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Paper 2.1 An approach for incorporating sub-grid variability information into air quality modeling

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1. INTRODUCTION

The Community Multiscale Air Quality model (CMAQ) predicts concentration fields of pollutants emitted into an evolving dispersive and chemically- reactive atmospheric environment. It is a property of such models that their quantitative outcomes are dependent on the selection of the grid cell size. For increased spatial resolution, methods can include adaptable grid meshes or "nested" sub-domains with decreasing grid sizes. While grid size can be user specified to be smaller than 1 km, requirements satisfying turbulence closure assumptions for scales less that 1 km are unsatisfied for typical boundary layers (Lumley and Panofsky, 1964). Thus, 1 km is considered a lower limit for models like CMAQ and its meteorological processor MM5.

Whatever is the finest grid size chosen, the CMAQ model predicts a single value for each grid cell for the hour of simulation. Unresolved spatial details, called sub-grid variability (SGV), exist within the grid cells. Obtaining information on SGV can be obtained for specialized situations with techniques such as modeling large buoyant stack plumes with Plume-in Grid (PinG) formulations (Karamchandani et al., 2002). Typically, however, most grid modeling is performed without explicit model provisions and representations of SGV.

There are various reasons for SGV in grid models. Grid models typically disperse emissions evenly across each grid cell. However, within-grid concentration variations exist because the real atmosphere does not disperse emissions homogeneously into grids. Thus, the resulting concentration inhomogeneities will yield distinct concentration distributions whose characteristics will depend on the source type, strength, and location in the grid, and the dispersion strength of the atmosphere. Dispersion in the real atmosphere varies temporally and spatially across individual grid cells because of within-grid variations in the meteorological variables and dispersion parameters that arise from differences in the land-use of the underlying surfaces, and the presence of heterogeneous features, such as buildings, street canyons, vegetation, soil moisture, or impervious surfaces. Significant SGV can also be caused by complex chemical-dynamical interactions in the PBL as a result of the within-grid inhomogeneities

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of chemical mixtures. Herwehe (2000) using a Large-Eddy Simulation model coupled with photochemistry (called LESChem) discussed and demonstrated how these processes contribute to SGV in air quality modeling.

There are several situations where considering SGVs may be important. For example, when comparing model predictions against observations, there will be differences between what is simulated and what is measured (Ching et al., 2005). This impacts the use of modeling for attainment demonstrations and model evaluation studies. Additionally, grid model simulations, being wave-number limited may not accurately characterize "hot spots" and may underestimate human exposure.

Several approaches are being investigated with the goal of describing and parameterizing SGV characteristics so they can be utilized in application assessments, (1) running CMAQ at urban scales (Ching et al., 2004a), (2) developing a hybrid approach that combines local scale dispersion modeling with CMAQ, (3) application of LESChem ((Herwehe, 2000) and (4) incorporating outputs from building scale and physical modeling studies.

Recognizing the existence of SGVs and assuming an eventual capability to model SGVs, we ask two questions: (1) how can SGV information be utilized? and (2) what air quality issues can it address? The remaining portions of this paper address these questions. We address the first question in the next section, where a simple operational method for incorporating SGV information into CMAQ is introduced. This is followed with preliminary results and a short discussion on potential merits of the method for several different applications to address the second question.

APPROACH

Let C_g be defined as the CMAQ gridded concentration values and C_{SGV}, the SGV concentration distribution about its grid cell value. Now, define the two additional terms, (1) concentration adjusted for SGV effects, SAC, and a non-dimensional weighting factor $f(C_{SGV})$. Thus,

$$SAC = C_g * f(C_{SGV}) \quad (1)$$

In principle, it would be desirable for each cell's C_{SGV} to reflect the properties of its SGV Distribution Function (DF). However, preliminary evidence suggests that the distribution function for SGVs differs throughout the modeling domain (Herwehe et al., 2004), and a robust description is not yet available. For this exercise, we use limited statistical descriptions that can still provide a representative metric for each grid cells DF. We explore the following three options for the non dimensional weighting factor:

