Air quality real-time operational forecasting system for large industrial plants: an application of MM5-CMAQ modelling system

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Abstract

The advances in air quality modelling have been substantial in the last decade. Nowadays, air quality modelling systems are capable to provide accurate information on the impact of different sources in relation to the total air pollution concentrations in real-time and in forecasting modes. In this contribution we show the results of the impact of five different industrial plants on a mesoscale domain by using MM5-CMAQ as the air pollution modelling system. The system has been implemented by using an emission model which includes antropogenic and biogenic emissions. The system is tested in real-time and in forecasting mode by implementing the “base case” in routine operational mode which includes emissions of five large industrial plants operating in a test area located at the south of the Madrid city domain. The sensitive cases include the impact of disconnecting the emissions of each of the industrial plants completely and also the scenario of disconnecting 50% of the total emissions for each industrial plant. The results show that the modelling system is capable of determining the impact of the different emission scenarios in real-time and in forecasting mode. The emission patterns have been implemented in a 72/120 hours pattern which means that after 72 hours the emissions are reduced completely or to 50% to evaluate the impact on the air pollution concentrations.
1 Introduction

The new generation 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 and the substantial increase in the knowledge in the atmospheric process have conducted to new possibilities. In this contribution we have used the OPANA V3.0 air quality modelling system which is a framework of different air quality models and utilities. The MM5 model (PSU/NCAR) [2] for producing meteorological fields in 4D mode and CMAQ model (Community Multiscale Air Quality Modelling System / Models-3 / EPA, U.S.) for chemical and dispersion of pollutants are used as part of OPANA V3 tool ([1]). CMAQ is a chemical dispersion model which is representative of the third generation of air quality models which includes clouds, aqueous and aerosol chemistry.

Industrial plants (including power generators) produce a considerable amount of pollution although in the last decade the technology has improved significantly and the total emissions have been reduced substantially. In spite of that, industrial sources are important cause of air pollution in the surrounding areas.
Table 1: Characteristics of the pollution emissions from the five different virtual industrial plants and geographical locations in the 3 km resolution domain (81 km x 99 km).

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>X (Lambert Conformal)</th>
<th>Y (Lambert Conformal)</th>
<th>Chimney Characteristics</th>
<th>All chimneys have the same characteristics</th>
<th>Emissions</th>
<th>All virtual industrial plants have the same emissions</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>500</td>
<td>500</td>
<td>Diameter</td>
<td>6.5 m</td>
<td>PM</td>
<td>1.9 g/s</td>
</tr>
<tr>
<td>B</td>
<td>20000</td>
<td>30000</td>
<td>Height</td>
<td>60 m</td>
<td>VOC</td>
<td>2.4 g/s</td>
</tr>
<tr>
<td>C</td>
<td>20000</td>
<td>-40000</td>
<td>Temperature</td>
<td>377 K</td>
<td>CO</td>
<td>8.9 g/s</td>
</tr>
<tr>
<td>D</td>
<td>0</td>
<td>-40000</td>
<td>Gas velocity</td>
<td>21.59 m⁻¹</td>
<td>NOx</td>
<td>34.56 g/s</td>
</tr>
<tr>
<td>E</td>
<td>-20000</td>
<td>-20000</td>
<td>Flux</td>
<td>716.38 m⁻¹</td>
<td>SO2</td>
<td>2.07 g/s</td>
</tr>
</tbody>
</table>

Figure 2: Scheme of the hardware and software architecture for the evaluation of the impact of the five virtual industrial plants with two different emission reduction scenarios for each one (100 - 50%).

In this contribution we will use state-of-the-art meteorological and chemical dispersion models (MM5/CMAQ) [3,4,5] for obtaining the impact in time (120 hours) and space (4D and 2 nesting levels) of the industrial emissions in the air pollution concentrations. The complete software tool, OPANA V3, shows the
portion of air pollution concentration (for all pollutants), in absolute and relative value, due to the industrial plant emissions. Furthermore, in this contribution we have simulated five different virtual industrial plants in a domain located in the South East area of Madrid city. Simulations involving the impact of the five sources and the impact of 50% emission reductions are reported. Results show that the tool is capable to control the impact of several industrial plants simultaneously and even different emission reduction strategies.

