The use of MM5 for operational ozone/NOx/aerosols prediction in Europe: strengths and weaknesses of MM5

R. Vautard[1], M. Beekmann[1], B. Bessagnet[2], N. Blond[3], A. Hodzic[1], C. Honoré[2], L. Malherbe[2], L. Menut[3], L. Rouil[2], J. Roux[1]

1: Institut Pierre-Simon Laplace, CNRS, Paris, France
2: INERIS, Verneuil en Halatte, France
3: Laboratoire interuniversitaire des Systèmes Atmosphériques, CNRS, Créteil, France

1. Introduction

During the last twenty years or so, the routine operational air quality forecasts have been carried out by statistical models, mostly because (i) these models are easy to handle and tune and (ii) photochemical smog is fairly well correlated to a few number of variables like temperature and wind. chemistry-transport models (CTMs), on the other side, even though possibly less accurate than statistical models in predicting air quality indices carry much more useful deterministic information, for instance about the origin of bad air quality. The progresses in chemistry-transport modelling nowadays allows the use of these models as predicting tools, both for short-term forecasts and for the evaluation of long-term emission abatement strategies.

Several European CTMs predict pollutant concentrations in forecast (Tilmes et al., 2000; Vautard et al., 2001) or simulation mode. The system that we describe here is based on the CHIMERE model (Schmidt et al., 2001; Bessagnet et al., 2004, see also the web site http://euler.lmd.polytechnique.fr/chimere) and was among the first to deliver, on a public basis, real-time ozone forecasts, since Summer 2000. This system has undergone evaluation and improvements based on experimental forecasts during the PIONEER (Prévision et Incertitude de l'Ozone à l'Echelle Européenne et Régionale) project in 2001 and 2002 (see web site http://euler.lmd.polytechnique.fr/pioneer). During this phase, chemical forecasts were forced by large-scale meteorological forecasts coming from the ECMWF, NCEP and Météo-France weather services.

Since Summer 2003, the French ministry of ecology and sustainable development supports the operational forecasting system (http://www.prevair.org) which is hosted by the INERIS institute and relies on MM5 european forecasts themselves forced by the NCEP AVN model. Forecasts of ozone, nitrogorgen dioxide, PM10 and PM2.5 are available on a routine basis. The whole air quality forecasting system also includes forecasts issued from another CTM, MOCAGE, developed by Météo-France. The two modelling system running in parallel allow comparisons and estimation of uncertainty. This operational service also provides routine ozone analyses for France based, like in meteorology, in a combination of observations and model forecasts.

At our institute (IPSL), and within a project with the Paris air quality monitoring organization, AIRPARIF, MM5 and CHIMERE forecasts are also carried out on an experimental basis at the smaller scale of the city of Paris and its suburbs, with a resolution of about 5 km.

The chain AVN+MM5+CHIMERE is not only used for forecasts but also for long-term simulations in order to verify the CTM skill in a pure simulation mode for ozone and aerosols.

In this paper, we report the skill of the whole system in simulating and forecasting ozone and aerosols and the ground level. The analysis of the skill suggests several problems linked with the mesoscale MM5 model and provide directions for improvement for the future WRF model as far as air quality is concerned

2. The air-quality simulation, forecast and analysis system

The air quality simulation/forecast system includes a version of MM5 over Western Europe with a 36 km resolution and 25 levels from surface to 100 hPa, including 17 layers for the description of the boundary layer below 700 hPa. MM5 is forced at the boundaries by AVN/NCEP 6-hourly analyses or forecasts. Nudging is applied over the whole simulation period in order for MM5 not to diverge from the original forecast. By trial and errors it was found that a nudging time scale of 10000 s for temperature and wind and 50000 s for humidity was optimal. MM5 is used with the Grell et al. (1994) parameterization for convection, the MRF boundary layer scheme, the RRTM radiation scheme, and the Schultz (1995) microphysics. In the boundary layer scheme, the convective velocity scale VCONV used to calculate friction velocity is replaced by VCONV=1.1w*, as suggested by Beljaars (1994). However, in order to ensure numerical stability, the standard convective velocity w* is not calculated using the actual boundary layer height, but rather a depth scale fixed to 1500m. The effect of this change is to reduce the excessive friction velocity obtained with the previous parameterization in the case of a high vertical resolution near the ground.

