CMAQ Modeling for Air Toxics at Fine Scales: A Prototype Study

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1. INTRODUCTION

Community Multi-scale Air Quality (CMAQ) has been applied to study the spatial and temporal variability of toxic air pollutants (TAPs) for identifying toxic hot spots, which are the areas that experience high levels of air toxics (AT)[1,2]. These areas are not only impacted by local sources but also by the secondary production of many air toxic compounds due to photochemistry and long range transport. For example, formaldehyde and acetaldehyde have secondary components because of oxidant photochemistry. The source distribution, photochemistry, dry and wet deposition of these compounds are scale dependent. Therefore, in order to capture the spatial and temporal variability of these compounds and identify air toxic hot spots, it is necessary to perform air quality simulations at fine scales.

CMAQ has been chosen to simulate air toxic concentrations at fine scale for a Delaware prototype study. The CMAQ modeling system has been selected because it can perform multiscale and multipollutant simulations for air toxics at a neighborhood scale of 1 km. CMAQ'S preprocessors, the NCAR-PSU Mesoscale Model Version 5 (MM5) and the Sparse Matrix Operator Kernel Emissions Model (SMOKE) provide the meteorological and emission fields at 1 km grid cell size. 1999 National Emissions Inventory (NEI) and 2001 meteorological databases are chosen for this study. The simulations are assessed to examine (a) the spatial and temporal variability of air toxics compounds, (b) the characteristics and nature of hot spots and their scale resolution requirements. This paper presents preliminary results for a case study period, showing examples of model outputs at different scales from the MM5 and CMAQ modeling systems, and for various pollutants, including photochemical oxidants and several AT species.

2. METHODOLOGY

The Carbon Bond IV chemical mechanism commonly used in the CMAQ modeling system has been modified to explicitly treat a number of gas-phase air toxics compounds. The resulting modeling system is identified as CMAQ-AT. Modeling from regional to finer scales is accomplished by nesting of CMAQ-AT. Simulations for this study are focused on Delaware area. MM5 and CMAQ-AT simulations have been performed for the entire calendar year of 2001using nests with 36, 12, and 4 km grid sizes at successively smaller domains, respectively, to provide the initial and boundary conditions for the simulations at 1 km grid size[1]. Simulations with 1 km grids were not performed on an annual basis; however, a one month period (July2001) for operational purposes was selected for the 1 km simulations to serve as a complement to the annual coarser grid size runs. A one month period is longer than a typical meteorological episode and serves as a surrogate for representing "seasonal" outputs and still be operationally expedient consistent with current computational speed and storage capabilities. For the 1 km grid runs, the emissions were spatially resolved for 1 km grids for the month of July 2001.

3. RESULTS

(a) Meteorology:

We now briefly examine the performance of the 1-km MM5 output. Fig. 1 depicts the time series of the MM5 predicted temperature at 10 m and the measured temperature at New Castle County airport for July 2001. Generally the model tracks well with the monitored temperature; occasionally, the monitored daily minimum temperature is lower than the predicted daily minimum. The MM5 predicted temperature had a bias of 0.24 K and a gross error of 2.4 K.

A case study approach illustrates important features and capabilities of the MM5 modeling system. Fig. 2 displays the MM5 temperature fields interpolated from layer 1 to 1.5 m predicted at 4 and 1 km grid cell sizes. The changes in temperature fields with MM5 modeling with 1 km grid (Fig. 2(b)) are not sudden but continuous. Also, 1km grid modeling shows lower temperature fields along the shore due to sea breeze flow from the shore, as indicated in Fig. 2(b). Furthermore, the 1km grid modeling provides good spatial structure to the temperature fields.

Fig. 3 shows an example 4- and 1-km grid size outputs of the planetary boundary layer (PBL) output parameters -

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PBL height, and cell-averaged friction velocity (ustar). Results indicate considerable additional texture in these and other fields as well as different magnitudes of these parameters at the 1 km grid size. We know, for example, that some of these differences arise because of the increased grid resolution of the input information such as land use, land cover and roughness lengths. The patterns and distribution of other meteorological variables such as incoming radiation, air temperature, wind speed, are also affected, and differ between the 4 and 1 km simulations; these differences will impact the modeling of the emission fields and the final air quality fields.

(b) CMAQ results: CMAQ-AT produced similar enhancement in spatial structure and concentrations of various pollutant species such as ozone, CO, NOx, and TAPs. Fig. 4 shows an example output for ozone resulting from the simulations performed through nested grid modeling with 36-, 12-, 4-, and 1-km grids. It shows the continued enhancements in spatial gradients and concentrations magnitudes with stronger ozone gradients with 36 and 12 km compared to 4 and 1km decreasing grid size. CMAQ-AT produces similar patterns for CO and NOx. The NOx titration effect on ozone along the I-95 corridor appear in both the 4-km and the 1 km simulation (Figs 4(c) and d).

