1.02 SENSITIVITY ANALYSIS OF OZONE LONG TERM SIMULATIONS TO GRID RESOLUTION

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INTRODUCTION

In the frame of the CAFE programme (*Commission of the European Communities*, 2001) modelling activities, the CityDelta (http://rea.ei.jrc.it/netshare/thunis/citydelta/) open model intercomparison exercise has been launched by the JRC-IES (Joint Research Centre – Institute for Environment and Sustainability) in collaboration with EMEP, IIASA and EUROTRAC to explore the changes in urban air quality (mainly ozone and particulate matter concentrations) predicted by different atmospheric chemistry-transport (CTM) dispersion models in response to changes in urban and regional emissions.

During the first phase of CityDelta exercise, four Italian groups cooperated in the preparation of the input data in order to perform simulations with three different atmospheric chemistrytransport models: CALGRID (Yamartino, R. J. et al., 1991), an Eulerian three-dimensional photochemical model for gas phase simulations. It implements an accurate advectiondiffusion scheme in terrain-following co-ordinates with vertical variable spacing. The CALGRID chemical module implements the SAPRC90 (Carter, W.P.L., 1990) and the CB4 (Gery, M. et al., 1989) mechanisms. The QSSA (Quasy Steady State Approximations) algorithm solves the kinetic equations (Hessvedt, E. et al., 1978); STEM-FCM (Silibello, C. et al., 2001) an Eulerian three-dimensional photochemical model that implements an accurate advection-diffusion scheme in terrain-following coordinates, with vertical variable spacing, and can take into account chemical transformations and deposition processes of both gas and aerosol species. The model uses SAPRC-90 mechanism (Carter, W.P.L., 1990), including 54 chemical species and 129 reactions. As for the kinetic equations integration, STEM-FCM implements the IEH solver (Sun, P. et al., 1994). Finally aerosol treatment is based on the size-resolved multicomponent aerosol module of (Wexler, A.J. et al., 1994); CAMx (Environ Corp., 2004), a comprehensive air quality computer modeling system publicly available for the integrated assessment of photochemical and particulate air pollution over many scales. CAMx provides the option to use two different chemical mechanisms: a) Carbon Bond 4 version 1999, modified to model for ozone and fine / coarse PM; b) SAPRC version 1999 (Carter, W.P.L., 2000). In addition CAMx provides two chemistry solver, IEH (Implicit-Explicit Hybrid) or CMC (developed by ENVIRON and based on an "adaptive-hybrid" approach). For the first phase of CityDelta SAPRC99 chemical mechanism and CMC solver were used.

The photochemical models have been applied over the Milan area defined in the frame of CityDelta intercomparison (300 x 300 km², Figure 1). The simulations concerned the 1999 six summery months (from April to September).

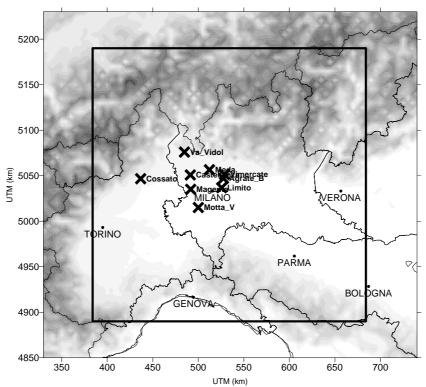


Figure 1. The CityDelta Milan domain. Air quality monitoring stations selected for model validation are also shown.

THE MODELS SENSITIVITY ANALYSIS

To better evaluate models reliability and cleverness in simulating the long-term dynamics of pollutants in the atmosphere, a comprehensive sensitivity analysis with regard to both model configuration and input data has been carried out. Models have been driven by same input fields, and in particular:

- ✓ the emissions over all the domain were provided by EMEP and JRC;
- ✓ the boundary concentrations were provided in the frame of CityDelta by EMEP;
- for the main meteorological fields (wind speed and direction, temperature, turbulence parameters) CALMET diagnostic model (*Scire, J.S. et al.*, 2000) was applied, whereas some other meteorological fields requested by CAMx (i.e. pressure, water vapour content, cloudiness, rain) were derived by Aladin data, provided in the frame of CityDelta by Météo France (http://www.meteo.fr/meteonet/).

