OBSERVED AND HIGH RESOLUTION MODELED POLLUTANT FIELDS USING FINE SCALE AND HYBRID MODELING APPROACHES FOR WILMINGTON, DELAWARE

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1. INTRODUCTION

Characterizing the spatial variability of air pollutants in an urban setting is critical for improved air toxics exposure assessments (Isakov et al., 2006; Touma et al., 2006), for model evaluation studies (Ching et al.,, 2006b), and for air quality regulatory applications. Photochemical air quality simulation models provide gridded concentration fields for air quality assessments and for air quality regulatory applications (Byun and Ching (1999). However, outputs of air quality models are grid size dependent. For urban applications, information is needed at fine scales for exposure assessments. For such applications, in principle, this need is met by applying nesting methods to grid models such as Community Multiscale Air Quality (CMAQ) model and other such models to the desired resolution. This approach has constraints; computational expenses increase as grid size decreases, and models are not recommended for running at grids smaller than ~1 km. Yet, it is known that significant spatial variability (hereinafter, sub-grid variability or SGV) occurs even at scales smaller than 1 km (Ching et al., 2006a & 2006b, 2005, Isakov et al., 2006, and Majeed et al., 2004,) due to various reasons including the presence of within-grid sources as well as photochemical-dynamic interactions. CMAQ provides multiscale, grid resolved concentrations. Modeling at neighborhood-scale is valuable when significant variability is present at that scale, but may still underestimate variability. Therefore, SGV should be derived from a combination of - fine-scale modeling with models such as CMAQ, modeling of local sources, and also from photochemistry in turbulent flows. SGV treated as concentration probability density functions (PDFs) are appropriate and provide essential information for improved human exposure assessments.

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2. OBJECTIVE OF STUDY

Previously, as discussed in Ching et al., 2005; et al., 2006a, b, there are various types of applications for which the introduction of SGV information would be a useful adjoint to the concentrations from air quality modeling results. They suggested relaxing grid model outputs from its current fully deterministic state to quasi stochastic fields in which the gridded fields are weighted with statistical parameters of the SGV. Simple examples could include such parameters as Coefficient of Variation (COV), a user specified percentile of the distribution, peak (or maximum) values or its comparable max-to-min range values. Several approaches are being investigated in parameterizing the SGV characteristics for applications in exposure assessments - running CMAQ at urban scales (Ching et al.,2004a), developing a hybrid approach that combines local scale dispersion modeling with CMAQ, application of Large Eddy Simulation with Chemistry models (e.g., LESChem (Herwehe, 2000) and incorporating outputs from building scale and physical modeling studies. Once such SGV information is derived, however, an approach to incorporate SGV for the CMAQ modeled concentration is needed. We present an approach here.

Let *Cg* be defined as the CMAQ gridded concentration values and *CSGV*, the *SGV* concentration distribution about its grid cell value. Now, define the two additional terms - concentration adjusted for *SGV* effects (*SAC*), and a non-dimensional weighting factor $f_1(CSGV)$ derived from modeling or monitoring. Furthermore, we introduce two additional factors – a factor f_2 which is a function dependent on surrogate exposure parameters (e.g., population residence distributions by distance for roadways, in the case of mobile sources) and another factor f_3 which is a function dependent on photochemical dynamical contributions.

$$SAC = C_g * f_1(CSGV) * f_2 * f_3 \qquad (1)$$

Function f_1 *(CSGV)* is the focus of current investigation. f_1 *(CSGV)* can be expressed in a number of ways. In principle, it would be desirable for each cell's CSGV to reflect the properties of its *SGV* distribution function (DF). However, preliminary evidence suggests that the distribution function for *SGVs* differ throughout the modeling domain (Herwehe et al., 2004). Here we use limited statistical descriptions that can still provide a representative metric for each grid cell's DF.

We explore the following three options for the non--dimensional weighting factor:

$$f_1(CSGV) = 1 + COV \qquad (2a)$$

$$f_1(CSGV) = 1 + 95^{th}\ \text{Percentile/GridValue} \qquad (2b)$$

$$f_1(CSGV) = 1 + \text{Peak/GridValue} \qquad (2c)$$

where *COV* is the standard deviation/grid value called the Coefficient of Variation, 95th (or other) percentile of the distribution/grid value and peak of the distribution/grid value. The factor in (2a), differs from (2b) and (2c) because it is computed about its grid mean value, (2b) and (2c) refer to the distribution itself.

