was calibrated for 60 days selected periods by using 5 day periods per month along one year. In order to strike a balance between the CPU time required for calibration and the need to select representative days from each month, a period of 60 days was chosen. This allows for enough time to calibrate the model while still being able to choose 5 days that are representative of each month. By selecting representative days, the model can better capture the variability of atmospheric conditions throughout the year and provide more accurate predictions of air quality. However, it is important to note that the choice of these representative days should be carefully considered and based on relevant meteorological and pollutant concentration data. 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.

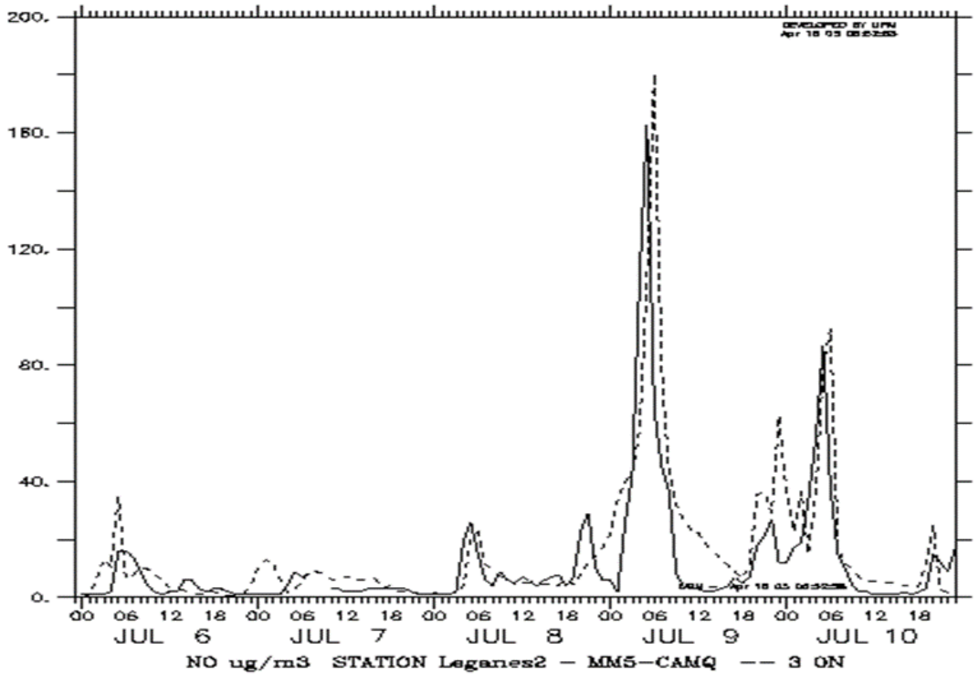

Figure 1. Comparison between NO observations and simulated data in Leganes (Spain) by using TEAP tool for analyzing the impact of emissions from combined cycle plants.

Figure 2 shows the comparison between hourly data during one year in Madrid area. The values presented in the figure are obtained after averaging the observed (monitoring stations) and simulated (cell averaging) values for the different monitoring stations. The correlation coefficient is excellent (0.8) if we take into account that typically the correlation coefficient for these type of experiments is around 0.6. In the context of air quality simulation, a correlation coefficient of 0.8 would be considered excellent because it indicates a strong positive correlation between the modeled and observed pollutant concentrations. This means that the model is able to accurately capture the trends and patterns of the observed data, and that the predicted pollutant concentrations are highly correlated with the actual concentrations. However, it is important to note that a correlation coefficient alone cannot provide a complete assessment of the model's performance. Other factors, such as the model's ability to capture the spatial and temporal variability of pollutant concentrations, should also be taken into account when evaluating the model's performance Clearly, the lowest values are much more difficult to match with the model but in this case, the model performs very well.