$f(C_{SGV}) = 1+COV$ (2a)
$f(C_{SGV}) = 95^{th}$ percentile /grid value (2b)
$f(C_{SGV}) =$ peak/grid value (2c)

where COV = the standard deviation /grid value) called the Coefficient of Variation, 95th (or other) percentile of the distribution/grid value and (3) peak of the distribution/grid value. The factor, 2a, differs from 2b and 2c because it is computed about its grid mean value, 2b c refer to the distribution itself. Results of 2a-c will be illustrated in the next section.

3. PRELIMINARY RESULTS

We illustrate the SAC methodology by using results of an air toxics version of CMAQ (Luecken et al., 2005) for a variety of model venues. The first case is for chronic exposure modeling of benzene for a one year

period. The second case, which is pertinent to acute exposure assessments, uses CMAQ simulations for more reactive pollutant species (e.g., formaldehyde) on an episodic basis.

CASE 3.1: CMAQ was run for the year 2001 as a pilot study to demonstrate how to link to the Hazardous Air Pollution and Exposure Model, Version 5 (HAPEM5) a screening model for exposure assessment (Ching et al., 2004b). Annual results for CMAQ are shown in Figure 1a (only grids for Philadelphia County are displayed). We chose benzene for this illustration because mobile emissions are a primary source category in this application. To resolve concentrations fields near roadways, we applied the ISCST3, a local scale modeling to mobile source emission allocated to individual road links (road segments). The roadway network is indicated in Figure 1. The distribution of the roadways varies greatly in density and pattern across the county. The ISCST3 model predicted annual average benzene concentrations at 200 m receptor spacing, thus providing the statistical descriptions of the concentration distributions to (but not altering the value of) the individual CMAQ grid cells. Figure 1b and 1c shows the standard deviation and the highest value (maximum or peak).

For the weighting factor, the descriptive statistics for SGV pertinent to this paper were prepared for each of the CMAQ grid cells. Figure 1 (d, e and f) shows results for SGV weighting functions, 2 a, b and c. In Figure 1f, the 95^{th} percentile values of the distribution for each 4 km cell are included; exposure models typically use the 95^{th} percentile as the statistical parameter of the general distribution of concentrations when introducing variability information. In the example shown in Figure 1f, the implication is that modeled exposure and population risk for benzene will increase by a factor which ranges from 1-5 as shown in Figure 1f.

For the annual benzene concentrations, the SGVs represented by peak/mean ratios are about an order of magnitude greater than the values of the COVs. We observe that spatial distribution of the various SAC factors is qualitatively similar across the County. All SAC factors are highly variable across the modeling domain. The SAC factors are lower in downtown areas with a high density of local roads and also high levels of mean concentrations. In other areas, SAC factors are variable and can be much higher in magnitude.

The comparison of SAC is shown in Figures 2 and 3 for two different grid sizes, 12 and 4 km grid sizes, respectively. Thus, while better able to discern the hot spot areas, it is clear that the results are sensitive to the size of the modeled grid used in the assessment.

CASE 3.2: The CMAQ grid at 1 km size was used to derive SGVs for a reactive pollutant species, formaldehyde. Results shown in Figures 4 and 5 are from nested runs at 1 km grids for a domain encompassing the State of Delaware and were prepared using outputs for July 2001 based on the 4 and 12 km runs from Case 3.1. SGVs were determined by aggregating information from 144 1-km grid cells in each of the 12 km cells. Time series are shown for three selected 12 km grid cells; two were of urban land use type and the third considered rural. Urban site (A) is just to the west of and urban site (B) was centered over Wilmington, DE. Rural site, (C) is located in Sussex County, Maryland, about halfway down and adjacent to the MD-DE border. In Figure 4, the time series of formaldehyde (HCHO) is shown for the CMAQ 12 km simulations. The time series for the three sites correlate with each other in

tracking the episodic swings during the month of simulation. The 95th percentile of the SGV as the weighting coefficient and resulting SAC are displayed for these grid locations. The time series results are shown on the top and the distributions in box-whisker format shown on the bottom. Generally, the grid concentrations and its SAC are larger for the urban grids than the rural grids. Figure 5 compares the time series of SAC using the 95th percentile of the SGV Distribution for HCHO for urban site (A).