The SGV within a regional-scale modeling grid exists for all the pollutants that are being modeled. For the pollutants that have primary and secondary components, SGVs do exist for each of them. The local-scale dispersion modeling is one of the tools available to us for assessing the SGV of primary components that exists within regional-scale modeling grids (Isakov et al., 2006; Touma et al., 2006). For this study we examine the use of local-scale dispersion models (AERMOD in this case) for assessing the SGV within the regional-scale modeling grids that result from various local sources. We are also interested in comparing such results against observations and for this purpose, we utilize data from the Enhanced Delaware Air Toxics and Assessment Study, E-DATAS (DNREC Report, 2006). Also, given that traffic is a major emissions source in urban areas, and because such emissions within a city have a high degree of complexity in their spatial distributions and source strengths, we expect them to contribute to a significant fraction of each model grid's SGV. For this study, we choose to examine the SGV of modeled formaldehyde (HCHO).

3. APPROACH

Our study involves using a hybrid modeling approach (Isakov et al., 2006; Touma et al., 2006) for determining the fine scale details of concentration fields and the E-DATAS database for corroboration. The E-DATAS was conducted in the Wilmington, Delaware (DNREC Report, 2006). During intensive fields study campaigns, a special set of continuous measurements of several air pollutant species including formaldehyde, ozone, Cr^{6+} and fine particles were made on board an instrumented van deployed in mobile transects of downtown Wilmington. Repeated sets of transects were performed, over a set, criss-cross type course that covered many of the streets; each transect taking approximately one hour to complete. Figure 1 shows the modeling domain and the sampling route of the mobile van. The sampling route provides a bases for spatial details of air pollutant characterization on scales finer than 1 km. (In this figure, the continuous data were binned at 100m intervals, and 3 hour averages computed from the morning runs. Such data provides information useful to compare with SGVs from model calculations.

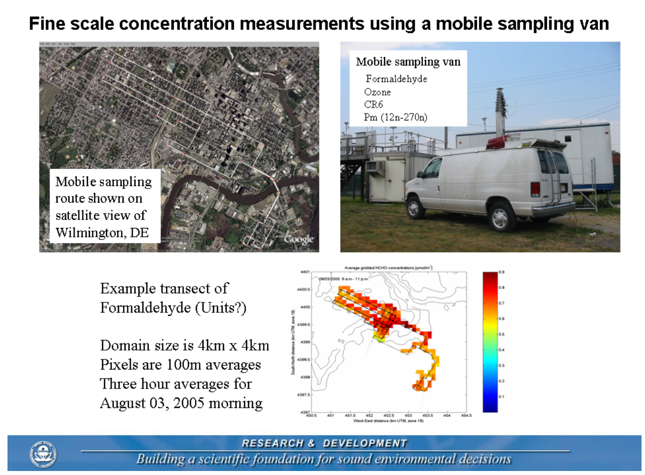

Fig. 1. Mobile sampling during E-DATAS. Study area is Wilmington, Delaware.

We performed a set of CMAQ simulations for 12km with nests at 4 km and 1 km grid sizes. The air toxics version of CMAQ that was used for this study utilized SAPRC-99 chemical mechanism for a Lambert-Conformal projection. The 1999 emissions inventory and 2001 meteorological datasets were utilized for the CMAQ runs. For the SGV, we hereinafter, only consider the primary sources; we model its contributions using a local scale model, AERMOD, to provide the fine scale distribution for CMAQ (Isakov et al., 2006). Local-scale modeling was conducted for all source categories; for the mobile sources the AERMOD was applied to link-based traffic emissions data. A comprehensive emissions inventory developed for calendar year 2003 was utilized for this purpose. However, the modeling was conducted for the calendar year 2001 so that the regional- and local-scale modeling can be related. While the CMAQ modeling is performed for Lambert Conformal and AERMOD for UTM projections, the 4 x 4 km CMAQ grid cell and the AERMOD 4 x 4 km modeling area overlap significantly. We then compute and compare distributions between model simulations and the mobile sampling data. Additionally, although the actual sampling (July-August, 2005) and the modeling period (July 2001) differed, it is assumed that the differences would be relatively small since (a) we do not expect the emissions to change significantly between 2001 and 2005 and (b) the simulations are for a month, and the sampling results are a one week average to minimize day-to-day variations.

4. RESULTS

Figure 2 is the result of CMAQ runs nested down to 4 km grid size. The 4X4 km cell is located over downtown Wilmington., DE. The results shown are the average diurnal variation Formaldehyde (HCHO) for July 2001. For formaldehyde, both primary and total HCHO are depicted for that 4X4 cell. We see the contribution of primary emissions for this cell ranging from to be about 1/5 to 1/3 of the total during the early morning to noon period with strong increases after sunrise from traffic and industry. The strong increase in the ratio of total to primary concentrations in the afternoon is a result of the increase in the height of the mixing layer. Also, photo-chemistry and regional transport processes becomes dominant factors in the afternoon; the total and the ratio show large increases and decreases respectively.

