J2.18 AIR QUALITY MODELING AT COARSE-TO-FINE SCALES IN URBAN AREAS

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1.0 INTRODUCTION

Consideration and movement for an urban air toxics control strategy is toward a community, exposure and risk-based modeling approach, with emphasis on assessments of areas that experience high air toxic concentration levels, the so-called “hot spots”. This strategy will require information that accurately maps and characterizes the spatial and temporal variability of such pollutants. Many air toxic pollutants are active in photochemistry and ambient concentration levels will, therefore, depend on both the magnitude of the secondary products from the inflow regional background as well as from fresh emissions. In principle, the Community Multi-scale Air Quality (CMAQ) modeling system, using multi-scale modeling attributes can provide the ambient concentrations of air toxics from both regional and local sources and through advanced treatment of chemical, transport and deposition pathways. This paper explores the CMAQ capability to model air toxics at fine scale to meet the desired air toxics assessments objectives.

2.0 METHODOLOGY:

We start by setting the nesting of CMAQ for modeling from regional to fine scales. Modeling results for various nests will be displayed and discussed. Given that exposure and risk assessments are typically focused on populations in urban and industrial areas, we review the requirements for modeling meteorological and air pollution fields in urban areas at grid resolutions of order 1 km. We subsequently utilize the 1.3 km grid simulations in CMAQ, as a basis for examining the inherent within-grid spatial variability unresolved at native coarser scales. We do note that there is additional sub-spatial grid variability at less than 1.3km, but their treatment and contribution to sub-grid variability are not discussed here. Rather, the methodology to attain information at grid scales smaller than 1.3 km will require utilizing dispersion and transport, and finer scale modeling, and that their outputs will be in the form of distribution functions to compliment the 1.3 km CMAQ simulations.

Simulations for this study were made on episodic bases and were focused on the Philadelphia area. MM5 and CMAQ simulations were performed using nests at 36, 12, 4 and 1.3 km resolutions and results are shown for July 12 and 14, 1995. At 1.3 km, urban canopy parameterizations, UCPs, were introduced into MM5 to account for the impact of urban building structures on the meteorological fields (Lacser and Otte, 2002, Dupont, et al., 2003, and Ching et al., 2003), based on Brown, 2000, and Martelli et al., 2002. Sensitivity studies (not shown here) have shown pronounced affects of the UCP on both the outputs of the MM5 and the subsequent CMAQ simulations. The emissions were also spatially resolved at 1.3 km grids. Ten (10) additional vertical layers were introduced into both MM5 and CMAQ to provide vertical resolution for implementing the UCP methodology. Sensitivity studies showed some, albeit relatively small sensitivities to the layer or layers nearest the surface in which small point, area and mobile sources were introduced.

3.0 RESULTS

Figure 1 shows an example output of the simulations for the four nested grids for CO. The results clearly showed continued enhancements of the spatial structure (gradients) and the concentration magnitudes with decreasing grid size. These features are even more pronounced (not shown here) in the case of photochemically active pollutants such as NO_x and O_3. Also, while not shown here, hot spot features do appear at the 1.3 km grid resolution for several toxic species such as formaldehyde and acetaldehyde. During this study, it was clear that for these latter two toxic pollutant species, the resultant concentrations consisted of a relatively large regional component.

We now investigate the relative sensitivity of the simulations to grid resolution. For this purpose, we assume the 1.3 km grid simulations as the base and by

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aggregating of these values to grids for the coarser grid modeling domain, we can examine the characteristics of their within-grid variability. Figure 2 shows results using the 1.3 km grid simulation for ozone at 4pm EDT aggregated to 12 km. The results from aggregating 1.3km simulations differ significantly from that of the native 12 km grid as seen in the right side of the figure.

Our neighborhood scale modeling paradigm for air toxics assumes that when significant within-grid concentration variability is known to exist, additional information on the characteristics of such distributions will be supplied to complement the grid resolved simulations for supporting risk-based population exposure assessments. The next series of figures provides illustrative statistics based on aggregating the 1.3 km grid results to 4 and 12 km to demonstrate the qualitative aspects of such distributions. For example, Figure 3 shows the standard deviation of the within-grid variability at 4 and 12 km (normalized by its respective grid value). Moreover, as shown in Figure 4, the distributions for each of the pollutants do exhibit a wide range in the value and sign of its skewness. No apparent form or structure emerges from these patterns; further, these distributions evolve with time.