4. SUMMARY AND DISCUSSION

We have shown examples to introduce SGV as outputs with CMAQ results embodied in Equation 1. We have illustrated the methodology using three indicators of SGVs, the ratio of standard deviation, the 95th percentile and the peak-to-mean values to the gridded concentrations from CMAQ at 12 km grid sizes. The SGVs for the relatively inert species, benzene, were obtained using local scale modeling. For the reactive species, HCHO, the fine scale details were obtained using CMAQ at a 1 km mesh size; however, we surmise that the SGV for HCHO will increase when contributions from both local scale modeling of primary emissions and the SGV variability due to coupled chemistry and turbulence are introduced. We have utilized various statistical descriptors as examples of the SGV distributions including their normalized standard deviation, peak, and percentile values. We find that these simple ratios can vary greatly across urban area modeling domains.

These early findings reveal that SAC results can be significantly larger than its parent CMAQ simulations. Their implication is for models to be able to predict a greater risk potential to populations exposed to air pollutants than from standard model results.

The following are three areas may benefit from the introduction of SAC methodology: (1) The SAC method provides more representative and defensible results for improved air toxics exposure modeling and their risk assessments for an improved characterization of toxics hot spots in the modeling domain. (2) For model evaluation, comparisons between model predictions from a grid volume to observations taken at a point could be based on a distribution of SGV grid values rather than a single cell value. Even though it is understood that the stochastic component imbedded in an observation can never be simulated by deterministic models and the SGV approach does not address that fundamental problem, the introduction of SACs can help establish upper and lower bounds for model evaluation studies. (3) It will be of interest to consider introducing SAC concepts to model attainment demonstrations required for State Implementation Plans. Under the provisions for a Weight-Of-Evidence (WOE) analysis, we suggest that SACs can provide an improved means for assessing and applying Relative Reduction Factors (RRFs) and future design values (DVFs). Per the Draft ozone modeling guidance, RRF is a single number, and it does not account for the SGV in the maxima of the future and base case. The application of SAC to the RRF could provide a range of DVFs. Exploratory studies are needed to determine what statistic provides a reasonable range of values for the RRF. The upper bound of the DVF would favor greater protection, while the lower bound would favor less protection.

SGV modeling is in its development stage. More model research and community dialogue will be needed to develop tools and methods for determining SGVs and subsequently in formulations for use of SGVs in practical modeling applications. The modeling of SGV for reactive species will

require modeling methods, such as coupled Large-Eddy Simulations with photochemistry models (e.g., LESCHEM, Herwehe, 2000) to provide a greater range of SGVs than can be obtained using fine scale CMAQ modeling alone. Local scale model tools should have the capability to accurately model dispersion of pollutants, especially those sources contributing to hot spots.

In addition to improving the tools for modeling the SGVs, we feel it is also important to derive parameterizations from gridded distributions to provide a fuller expression of the type and shape of the distribution functions for practical applications (Herwehe, et al., 2004). Also, this paper focused on a methodology as applied to concentration modeling. In principle, one could consider generalizing this approach to emission and meteorological grid model simulations.

