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Application of fine scale air toxics modeling with CMAQ to HAPEM5

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1. INTRODUCTION

The USEPA is developing the capability to link air toxics (AT) concentrations from an advanced photochemical grid model to the HAPEM (Hazardous Air Pollutant Exposure Model) www.epa.gov/ttn/atw/nata/modelexp.html. The basis for AT modeling is the Community Multi-scale Air Quality (CMAQ) modeling system (Byun and Ching, 1999), a "one-atmosphere" chemical transport model. Because the AT model must simulate the spatial distribution of "toxic hot spots" across an urban area, the CMAQ system needs to account for specific toxic compounds at a fine-scale grid resolution. This paper provides a preliminary demonstration towards applying the EPA neighborhood scale modeling paradigm for air toxics using CMAQ to the EPA advanced exposure model HAPEM5. For the HAPEM, the Version 5 replaces a previous version to be able to broaden the potential exposure to both temporal and spatial (sub-grid) variabilities in pollutant concentration. The temporal variability in the concentration field was computed from hourly outputs for the year and for each cell. The results of this application provide a more robust set of information than was possible using the traditional ISC approach to HAPEM. For the pilot study described in this paper, information provided to HAPEM5 includes the mean, median, and the 90th percentile of the concentration distribution. For this demonstration, annual simulations of CMAQ are performed at multiple scales including 36, 12 and 4 km grid sizes, the domain for the former was the continental US while the latter two sets were for smaller nested domains encompassing Philadelphia and the state of Delaware. The CMAQ-AT modeling system has been configured with a modified version of the Carbon Bond IV chemical mechanism that explicitly treats a number of gas-phase air toxic compounds. CMAQ-AT, was run using the 1999 National Emission Inventory (www.epa.gov/ttn/chief/net/) and meteorological outputs from 2001 simulations with the Penn State/NCAR Mesoscale Meteorological Model (MM5). Because our pilot study requires annual simulations, for operational purposes, the finest grid resolution has been a 4 km grid mesh to explore the feasibility of linking CMAQ-AT with human exposure models. We plan to introduce either finer-grid meshes and/or the use of the Industrial Source Complex (ISC) model with a high-resolution receptor network capable of providing within-grid concentration distributions of slow reacting species to provide sub-grid spatial variability information to the HAPEM5.

The HAPEM5 is a screening-level exposure model designed to predict the "apparent" inhalation exposure for the general population, or a specific sub-population, over spatial scales ranging from urban environment to nationwide. HAPEM5 uses the general approach of tracking representatives of specified demographic groups as they move among indoor and outdoor microenvironments and among geographic locations. The estimated pollutant concentrations in each microenvironment visited are combined into a time-weighted average concentration, which is assigned to members of the demographic group. HAPEM5 uses four primary sources of information: population data from the US Census, population activity data from human diary data, microenvironmental data, contained within the model and air quality data that is provided for the study region.

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As human activity data generally exhibits a diurnal pattern the air quality data provided to HAPEM5 must capture the expected diurnal pattern. The hourly CMAQ results were utilized to build a diurnal temporal pattern by averaging the model results over 3-hour blocks (i.e., midnight - 3am, 3am-6am…) for the entire year. To help exhibit the range in the diurnal pattern, similar patterns were built utilizing the median and 90th percentile ambient levels. Such temporal information is useful for risk assessment in both bounding the range of potential exposure levels and in helping to define the annual variability in exposure. Since the HAPEM5 model is designed to perform its exposure assessments on census tract bases, the gridded CMAQ air quality estimates were mapped to each census tract centroid. In an urban area, such as the Philadelphia study area, even with a 4 km grid, this generally results in multiple census tracts residing a single grid cell. The study area for HAPEM5 included the 381 census tracts in the Philadelphia area.

This paper highlights (a) annual outputs of CMAQ-AT; (b) comparisons of model outputs to observations from an available monitoring site; and, (c) linkages of annual concentrations from CMAQ-AT to HAPEM-5.

2. RESULTS

2.1 CMAQ-AT results:

The benefit of the CMAQ system is its ability to model both the transport and photochemistry of air pollutants. Annual time series for both primary and secondary formaldehyde concentrations predicted using CMAQ-AT from the first layer of a 4-km grid cell in central Philadelphia are shown in Fig 1.