Since exposure estimates depend on concentration and dosage, the magnitude of the range of the within-grid variability becomes an important measure of risk. Figure 5 shows such range computed from the difference in the peak and minimum values of the 1.3 km results for each cell of the 12 and 4 km simulations (normalized by their respective coarse scale aggregated grid mean). In this case, we see in the central Philadelphia area, that the range can exceed the mean by up to a factor of 2. No characteristic pattern of variability of the features on range emerges within this domain.

Figure 6 shows concentration distribution histograms from CMAQ simulations for a 12 km grid in central Philadelphia July 14, 1995 for the time sequence 17-20 GMT. Here, we can see that the histograms can change rapidly in time, and their characteristics also differ between the different pollutants. Several of the distributions exhibit multimode character and such shapes changes in time.

4.0 DISCUSSION AND SUMMARY

From this limited set of model runs, a few noteworthy and general points emerge:

(1) The introduction of UCPs impacts the resulting modeled flow and air quality fields.
(2) Resolving the flow and air quality at fine scales will significantly increase the level of detail in the spatial features, in the magnitudes of the concentration gradients and their extreme values.
(3) Compositing neighborhood scale simulations to coarser scales yields different results when compared to coarse grid native simulations; further the fine scale grid simulations provide indications of variability in coarser grid solutions. The character of these results differs depending on the scale of the coarse grid mesh.
(4) The degree of within-grid variability is a function of the grid resolution and pollutant species and of course the characteristics of such variability are dependent on many factors, including complexity of the urban area, its source distribution etc.
(5) While not presented, within-grid variability will generally be present even at the 1 km mesh resolution (These will arise as a combination of variability due to within grid source configurations and distribution as well as inherently due to chemistry and turbulent interactions (Ching et al., 2003). Investigations of methods to derive such distributions are underway.
(6) There is also an important implication arising from the results of fine scale modeling to model evaluation. This study suggests that in areas for which within-grid air quality has an inherently high degree of spatial variability, a comparison of model results should factor-in such variability. Since monitors will not, in general, be adequately sited to represent the grid resolved value, it follows that model comparison and evaluation should introduce some measure of this variability.

Disclaimer: *This paper has been reviewed in accordance with United States Environmental Protection Agency's peer and administrative review policies and approved for presentation and publication.*

5.0 References

Brown, M.J., 2000: Urban parameterizations for mesoscale meteorological models, in: *Mesoscale Atmospheric Dispersion*. Ed Z Boybeyi, Wessex Press, 448 pp.

Ching, J., A. Lacser, T. Otte, and S. Dupont, 2003: Air quality simulations at neighborhood scales with CMAQ. Proceedings of the Fourth Int'l Conference on Urban Air Quality, Measurements, Modeling and Management, Prague, CZ.

Dupont, S., T. Otte, and J. Ching, 2003: Simulation of Meteorological fields within and above urban and rural canopies with a mesoscale model (MM5) *Bound. Layer Meteorology. (submitted)*

Lacser, A. and T. Otte, 2002: Implementation of an urban canopy parameterization in MM5. Preprints, Fourth Symposium of Urban Environment. Norfolk, VA. American Meteorological Society, 153-154.

Martelli, A., A. Clappier, and M.W. Rotach, 2002: An urban surface exchange parameterizations for mesoscale models. *Bound. Layer Meteor.*, 261-304.