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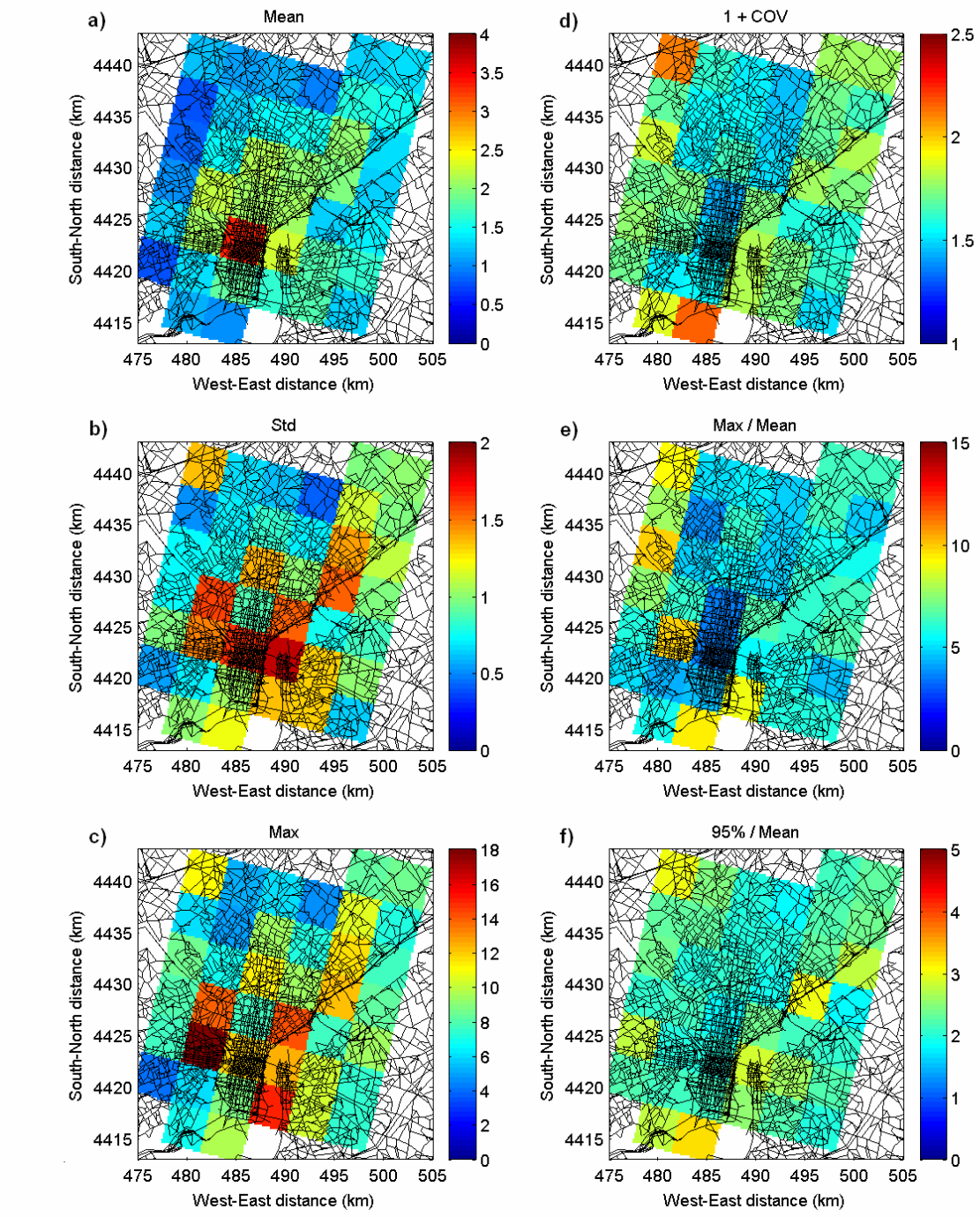

Figure 1. Benzene simulation results from CMAQ for annual (2001) simulations using 4 km grid size. Included are the (a) mean [μg/m^3], (b) standard deviation, STD [μg/m^3], (c) peak [μg/m^3], and SGV dimensionless factors for: (d) COV, (e) Peak/mean, and (f) 95th percentile/mean. The SGV values are derived from ISCST3. The road links are shown as background.