Figure 1 shows an example of the MM5 wind field. simulated in an extremelely anticyclonic hot weather condition during the August 2003 european heat wave. The MM5 output fields are then provided to the CHIMERE CTM (Schmidt et al., 2001; Vautard et al., 2003; Bessagnet et al., 2004) in order to make a chemical simulation or forecast. Wind fields are used to transport pollutants. 3D Temperature and humidity are used in the chemical module, surface parameters (friction velocity, fluxes) are used to recalculate vertical diffusivities and parameters for dry deposition. Liquid water and precipitations are used for wet scavenging of aerosols. Biogenic emissions of isoprene, alpha-pinene, and nitrogen monoxide (due to microbiological transformations of fertilizers) use 2m-temperature. Finally, in the latest versions of the model, simplified parameterizations of erosion and subsequent dust emission, as well as aerosol re-suspension are taken into account, which use the friction velocity parameter.

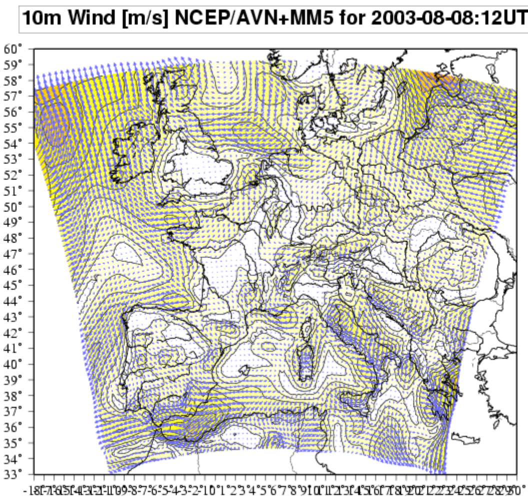

Figure 1: The MM5 simulation domain and the wind field simulated for 08/08/2003.

CHIMERE and its chemical mechanism describe the evolution of 44 gaseous species and 118 gas-phase reactions. The aerosol module describes the concentrations of aerosols into 6 chemical families: primary particulate matter (PM), sulphate, nitrate, ammonium, anthropic and biogenic secondary organic aerosol. These are distributed into 6 size bins from 40 nm to 40 µm. The aerosol processes include nucleation, coagulation and adsorption, wet and dry deposition. Heterogeneous chemistry of sulphate and nitrates is considered. The emissions are derived from the EMEP data base (Vestreng, 2003).

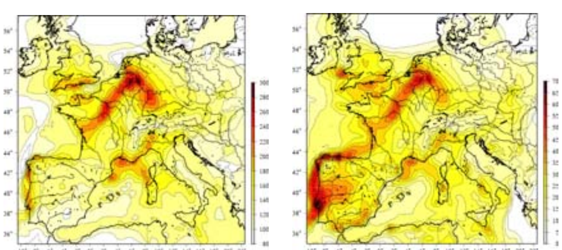

Figure 2: left: surface ozone concentration field (µg/m^3) and right: surface PM10 concentration field (µg/m^3) simulated by CHIMERE forced by MM5.

Figure 2 shows an example of ozone and PM10 simulated field, for the same date as the wind field of Figure 1. The large concentrations of ozone and PM10 in a band from Germany to Western France are due to the exceptional stagnation that occurred during August 2003, when temperatures reached record or near-record values for 2 consecutive weeks. The high PM10 values simulated over Western Spain are, by contrast, due (in the model) to erosion of extremely dry soil during this period.

The only differences between forecasts and simulations lie in the use of meteorological analyses instead of meteorological forecasts, in all cases provided every 6 hours. Real-time forecasts are issued every day at the end of the day, starting with analyses at 00Z, 06Z and 12Z, but using meteorological forecasts at 18Z and over the next 3 days. Since the results are usually available only on the next morning of the forecast, we call Day-1 the first "forecast" day, Day+0 the second, Day+1 the third and Day+2 the last one.

3. Simulation and forecast skill

We first discuss the model skill in simulating the ozone daily maxima. A long-term simulation is initiated on April 26th 2003 and is carried out through September 2nd 2003. Simulated ozone daily maxima are then compared to their observed counterparts over about 250 "background" stations in Europe, located in France, Germany, Switzerland, Belgium, Netherlands, England and the Czech republic.