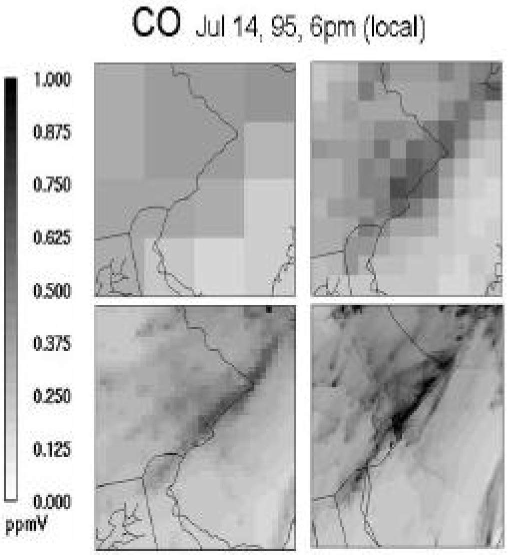

Figure 1. CMAQ simulation of CO: Top (left: 36km, right: 12 km), Bottom (left: 4 km, right: 1.3km)

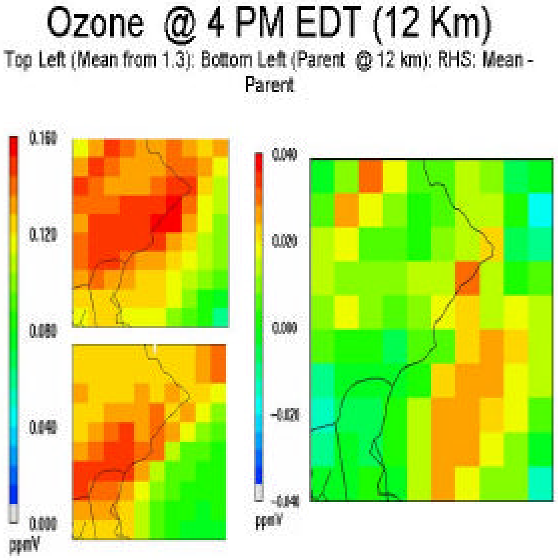

Figure 2. CMAQ simulation of ozone, July 12, 1995.

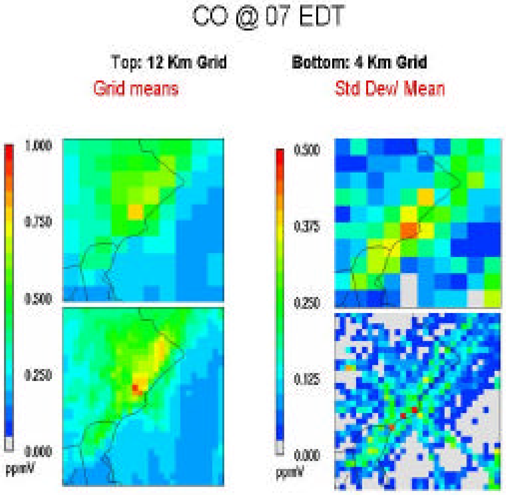

Figure 3. CMAQ simulations of CO for July 12, 1995.

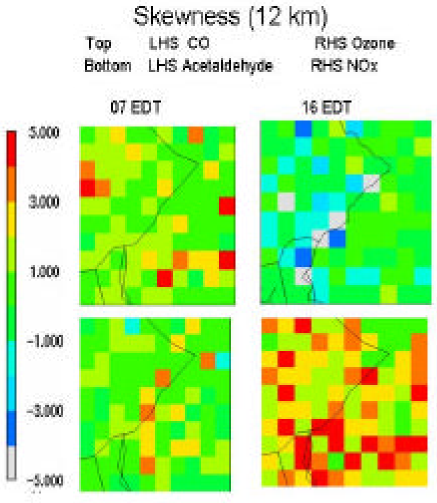

Figure 4. Skewness at 12 km grid resolution derived from 1.3 km simulations for July 12, 1995

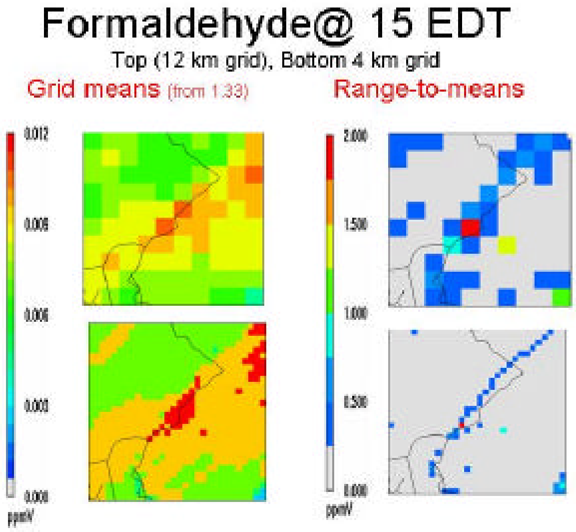

Figure 5. Grid and range-to-mean derived from 1.3 km simulations for July 12, 1995