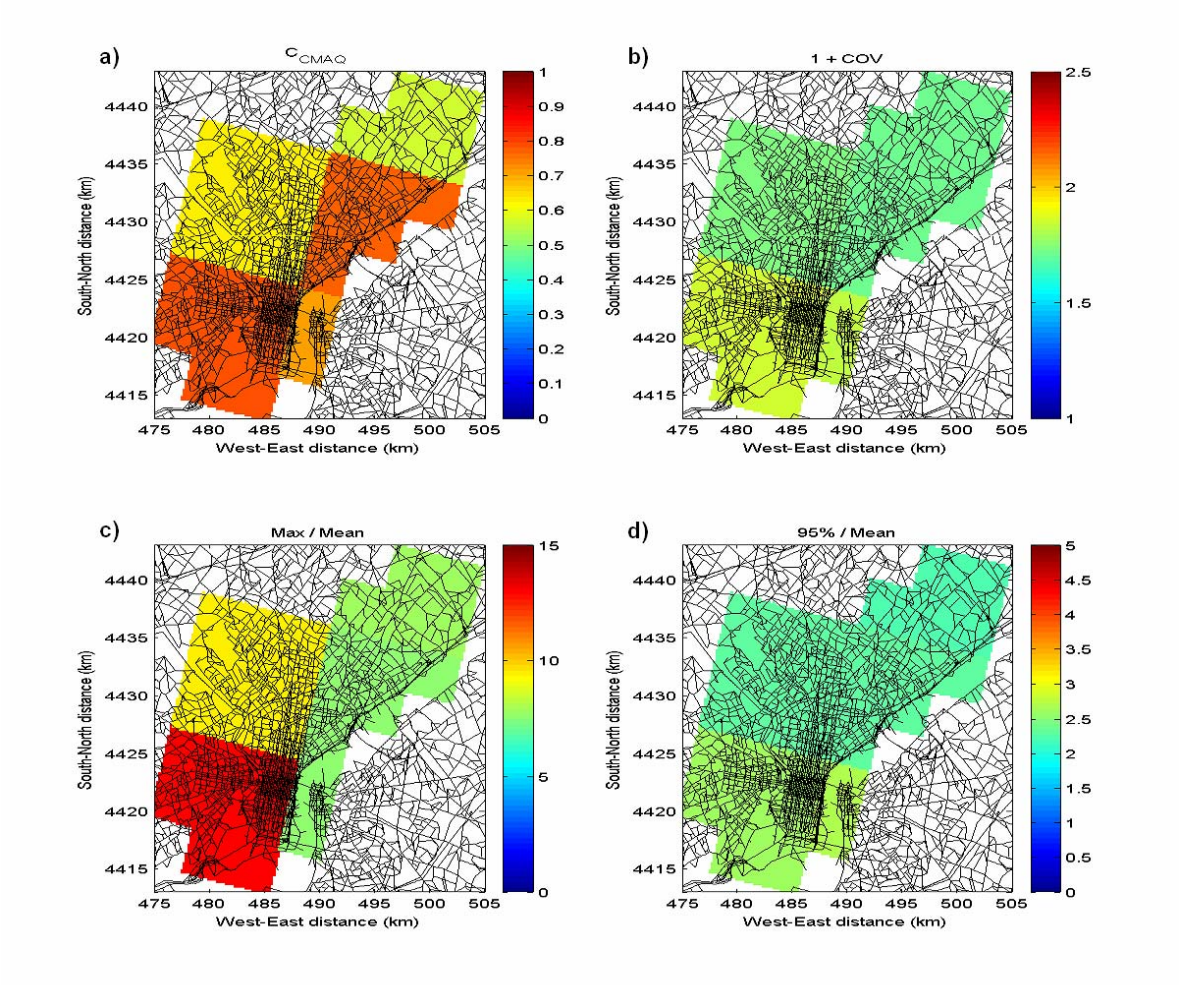

Figure 2. Benzene concentrations [μg/m^3] from annual (2001) CMAQ simulations using 12 km grid size: (a) grid cell mean values [μg/m^3], and various SGV adjustment factors: (b) 1+COV, (c) peak to mean ratio, and (d) 95th percentile to mean ratio. The SGV values are derived from ISCST3. The road links are shown as background.