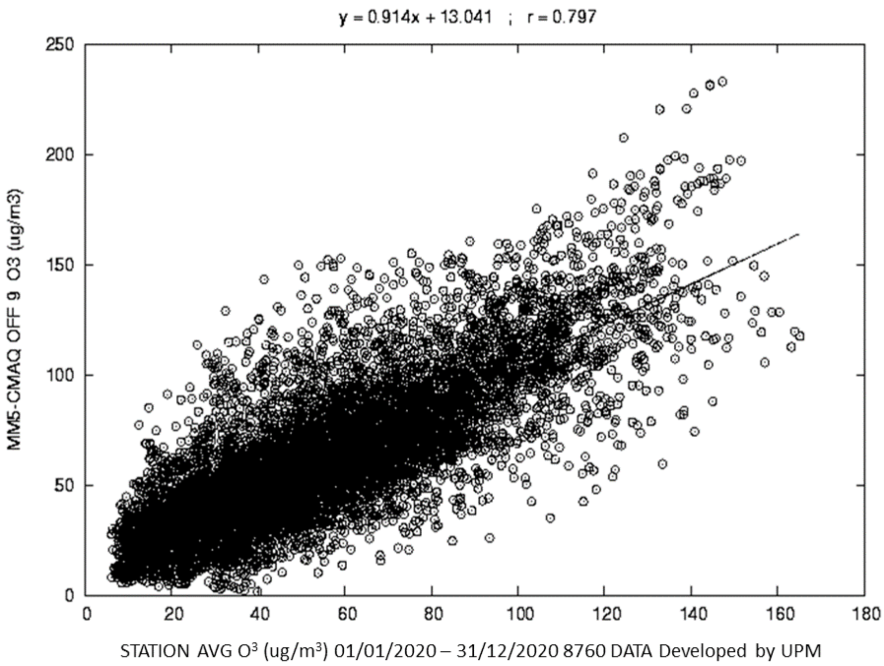

Figure 2. Comparison between observed and modelled data for hourly data during one year. The observed data is an average of Madrid community monitoring stations on an hourly basis and the simulated data is an average of the simulated hourly values in the grid cells where monitoring data is located. The correlation coefficient is 0,797.

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. The excellent correlation coefficients shown can be imp-proved mainly with better emission data. The emission data is the module with the highest uncertainty in the whole system. The system is the first operating in Spain by using such a sophisticated 3rd Generation Air Quality Modelling System. 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 was applied in a Combined Cycle Power Plant located in the south area of Madrid and a third application was implemented for a cement company located in the southeast part of Madrid. Figure 3 shows two examples of the web site which is restricted to environmental authorities and company users.

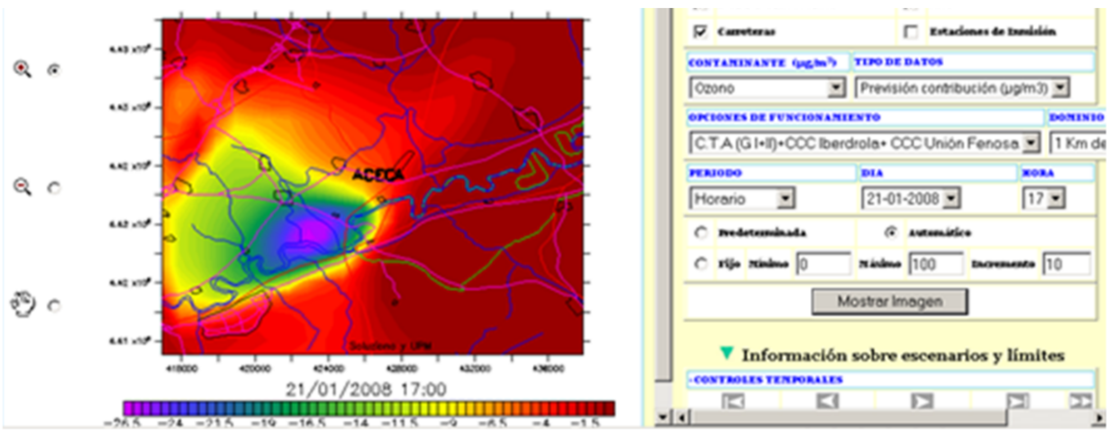

Figure 3. Power plant air quality impact operational system located in the south region of Madrid, Spain

In Figure 4 we see the percentage of O3 contribution of the power plant to the surrounding area (81 × 93 km). We observe that with very low average winds (see small arrows in the map) there are two clearly detected hot spots, one red hot spot with increased impacts up to 4 % and one blue hot spot with decreased impacts up to 5,4 %. In all cases and in general terms the impacts are small but the tool is clearly very precise in detecting the areas in time and space. In this particular case the forecast is done with 24 hours but in other applications we have scenarios up to 7 days' forecasts. In Figure 5 we observe the time evolution of the SO2, O3 and NO2 concentration in a specific location of the high spatial resolution domain (1 km and 24 km x 24 km). The SO2 contribution percentage does not have any change during this day because no emissions from the power plant occurred; however, the percentage contributions to O3 and NO2 are changing from positive contributions (increases) and negative contributions (decreases). The maximum contributions on this day are ranged between +17% to -12 % at different hours and for that specific location (close to the power plant position).