For the sake of comparison with other meteorological forcing, we also reproduce this experiment using ECMWF 3-hourly sampled short-term forecasts (with 3 and 6 hour lead times), interpolated hourly.

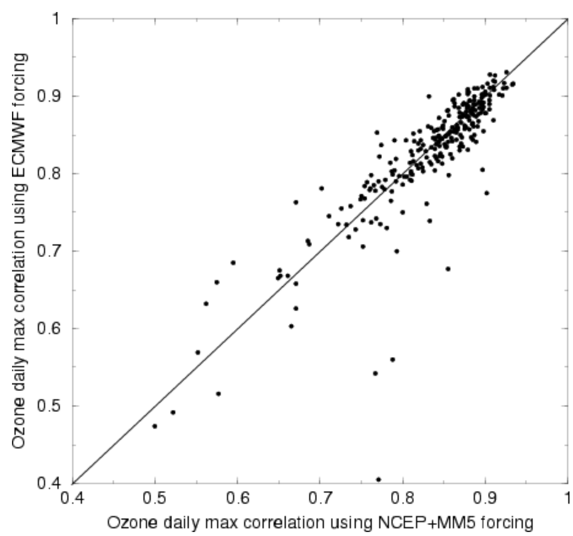

Figure 3: Time correlations obtained by comparison of the Summer 2003 CHIMERE+ECMWF vs. CHIMERE+MM5 simulations of ozone daily maxima and the observed ones. Each point on the graph corresponds to a monitoring station.

Figure 3 shows the time correlations obtained for the ozone daily maxima for the ECMWF forcing vs. those obtained for the NCEP+MM5 forcing. For most monitoring stations (about 75%) the correlation lies above 0.8 for both forcings, and the average correlation is 0.83 in both cases. Figure 4 shows the observed vs. simulated means of the ozone daily max. For both forcings, the scatter plot is well correlated, indicating that high ozone values are generally simulated at the right locations in Europe. However, the model underestimates high values. This is probably due to a lack of resolution for stations near big cities, where strong plumes develop, which cannot be resolved at a ½ degree resolution. This bias seems to be more pronounced with ECMWF than with MM5 forcing, indicating a better ability of MM5 to capture flows with stronger local forcings. Finally, RMS errors generally lie below 20 µg/m^3.

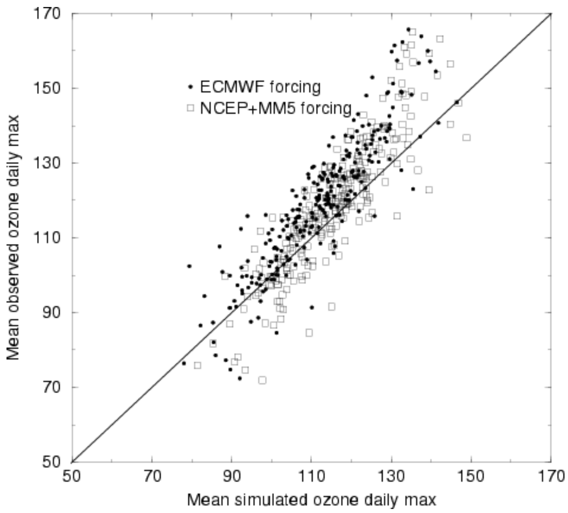

Figure 4: Grand means of observed vs. simulated ozone daily maxima in µg/m^3.

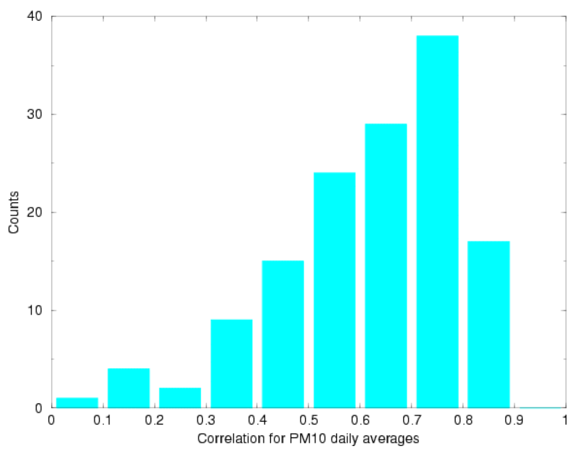

Figure 5: Histogram of correlations between simulated and observed PM10 values for the MM5-forced simulation. There are now only 142 monitoring stations.