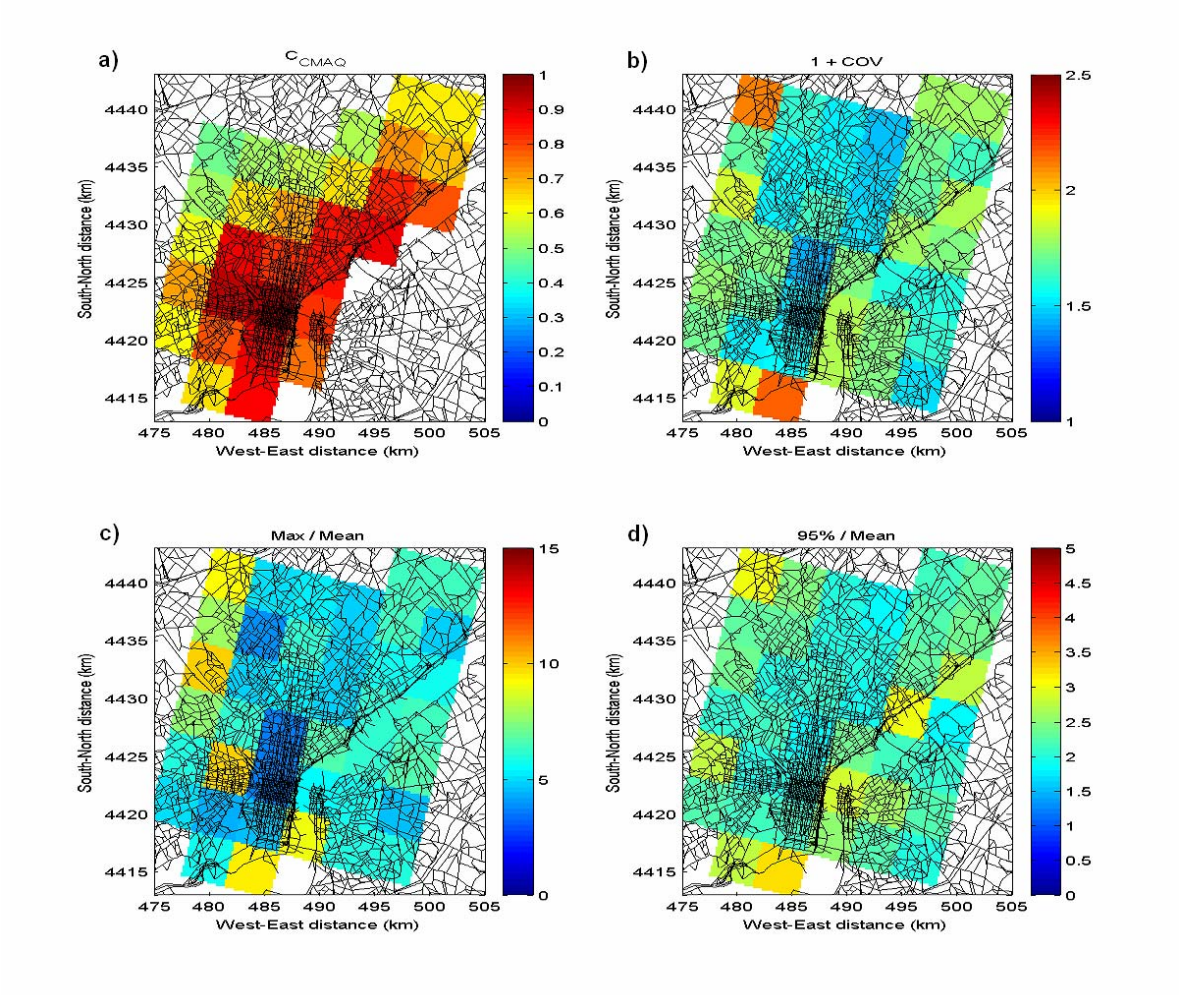

Figure 3. Benzene concentrations from annual (2001) CMAQ simulations using 4 km grid size: (a) grid cell mean values [μg/m^3], and various SGV adjustment factors: (b) 1+COV, (c) peak to mean ratio, and (d) 95th percentile to mean ratio. The SGV values are derived from ISCST3. The road links are shown as background.