Comparing model outputs obtained with the same input fields and the same configuration (in terms of horizontal and vertical resolution, for example) has allowed to highlight differences only due to models response. In particular, three main aspects were investigated: a) horizontal grid resolution, b) meteorology fields and c) chemical mechanisms and integrators. This work deals with the first one: the influence of horizontal grid resolution

GRID RESOLUTION INFLUENCE

Analysis of the horizontal grid resolution influence (varying from 5 to 10 km) represents one of the main issues of CityDelta project and has been addressed both to Base Case and to hypothesised future scenarios.

The results obtained with the three models for the different scenarios were evaluated by means of a statistical tool provided by JRC. Several statistical parameters were taken into account, all based on the ozone and NO₂ six months hourly concentrations. The evaluation

was performed in relation to nine geographical points selected by JRC and corresponding to the air quality monitoring stations concerning the base case (validation) and to 'significant' locations concerning the future scenarios.

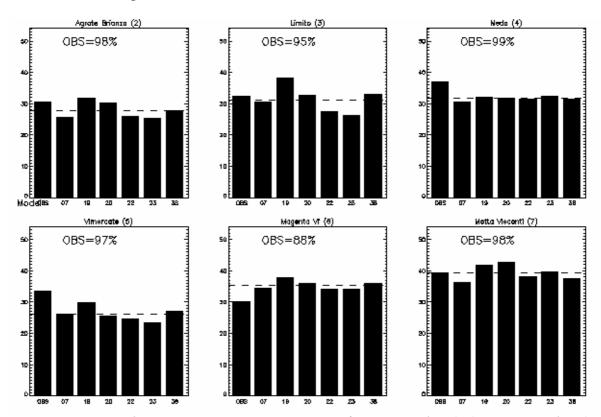


Figure 2. Six months mean ozone concentrations of CAMx 10 km (07), STEM 10 km (19), STEM 5 km (20), CALGRID 5 km (22), CAMx 5 km (23), CALGRID 10 km (38) for some monitoring stations. Observations are shown as first column.

The analysis demonstrates that ozone concentrations seem quite insensitive to grid resolution as for mean statistical parameters. For example, Figure 2 shows the mean ozone concentrations over the summery months for six monitoring stations. As we can see the results of the same model are comparable in relation to the two grid resolutions, even if some differences can be found at Limito station. Similar conclusions can be drawn for other mean parameters like correlation coefficient and BIAS. For some models, on the contrary, extreme values statistics can be more sensible to horizontal resolution. For example, exceedance days of 60 (ppb) threshold for 8 hourly ozone concentration can vary up to 15-20 % (Figure 3). Similar results can observed also for hourly exceedances or AOTx.

Concerning the nitrogen dioxide, concentrations seem to be more sensitive than ozone to the grid spatial resolution, as they are more linked to emissions. In Figure 4, for example, the NO₂ mean concentrations over six months differ in relation to the grid horizontal resolution, particularly near the urban area (station n. 3, Limito). Moreover NO₂ variations are coherent with the corresponding modifications in ozone concentrations, even in an opposite sense. Finally, observed behaviours seem to be coherent among base case and hypothesised future scenarios.

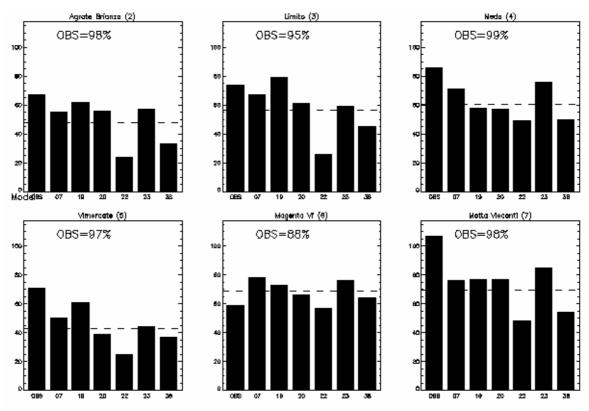


Figure 3. Exceedance days of the 60 (ppb) threshold for 8 hourly mean ozone concentration.