The skill of the model for the simulation of aerosols can also be assessed using the same statistical indices. However we use for validation the daily average of PM10 here instead of daily maximum.

Figure 5 demonstrates that PM10 is simulated with successful skill, although it is inferior to that obtained for ozone daily maxima. There is a group of stations with very poor skill (say less than 0.5). Most of these stations lie along coasts where sea salt aerosol emissions, not accounted for in the model, can be a dominant process. The scores are particularly high in the northern plains of Europe. A key process for aerosol skilful prediction seems to be the re-suspension of deposited material or the erosion. These processes are particularly important during summertime droughts as the one which occurred in August 2003.

In forecast mode, the performance of the model is similar, with a moderate modulation due to the lead time of the forecast. Figure 6 shows that the normalized mean square error for the ozone daily maximum increases from about 18% to 22% while the correlation drops down from 0.83 to 0.77 over the French rural stations.

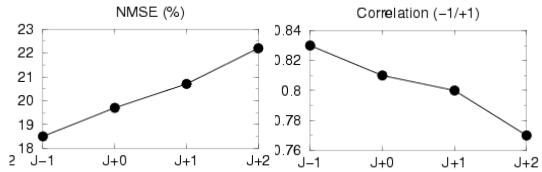

Figure 6: Forecast skill as a function of lead time (J-1 means Day-1, J+0 is Day+0 etc…), of the NCEP+MM5+CHIMERE model chain for the forecast of daily ozone maxima, calculated only over the subset of the French rural stations. These comparisons are made using the PREV'AIR operational forecast system over Summer 2003 (http://www.prevair.org).

Several other skill scores have been established on other regions (the neighbourhood of Paris at higher resolution), but are not discussed here for the sake of conciseness.

4. Problems encountered with MM5 and consequences for air quality simulation

The analysis of the skill of the simulation reveals several problems due, at least in part, to the meteorological driver MM5. These come from various origins.

4.1 Dynamical problems and their impact

The flow itself is generally very well simulated, and MM5 has been tested against wind observations in numerous instances. However, as mentioned in Section 2, a major problem arises with the MRF PBL scheme in free or almost free convection conditions, due to the parameterization of the convective velocity scale. The direct effect is an excessive friction velocity, often reaching 0.5-0.8 m/s in free convective regime. The most important impact on air quality simulation is a too-light near-surface wind and a too-small aerodynamic resistance, which therefore increases dry deposition of ozone and other important species such as nitric acid. To a degree, these effects on ozone compensate each other. However we found by numerical tests that the net effect on ozone is an underestimation, of the order of about 10%. At urban scale, the underestimation of near-surface winds tend to make the model develop plumes that are not extended and diluted enough, leading to an overestimation of the ozone plume maximum and an error in location.

Another important effect is on fugitive dust emission fluxes, which, according to various authors (see e.g. Marticorena and Bergametti, 1995), depend on a power 3 to 4 of the friction velocity, making them very sensitive to this parameter.

The structure of the boundary layer and its height do not seem particularly biased, as compared to backscatter lidar measurements (Hodzic et al., 2004) made on a site (SIRTA) near Paris.

4.2 Cloud/Radiation problems

Radiation, especially in conditions near the saturation or in the presence of clouds, is difficult to predict. Problems due to the microphysics are not easy to diagnose. However, in a companion paper presented at this workshop (Chiriaco et al., 2004, this issue), systematic comparisons of model high cloud characteristics with numerous lidar measurements are carried out on the SIRTA site near Paris. They indicate that the Schultz scheme systematically underestimates cirrus ice concentration. The consequence is an overestimation of ozone production, especially before the fronts where simultaneously temperature is hot, cirrus are numerous and ozone is high.

Another problem arises from the lack of detailed cloud fraction, especially in the boundary layer with cumulus clouds. In many instances, the relative humidity profile reaches values near saturation without making significant cloud water, while the variability of humidity is often such that cumulus clouds start to form with values near 80% relative humidity or so.