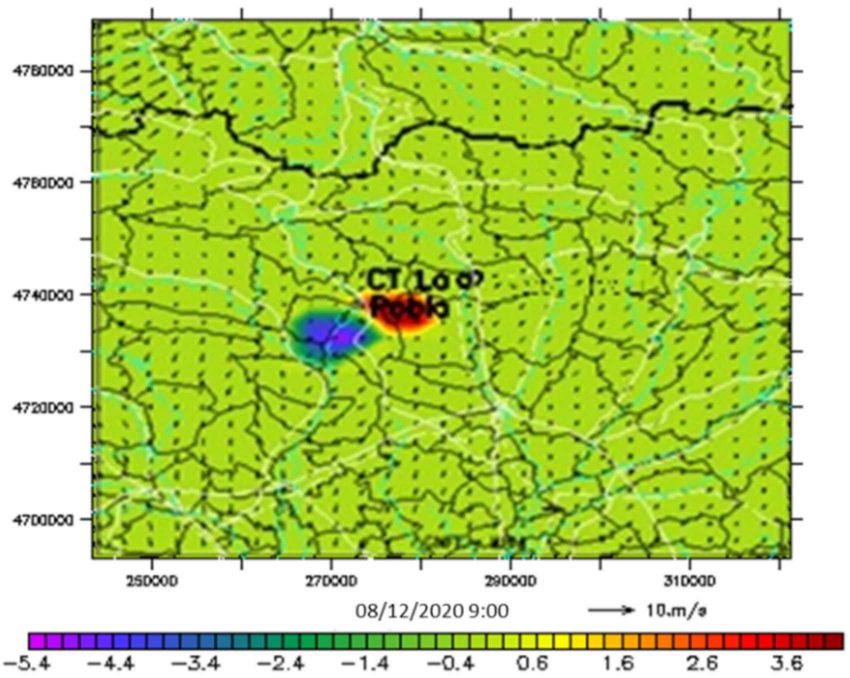

Figure 4. Contribution to O3 concentrations (%) due to emissions of the power plant

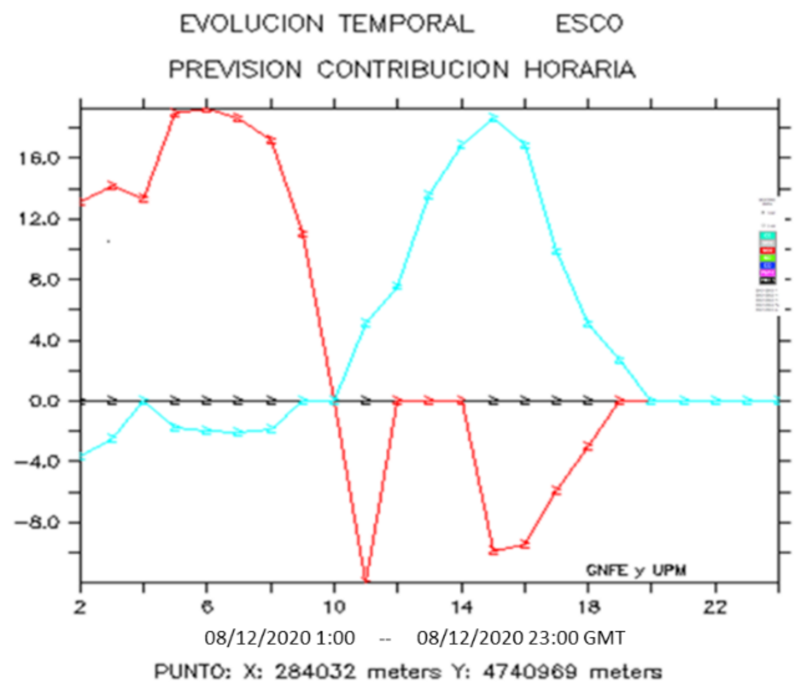

Figure 5. Time evolution of the contribution of the power plant to the O3, NO2 and SO2 air concentrations in the high spatial resolution domain

5. CONCLUSIONS

We have developed an air quality complex modeling system based on MM5-CMAQ-EMIMO system, which incorporated full chemical mechanisms and runs in operational mode to produce daily air quality forecasts of the different emission scenarios based on the so-called ON and OFF modelling approach. This means that the system includes all emission data—traffic, surrounding industry, biogenic emissions, etc.—in order to simulate the observational data set obtained in the pollution monitoring network located in the area, in the ON mode. The OFF mode is exactly the same that the ON mode but switching off the emissions of the scenario to consider in the industrial plant. The results offer detailed full information for the next 72 hours of the impact on ozone, NOx, etc. concentrations of the emissions of the different industrial operational modes. The system is successfully operating in two industrial plants located in the surrounding area of Madrid. he confidence and accuracy of the atmospheric model is critical for the performance of the complex system. New generation of on-line air quality models such as WRF/Chem are expected to be used in the near future to improve the accuracy and confidence of the air forecasted air concentration levels. The forecasted industrial emissions are also a key element in the complexity of the system. The industrial emission forecasts are produced by the industrial company and are also affected by the corresponding uncertainty. Additional efforts are needed to reduce the uncertainty of the emission sources and the physical and chemical parameterizations included in the atmospheric dispersion and chemical models. The system is 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.

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