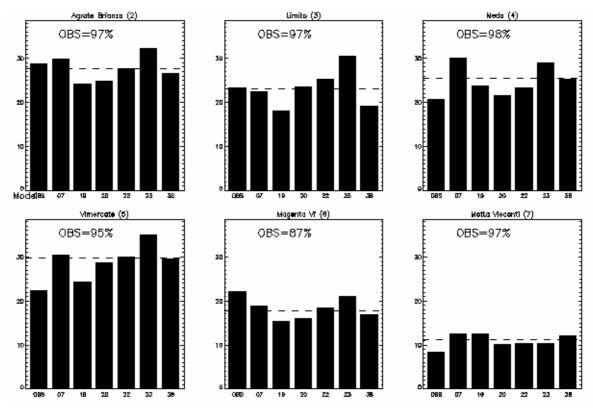


Figure 4. Six months mean NO_2 concentrations.

CONCLUSIONS

Performed analysis suggest that varying horizontal grid resolution from 5 to 10 km doesn't induce significant variations in ozone models performance (maybe except for the exceedance

parameters), while could be in some ways more critical with regard to NO₂. In any case, observed variations don't put in evidence a clear worsening in model performances due to a reduction of spatial resolution. Generally nitrogen dioxide seems to be more sensitive, suggesting that grid resolution could be more influent on emission reconstruction than on transport or chemical transformations. On the other hand, increasing grid step reduces computational resources requirement, that represents an important issue in regulatory context. Consequently, modifying spatial resolution can represent a rational decision on condition that full model sensitivity has carried out taking into account different chemical species and performance indicators, in order to correctly set grid configuration.

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REFERENCES

- Carter, W.P.L., 1990: A detailed mechanism for the gas-phase atmospheric reactions of organic compounds. Atmospheric Environment, 24, 481-518.
- Carter, W.P.L., 2000: Documentation of the SAPRC-99 chemical mechanism for VOC reactivity assessment. Final Report to California Air Resources Board, Riverside CA, U.S.A., May 2000.
- Commission of the European Communities, 2001: Communication from the Commission The Clean Air for Europe (CAFE) Programme: Towards a Thematic Strategy for Air Quality. COM(2001) 245 final, Brussels, 2001
- ENVIRON International Corporation, 2004: User's guide to the Comprehensive Air Quality Model with Extensions Ver 4.0. *Technical Report*, Novato CA, U.S.A., January 2004.
- Gery, M., Whitten, G., Killus, J., 1989: A photochemical mechanism for urban and regional scale computer modeling. J. Geophys. Res., 94, 12925-12956.
- Hessvedt, E., Hov, O., Isaksen, I., 1978: Quasi Steady State Approximation in Air Pollution Modeling. Intern. J. Chem. Kin., 10, 971-994.
- Scire, J.S., F.R. Robe, M.E. Fernau e R.J. Yamartino, 2000: A User's Guide for the CALMET Meteorological Model (Version 5). Technical Report Earth Tech Inc., Concord MA, U.S.A., January 2000.
- Silibello, C., G. Calori, G. Pirovano, and G.R. Carmichael, 2001: Development of STEM-FCM modelling system: Chemical mechanisms sensitivity evaluated on a photochemical episode. *Proceedings of APMS'01 International Conference*, Paris, April 2001.
- Sun, P., Chock, D. P. and Winkler, S. L., 1994: An implicit-explicit hybrid solver for a system of stiff kinetic equations. *Journal Of Comp. Physics*, **115**, 515-523.
- Wexler, A.J., Lurmann, F.W., Seinfeld J.H., 1994: Modelling urban and regional aerosols I. Model development. Atmospheric Environment, 28, 3, 531-546.
- *Yamartino, R. J., J.S. Scire, G. R. Charcichael and Y. S. Chang*, 1991: The Calgrid mesoscale photochemical grid model I. Model formulation. *Atmospheric Environment*, Vol. **26**, 3, 1493-1512.