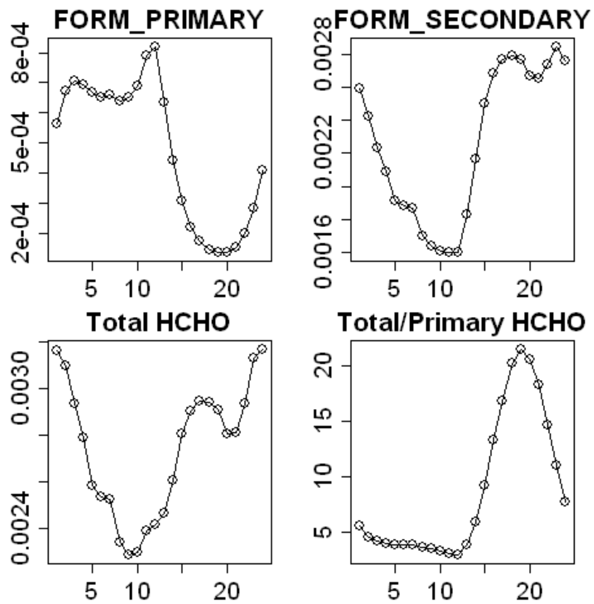

Fig. 2. Results of CMAQ simulations for July 2001 showing sample diurnal variations for a 4X4 km grid cell over downtown Wilmington, DE.

Figure 3 shows an example of the AERMOD model results for HCHO. Values shown are normalized to the modeled peak value of the month. The AERMOD simulations shown are for receptor grids of 200m in UTM coordinates for a domain of approximately 10X10 km. The figure also shows the mobile sampling route implemented during the E-DATAS. The primary sources include all point, area and line sources; the latter from road link-based emissions data. The results shown are the July 2001 average for 1200 EDT, 2001. For the total concentration field, one would need to incorporate the primary contribution from AERMOD with the CMAQ results (Isakov, et al., 2006). The AERMOD simulation shown is arbitrarily chosen for 1200 EDT. While the magnitudes changed over the course of a day, only slight changes in the spatial patterns are noted over the course of a day. From the AERMOD simulation, we observe a significant amount of spatial variability. Variability at this scale is not possible using CMAQ alone for typical urban scale applications of 1 km grid size for CMAQ. The results show clearly, the significant contributions from the highway sources to the variability pattern. Additionally local hot spots of emissions are apparent.

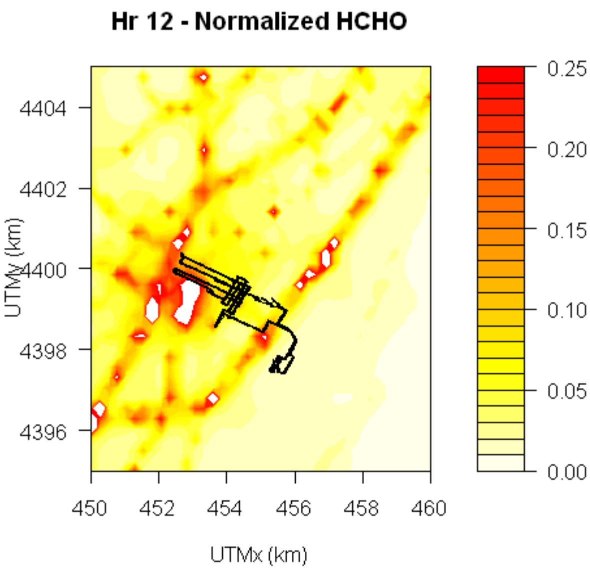

Fig. 3. AERMOD simulation of primary emissions of HCHO in the Wilmington, DE area. The mobile sampling route in the E-DATAS project is indicated. The simulations were made in UTM coordinates for July 2001 @ 1200 EDT.

Figure 4 presents time series plots for three SGVs as defined by (2a), (2b) and (2c) for the mobile van measurements made during the summer 2005 campaign July 31st through August 5th. These measurements were made during the hours of 8 am through 5 pm. The mean, 95 percentile and peak concentrations utilized in the estimation of these SGVs are based on the hourly datasets, that is, measurements for the hours of 8 am to 5 pm. Van measurements indicate that the SGVs based on COV can be as high as [1.1, 1.4], SGVs based on 1+ 95 Percentile/Mean can be as high as [2.1, 2.6], and those based on 1 + Peak/Mean can be as high as [2.1, 3.0].