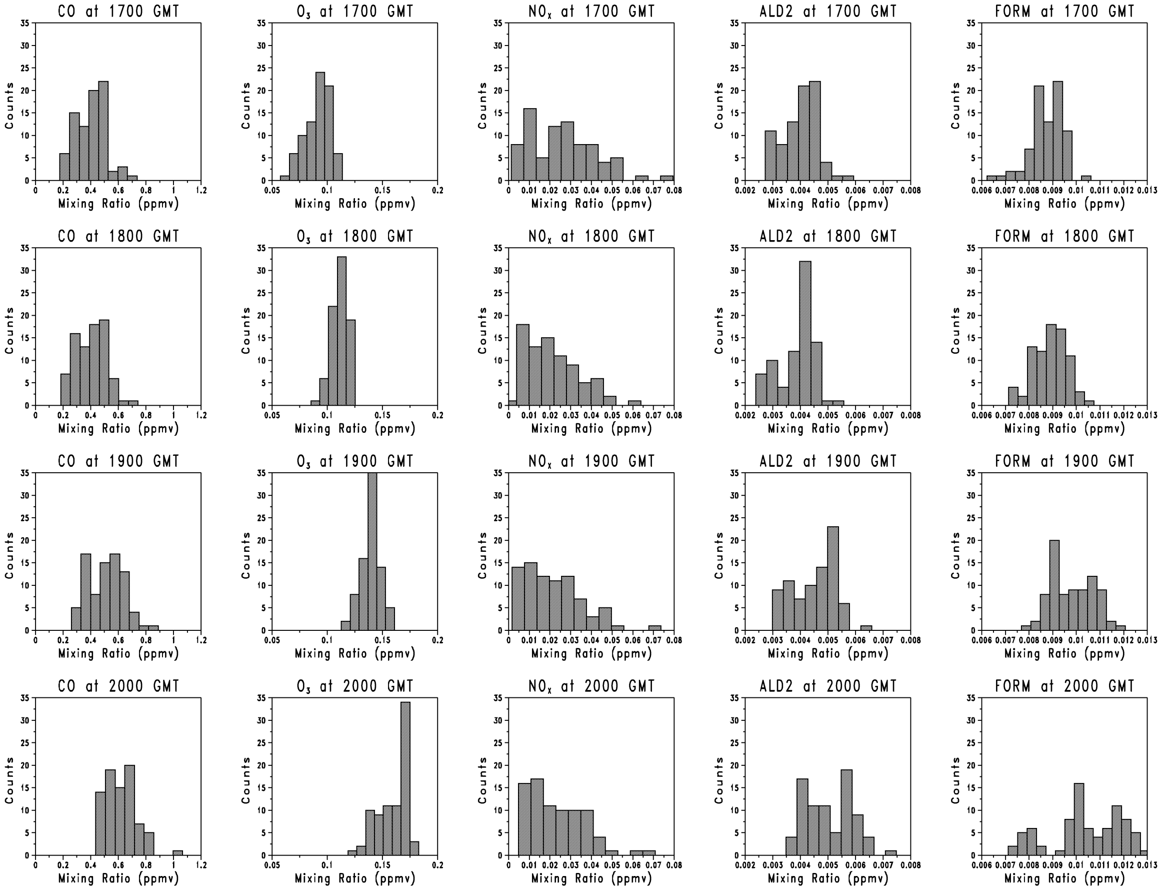

Figure 6. Concentration distribution histogram for 12 km cell in Central Philadelphia. From left: CO, O_3, NO_x, Acetaldehyde and Formaldehyde. From top, 1700, 1800, 1900, and 2000 GMT, July 14, 1995