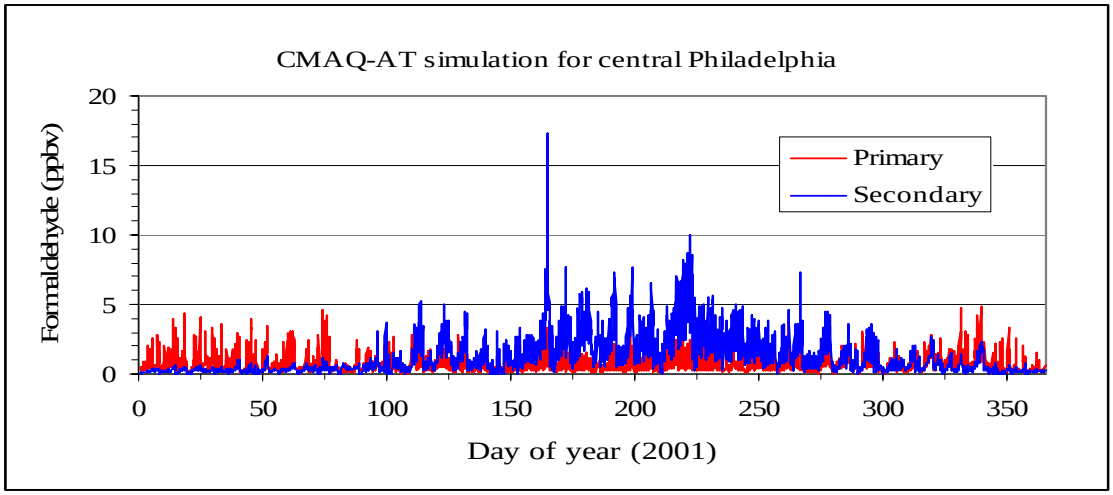

Figure 1. CMAQ modeled concentrations of formaldehyde for 2001 over central Philadelphia. Data are three hour averages of primary and secondary formaldehyde.

The contribution of the primary species to total formaldehyde during the winter period is typically larger than that of the secondary species in central Philadelphia, and comparable elsewhere. The secondary contribution is larger than the primary though out most of the domain in the summer and in some areas can exceed the primary contribution by an order of magnitude. The secondary contribution result in large part from photochemical reactions, including the reaction of isoprene primarily from biogenic sources and the aromatics and olefins from anthropogenic sources with the hydroxyl radical. The primary species varies less on a seasonal basis than the secondary species. Results for a slower reacting compound, benzene, are similar to that seen for the primary contribution of formaldehyde species, with peak values occurring during the colder months. This is attributed to the trapping of the pollutants during periods of lower mixing heights. Primary formaldehyde can be linked to the direct emission of formaldehyde, while secondary formaldehyde.

The 90th percentile of the annual concentration was computed for each of the three hour time-of-day blocks. The ratio of the 90th percentile value to the mean value for three toxic pollutants are shown in Figure 2. In general, the results the ratio is about a factor of two for formaldehyde,

aceteldehyde and acrolein. Differences in the ratios are surprisingly small between the three pollutants. Diurnally, the ratio shows some variability with higher values for formaldeyde during the early morning (03-06) and for acrolein during the late afternoon (15-18).

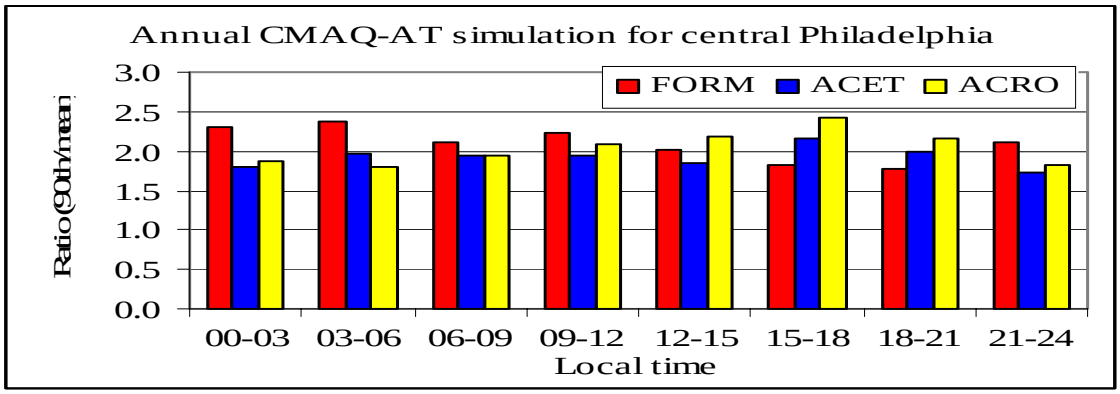

Figure 2. Comparison of 90th percentile versus mean values of formaldehyde (FORM), acetaldehyde (ACET), and acrolein (ACRO) as computed for each diurnal time period (3-hour averages) over central Philadelphia.