The next set of figures are based on the 1 km simulations. CMAQ-AT tracks primary and secondary species of three carbonyl compounds - formaldehyde, acetaldehyde and acrolein. Primary species are the result of direct emissions from both anthropogenic and natural sources, whereas the secondary are the result of photochemical reactions. Figs. 5 (a & b) show that the primary formaldehyde emissions are negligible, and that most of the formaldehyde is due to the secondary species. Isoprene reaction with hydroxyl radical contributes significantly to the secondary formaldehyde during the summer season (Fig 5c). Note that formaldehyde hotspots occur where isoprene emissions are significant (Fig. 5b). The secondary component is likely to be considerably smaller in the winter periods when photochemical activity is diminished [1].

CMAQ-AT predictions for acetaldehyde are similar to formaldehyde, see Fig. 6(a & b). The peaks in secondary acetaldehyde occur where the concentrations in benzene (Fig. 6(c)) and CO (Fig. 6(d)) are high, which can be attributed primarily to emissions from mobile sources. This indicates that the peaks of secondary acetaldehyde are related to mobile source emissions. Furthermore, Fig 6 (b) indicates that the acetaldehyde hotspots occur where benzene emissions are significant. The behavior of acrolein (Fig. 7) is different from formaldehyde and acetaldehyde. The primary contribution to acrolein dominates; primary acrolein is attributed primarily to mobile source emissions. Furthermore, Fig. 7(a) indicates that acrolein hotspots to be generally collocated where benzene emissions are high (Figure 6(c)). A comparison of Fig. 5-7 indicates that formaldehyde and acetaldehyde are impacted by long-range transport, while acrolein from more local contributions.

4. SUMMARY AND CONCLUSIONS

Modeling MM5 at 1 km grid resolution produces different meteorology and dispersion fields than those at 4km contributing in part to the difference between the coarse and finer scale simulations of air pollution. This research with CMAQ-AT fine-scale modeling demonstrated that fine-scale modeling captures spatial and temporal variability of the air toxics compounds, and also fine-scale modeling provides the spatial gradients and concentration magnitudes which help identify and characterize the hot spots of air toxics compounds. The CMAQ multiscale simulation results provide evidence of the important role of photochemistry in modeling the carbonyl species; we see its dominance of the secondary component to the total formaldehyde and acetaldehyde concentrations during the summer months.

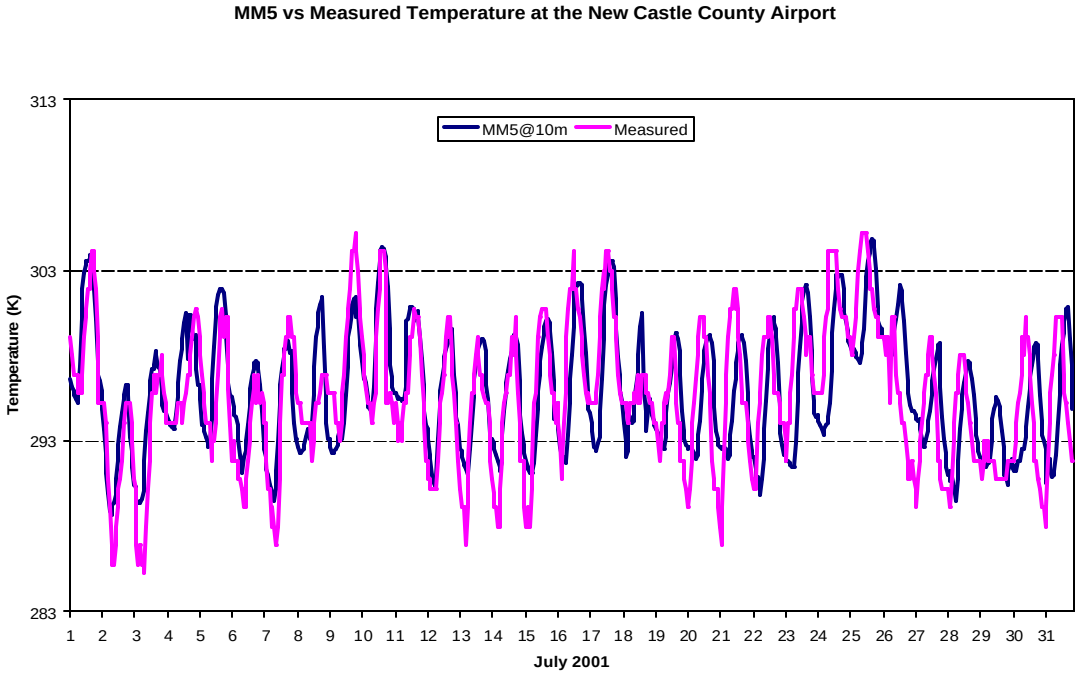

Figure 1. Temperature time series for MM5 predicted and monitored at the New Castle County Airport.