![Graph showing ozone concentration comparison](image)

**Figure 3:** Comparison between ozone observed concentrations at Coslada air quality monitoring station (in the south area of Madrid city) and modelled with MM5-CMAQ switching off the five virtual industrial plants.

## 2 Methodology

Traditionally Eulerian models have not been used for evaluating the air quality of industrial plants because the complexity of the models and the low sensitivity to determine the portion in the inmission due to industrial plant emissions. Local
meteorology has a significant impact on the impact of industrial sources. MM5/CMAQ has the capability to quantify and qualify the impact on air pollution concentrations of different emission sources because of the high sensitivity of the architecture and atmospheric science included. Chemical mechanisms (CBM-IV, RADM, SAPRAC, etc.) can trace the pollution concentration changes with high degree of accuracy.

![Figure 4: Regression analysis between observed data and simulated data during this experiment when all virtual industrial plants are emitting (ON mode).](image)

The methodology involved in this contribution is to simulate the atmospheric process over a domain (2 nesting levels) with MM5-CMAQ and an emission model (in our case, EMIMO) to obtain a 4D dataset with the pollution concentrations in time and space for the simulation period. Five different virtual industrial sources have been implemented in the area domain. This is called ON mode. The model has been implemented over one domain of 9 km resolution and the area domain is 405 km and for the 3 km spatial resolution model domain with the dimensions of 81 km x 99 km. These are CMAQ model dimensions.

In all cases (MM5 and CMAQ [6,7]) 23 vertical layers are used with 100 mb as top level height. Five different vertical industrial emission sources have been implemented in the 3 km model domain (81 km x 99 km). Table 1 shows the UTM coordinates for the five virtual industrial sources. Figure 2 shows the architecture of the software and hardware design for five different virtual...
industrial sources (although with the same geometrical and emission characteristics).

Figure 5: Boundary Layer height surface pattern at 05h00 GMT on July, 10, 2002 by using the MM5-CMAQ air quality modelling system.

The full system was designed to run the ON scenario as reference case and the two different emission reduction scenarios (50, 100%) for each virtual industrial source for 120 hours, July, 8-12, 2002. The calibration phase consisted to run the full system without emissions from the five different virtual industrial plants and compare the results with the air quality monitoring network in Madrid domain. Figure 3 shows a comparison between observed and modelled ozone concentrations at Coslada air quality monitoring station (located at the East area of Madrid). Figure 4 shows the linear regression analysis for Figure 3 data sets.
3 Results

The system took 140 CPU hours in a Pentium IV, 3.06 Ghz, 1 Gbyte RAM. The 12 CMAQ simulations – two emission reduction scenarios (50 and 100%) for each virtual industrial plant and one for ON mode (all virtual industrial plants emitting) and CAL mode (the five virtual industrial plants are not emitting at all) for 9 km and 3 km spatial resolutions took 70% of the total CPU time. Post-processing analysis took 25% of the total CPU time. The system could be mounted in a PC cluster with 20 PC to obtain about 10 times speed-up in the CPU time which will make the system to be “operational” under daily basis operations since the total CPU time will be about 14 hours.

Figure 6: Percentage of change for NO2 at 03h00 GMT on July, 12, 2002 between ON mode and CAL mode (switching off the five virtual industrial plants) ((ON-OFF)/ON*100).

The system generated a total of 134139 files which mostly are hourly images of the different combinations between OFF, 50%OFF and ON (excluding switching off more than one virtual industrial plant). A total of 2,91 Gbytes were generated. Figure 5 shows – as an example – the boundary layer height (in
geographical projection) at 05h00 GMT on July, 10, 2002. Figure 6 shows the percentage differences between ON mode and switching off all virtual industrial plants (mode CAL) for NO2 on July, 12, 2002, 03h00 GMT.

4 Conclusions

We have built a tool which implements an adaptation of the MM5-CMAQ modelling system named OPANA V3. The system shows an extraordinary capability to simulate all changes produced when five different virtual industrial plants are implemented in the 3 km resolution and 9 km resolution model domains. We have analysed more 11 scenarios corresponding to 100% and 50% emission reduction for each virtual industrial plant and CAL scenario (all virtual industrial plants are switched off). The results show that the system can be used as a real-time and forecasting air quality management system for industrial plants. The system requires to be mounted in a cluster platform in order to handle the CPU times required for such daily simulations.

Acknowledgements

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References