In many instances during the fall period we noticed that near-surface clouds form in the model but not in reality, which has a strong impact on surface temperature and therefore vertical mixing of primary pollutants. Errors of more than 4-5 degrees have been sometimes encountered, while when both models predict clear sky the temperature seems unbiased. The presence of stratocumulus clouds associated with significant "radiatively-driven" down-mixing can also significantly spoil the primary pollutants simulation because the boundary layer scheme does not account for such a mixing process. In the CHIMERE model, a minimal vertical diffusivity is assumed in the case of clouds in order to reduce this problem.

4.3 Urban heat island

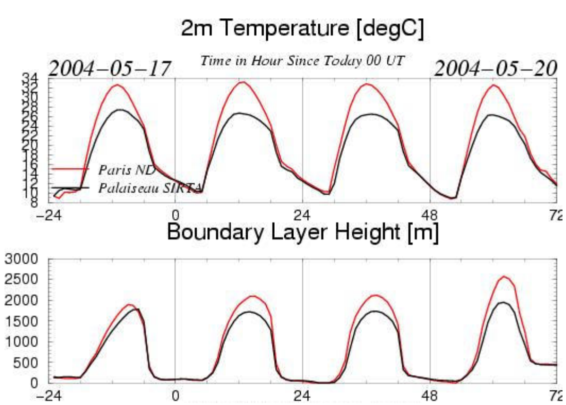

Figure 7: 4-day forecast of temperature and boundary layer height issued on 17/05/2004 for the centre of Paris (red curve) and the SIRTA site, about 25 km away from the city centre.

MM5 simulations carried out at urban scale do not account properly for heat storage in the urban canopy, especially during summertime. The MM5 urban heat island displays a maximum during daytime while it is minimal at nighttime (see Figure 7). In reality the reverse situation occurs. The impacts of this problem can be numerous: first the underestimation of the nighttime urban heat island leaves the city with a very stable air near the ground, blocking dispersion of primary pollutants. Second, the overestimation of sensible heat fluxes and surface temperature during daytime over the city leads to an overestimated boundary layer and mixing which can significantly modify the structure of the pollutant concentrations near the city.

5. Conclusion

MM5 simulates the flow and meteorological parameters with a sufficient skill to allow its use for operational air quality forecasts in Europe. However the routine analysis of the errors made by the operational air quality modelling system using MM5 and the CHIMERE chemistry-transport model points towards problems that need to be addressed in future developments. The most important are: (i) An accurate representation of the surface momentum and heat fluxes are required (ii) microphysics scheme are too simplified and need to taken better into account high clouds, cumulus and stratocumulus clouds and their turbulent properties, (iii) there is a crucial need for the development of a consistent urban canopy and soil scheme.

References

Beljaars, A.C.M., 1994: The parameterization of surface fluxes in large-scale models under free convection. *Quart. J. Royal Met. Soc*., **121**, 255-270.

Bessagnet, B., et al., 2004: Aerosol modelling with CHIMERE – Prelmiminary evaluation at continental scale. *Atmospheric Environment*, **38**, 2803-2817.

Grell, G. A., J. Dudhia and D. R. Stauffer, 1994: A description of the fifth-generation Penn State/NCAR mesoscale model (MM5). *NCAR Technical Note*, NCAR/TN-398+STR, 117 pp.

Hodzic, A., et al., 2004: comparison of aerosol chemistry-transport model simulations with lidar and sun-photometer observations at a site near Paris. *J. Geophys. Res*., sub judice.

Marticorena, B., and Bergametti, G., 1995: modeling the atmospheric dust cycle. *J. Geophys. Res*., **100**, 16415-16430.

Schultz, P., 1995: An explicit cloud physics parameterization for operational numerical weather prediction. *Mon. Wea. Rev.*, 123, 3331-3343.

Schmidt, H., Derognat, C., Vautard, R., Beekmann, M., 2001: A comparison of simulated and observed ozone mixing ratios for the summer of 1998 in Western Europe. *Atmos. Environ*., **35**, 6277-6297.

Tilmes, S., et al., 2000, Comparison of five eulerian ozone prediction systems for Summer 1999 using the German monitoring data. J. Atmos. Chem., in press.

Vautard, R., Beekmann, M., Roux, J., and Gombert, D., 2001. Validation of a hybrid forecasting system for the ozone concentrations over the Paris area. *Atmospheric Environment*, **35**, 2449-2461.

Vestreng, V., 2003: Review and revision of Emission data reported to CLRTAP, EMEP Status report July 2003.