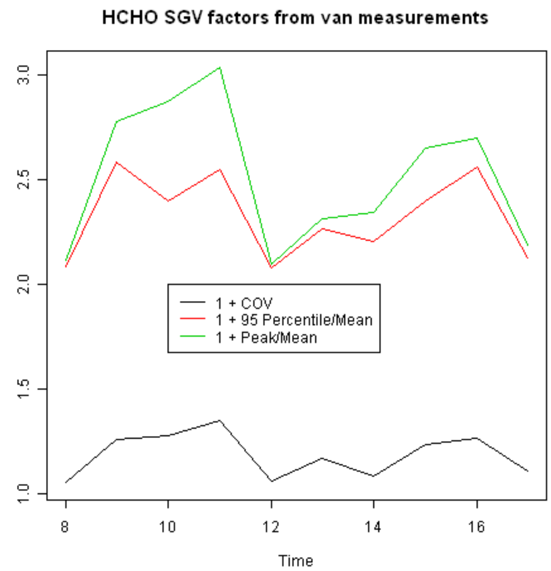

Fig. 4. Three different forms of SGV parameterization derived from mobile van measurements during the July 31 – August 5, 2005 summer campaign

The type of results shown in Figure 4 will, in principle, be an indicator of the magnitude and characteristics of the sub-grid variability of a grid model of 4X4 km size over Wilmington, DE. Figure 5 displays time series of three possible parameters representing SGV (top) and the SGV adjusted concentrations, SACs, grid concentrations influenced or adjusted fields (bottom) based on the SGV parameters from local scale modeling. The SACS shown here are the adjusted CMAQ results shown in Figure 2 for HCHO. Each of the SACs shown is defined using the CMAQ mean for the hour. This introduces a sensitivity resulting in large SACs when the mean is small, especially for example, the example of peak-to-mean. Other definitions may be more satisfactory and are being explored. We can also note that the SGVs estimated from the van measurements and modeling are comparable.

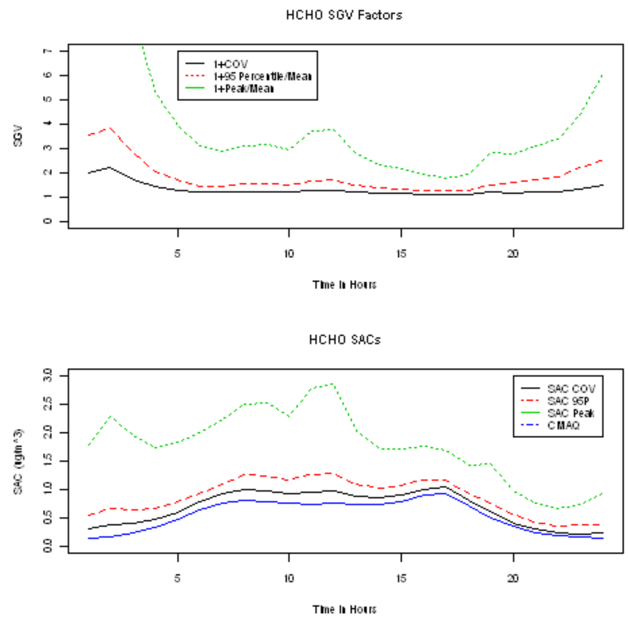

Fig.5. Three different forms of SGV parameterization derived from results of AERMOD modeling of the 4X4 km cell over Wilmington DE for HCHO for July 2001 (top). SGV weighted HCHO concentrations from CMAQ using corresponding SGV parameterizations.

5. DISCUSSIONS AND SUMMARY

We recognize that variability exists at scales smaller than can be resolved with photochemical grid models. Under the assumption that such variability can be important in exposure assessments, we have been attempting to develop modeling tools that will provide this additional dimension of information. To this end, this paper has applied local scale modeling (AERMOD) to provide an estimate of variability from primary emissions. The results of this study substantiates our hypotheses that significant amounts of spatial variability do exist; that application of dispersion models can provide a means to characterize and estimate such variabilities for a primary pollutant species, here HCHO. We note, however, that the modeling results and comparisons with observations noted here have invoked many assumptions, e.g., model and measurement periods differed. Local scale modeling will be inadequate for reactive species and thus, we still see a need for modeling tools such as coupled Large-Eddy Simulations with photoChemistry models (e.g., LESChem, Herwehe, 2000) or local-scale models capable of addressing chemistry to assess secondary components correctly as to provide a greater range of SGVs than can be obtained using local scale and fine scale CMAQ modeling alone. Future efforts will utilize the SGVs from these various modeling tools to applications that include exposure assessments, model evaluations and weight-of-evidence analyses in regulatory models. Regarding SACs, the examples shown here show that sensitivity to some definitions e.g., peak/mean may be excessive; thus, the SAC definitions shown here are to be considered preliminary. Clearly, this situation is to be considered an opportunity for the air quality communities to provide input and guidance on appropriate SAC definitions for different applications.

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