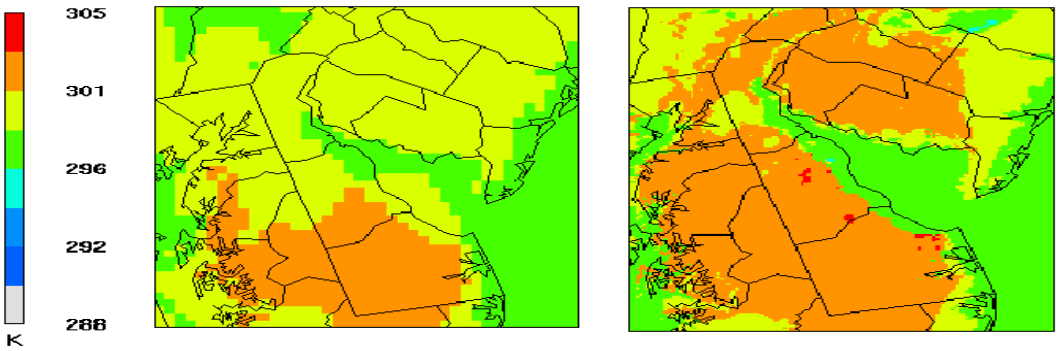

Figure 2. Temperature fields interpolated from MM5 layer 1 to 1.5 m for July 4th 2001 at 6:00 pm EST; left 4-km run and right 1-km run.

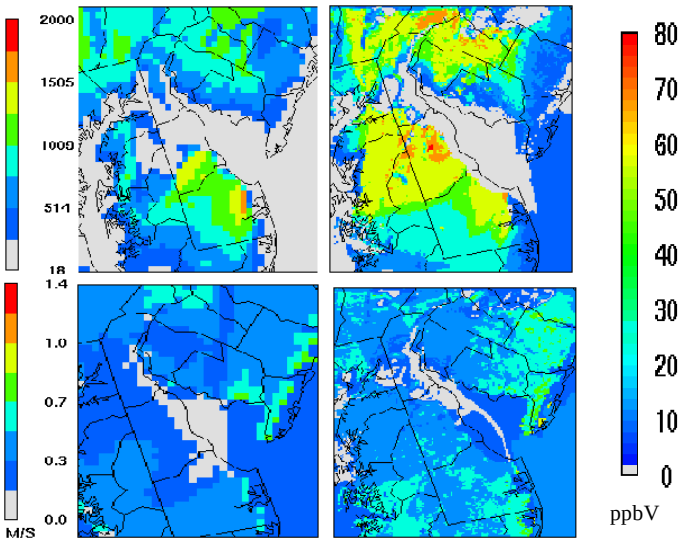

Figure 3. Dispersion parameters for July 4th 2001 at 6:00 pm EST: left side is 4-km grid; right side is 1-km grid. Top is PBL height (m); bottom is ustar (m/s).

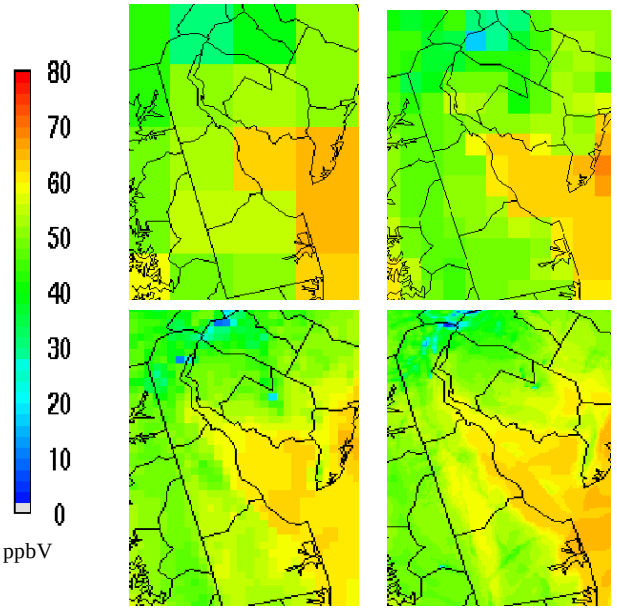

Figure 4. CMAQ-AT ozone simulation for July 2nd 2001 at 7:00 pm EST. Top (36-km and 12-km); bottom (4-km and1-km).