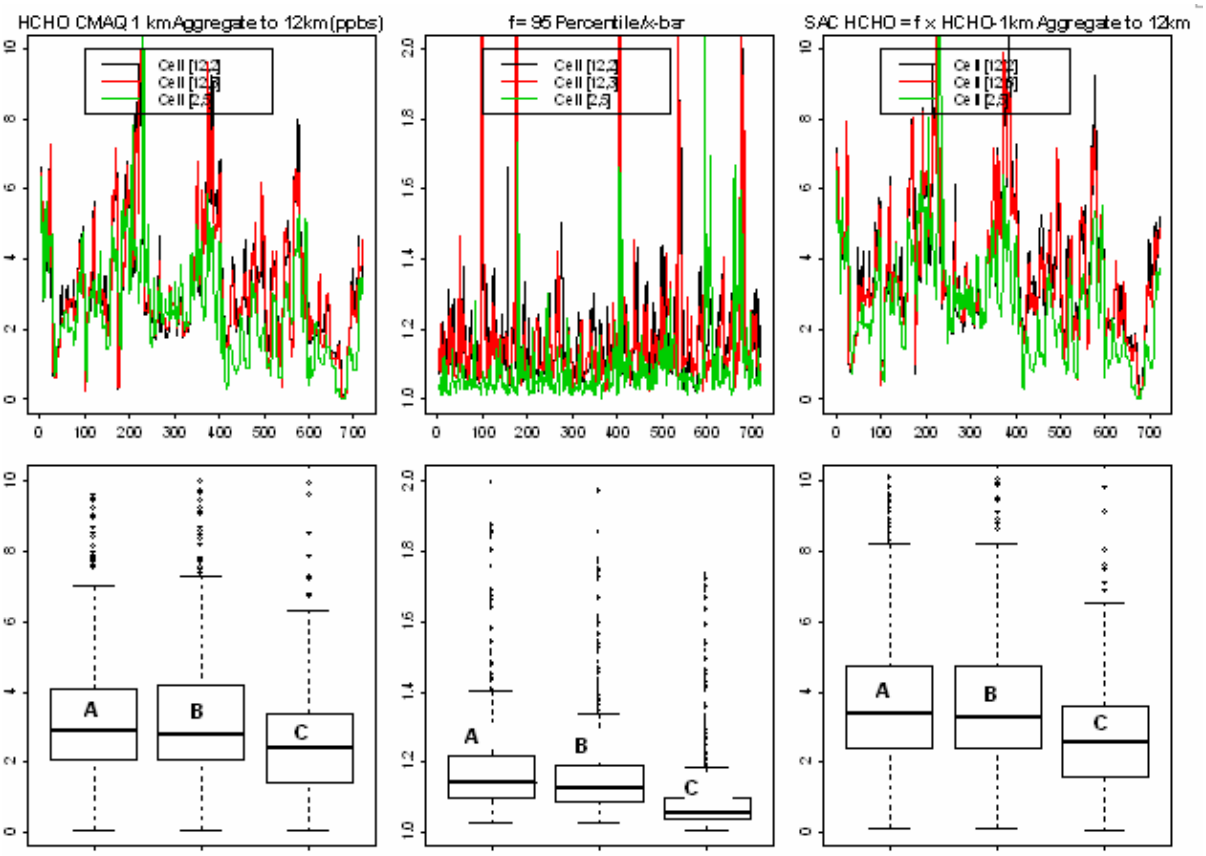

Figure 4. CMAQ time series (left side) and SGV weighting function (middle) and SAC (right side) for 95th percentile of SGV for HCHO for July 2001. Results are for three 12 km cells, Urban cell (A) west of Wilmington DE)(black), Urban cell (B) for Wilmington DE (red) and Upwind rural cell (C) (green).