2.2 Comparison of monitoring and model outputs

Although detailed field observations for the Philadelphia modeling domain are lacking, air toxic concentration measurements are available from a single monitor in Camden, New Jersey that is part of EPA's Urban Air Toxic Monitoring Program (UATMP) (ERG, 2002). The Camden site is located just east of Philadelphia in a semi-industrial area. The primary emission sources are located mainly to the west and to the north of the Camden site. Further details on the site and the sampling protocol are available from ERG (2002). Concentrations from layer 1 of the grid cell overlaying the Camden site were extracted from the two CMAQ-AT simulations (Table 1). With the exception of 1,3 butadiene, in general, the modeled mean values compared reasonably well against the observed values, and the means, standard deviations, and correlations from the 4 km version of CMAQ-AT compared more closely with the observed values than the modeled values extracted from the 36 km version of CMAQ-AT.

2.3 HAPEM5 Results

A total of six HAPEM5 simulations were made using the three diurnal distributions and two pollutants (benzene and formaldehyde). The average exposure for the Philadelphia area estimated from these simulations, along with the draft 1999 NATA HAPEM5 results which uses a Gaussian plume model (USEPA, 2004), is presented in Table 2. Future analyses will examine the spatial variability of these exposure estimates across the individual census tracts in Philadelphia. As a benchmark, the CMAQ results are compared to the HAPEM5 model results from the 1999 National Air Toxic Assessment (NATA). The CMAQ-AT's estimates for benzene are about half of that predicted by NATA and about 85% of the NATA estimated formaldehyde exposure values. An examination of the temporal variation of the diurnal patterns shows that exposure levels are almost doubled as compared to using average annual patterns. The 90th percentile estimate provides an upper estimate that is comparable to day-to-day variations in ambient levels. Toxicologists believe that capturing this variation is important in characterizing both acute as well as chronic risk (USEPA, 2001).

3. DISCUSSION and SUMMARY

Incorporating variability information at sub-4 km grid resolution will be needed to improve the HAPEM 5 exposure estimates. The current 4 km grid size for the annual CMAQ simulation available underestimates the HAPEM exposure estimates when significant sub-4km grid spatial variations are present. Modeling studies at finer scales for Philadelphia have been conducted. These results provide evidence of significant sub-grid spatial variability below 4 km grid sizes (Ching et al., 2004). Currently, investigations are underway to provide this information to the HAPEM5 system.

We have demonstrated that a sophisticated chemical grid model can be used to provide the air

toxic concentration fields needed to drive an exposure model. A comparison of the model results with a limited set of observations suggests that the model performance is reasonable.

For this pilot study, air toxic concentrations generated by the CMAQ-AT model for a 4 km grid mesh overlaying Philadelphia were successfully formatted for direct input to the human exposure model HAPEM5.

Table 1. Comparison of air toxic concentrations measured at the Camden, NJ, site to CMAQ-AT (layer 1). All samples, except benzene, are 24-hour averages; benzene is a 1-hour average.

Compound	n	Mean (ug/m^3)			Std. deviation (ug/m^3)			Correlation with Observations	
		Obs	4 km	36 km	Obs	4 km	36 km	4 km	36 km
1,3-Butadiene	28	0.33	0.18	0.12	0.34	0.12	0.08	0.07	0.09
Formaldehyde	44	3.68	2.91	2.25	3.21	2.13	1.52	0.42	0.38
Acetaldehyde	44	2.09	2.49	1.92	1.42	1.20	0.78	0.45	0.44
Benzene	1328	1.11	1.02	0.77	1.06	0.71	0.40	0.48	0.41

Table 2. Average Philadelphia exposure levels (ug/m^3) computed with HAPEM5.

Compound	CMAQ-AT 4 km			NATA
	Mean DD	Median DD	90% DD	Mean DD
Benzene	1.26	0.96	2.63	2.23
Formaldehyde	2.15	1.63	4.60	2.57

DD= diurnal distributions pattern

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. REFERENCES

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