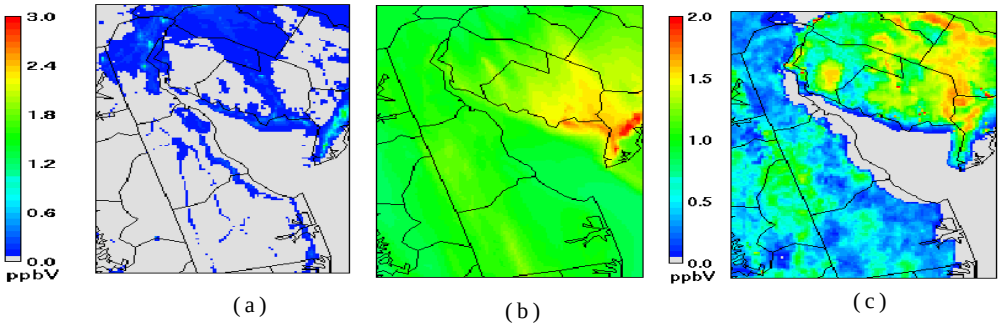

Figure 5. (a) primary formaldehyde, (b) secondary formaldehyde, (c) isoprene at 4:00 PM EST July 2nd, 2001.

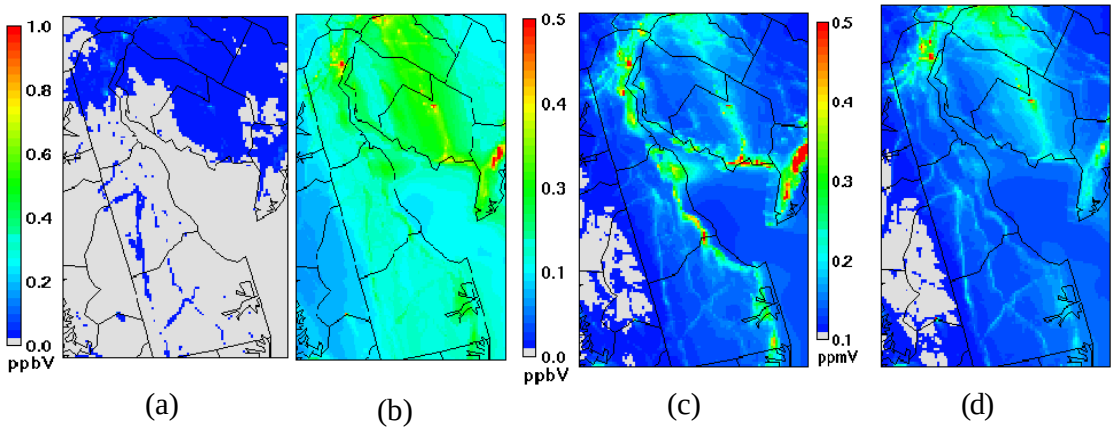

Figure 6. Same as Figure 5: (a) primary acetaldehyde, (b) secondary acetaldehyde, (c) benzene and (d) CO. at 5:00 PM EST July 2nd, 2001

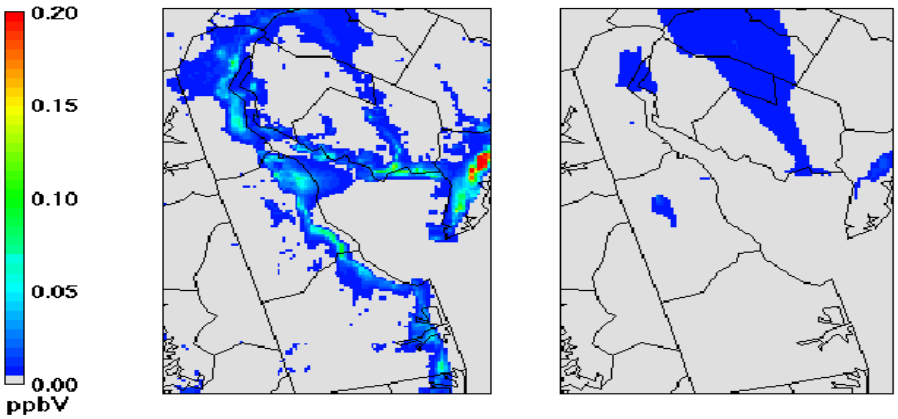

Figure 7. Same as Figure 6: (a) primary acrolein, (b) secondary acrolein

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

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2. Ching, J., Dupont, S., Herwehe, J., Otte, T., Lacser, A., Byun, D., and Tang, R.: Air quality modeling at coarse-to-fine scales in urban areas, In *Proceedings of the Sixth AMS Conference on Atmospheric Chemistry: Air Quality in Megacities*, American Meteorological Society, Seattle, Washington, January 11-15, 2004.