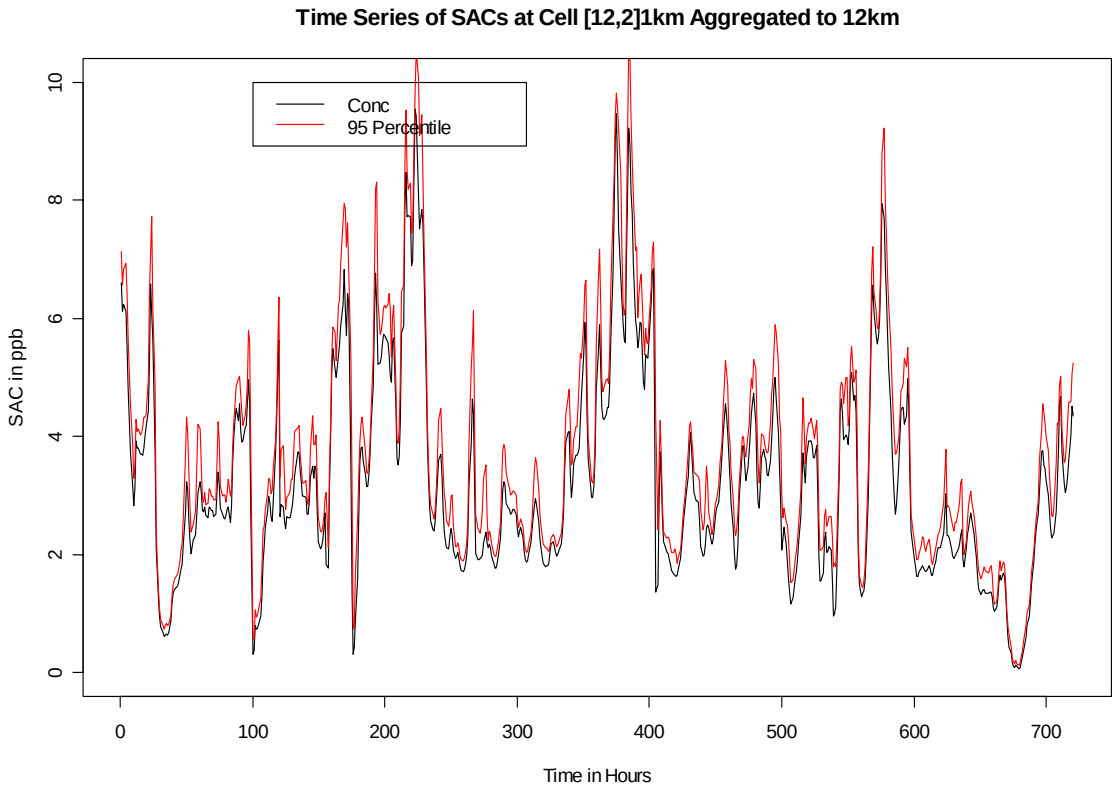

Figure 5. Time series from CMAQ (12km grid concentrations from aggregation of 1 km cell values) simulations and weighted results for 95th percentile SGV of HCHO from July 1 to July 31, 2001. Results are for an urban grid cell (A of Figure 4) of 12 km size located west of Wilmington DE.