

On joint deterministic grid modeling and sub-grid variability conceptual framework for model evaluation

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Abstract

The general situation (but exemplified in urban areas), where a significant degree of sub-grid variability (SGV) exists in grid models poses problems when comparing grid-based air-quality modeling results with observations. Typically, grid models ignore or parameterize processes and features that are at their sub-grid scale. Also, observations may be obtained in an area where significant spatial variability in the concentration fields exists. Consequently, model results and observations cannot be expected to be equal. To address this issue, we suggest a framework that can provide for qualitative judgments on model performance based on comparing observations to the grid predictions and its SGV distribution. Further, we (a) explore some characteristics of SGV, (b) comment on the contributions to SGV and (c) examine the implications to the modeling results at coarse grid resolution using examples from fine scale grid modeling of the Community Multi-scale Air Quality (CMAQ) modeling system.

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1. Introduction

Comparison of meteorological and air-quality grid model simulations with point measurements is problematic. In statistical terms, this is considered a “change of support” problem in which inferences are made about differences between point-based measurements to model-predicted values that represent volume average concentration (Gelfand et al., 2001). There is an extensive body of literature that recognizes and discusses sources of modeling

uncertainties and methods for evaluating them. For example, Fine et al. (2003) review the issues associated with evaluation of model uncertainties (MU) in photochemical models. They explore the range of sensitivity, diagnostic and other useful studies used in performing uncertainty analyses. MU, in general, consists of contributions from all sources in varying degrees, to be both epistemic and aleatory (i.e., due to deterministic or stochastic causes, respectively) (Lohman et al., 2000). The classes of epistemic MU are those inclusive of model inputs such as emissions, meteorology, land-use, initial and boundary conditions, and imperfections in model formulations (parameterizations) of various physical and chemical processes (NRC, 1991; Russell and Dennis, 2000). The aleatory classes of

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MU are stochastic variability due to turbulence and other random processes not simulated by deterministic models.

In addition to the MU from both epistemic and aleatory classes, there is an additional consideration, which arises from the scale dependency of models. A fundamental attribute of deterministically modeled air-pollutant concentrations is that they are grid size-dependent (Odman and Russell, 1991; Jang et al., 1995). Thus, quantitative comparisons of modeled concentrations with observations will change merely due to a different choice in the size of the grid cell chosen for the simulation. Further, attributes of inherent within-grid spatial variability, also known as sub-grid variability (SGV), which, by definition, is not simulated by grid models, are dependent on the parent model grid size. When SGV is significant, the comparison of grid model outputs against one or more point measurements cannot be expected to be encouraging, except under very limited circumstances. Moreover, any observation reflects an event out of a population, while model predictions represent an average of the population.

2. Concept and approach

One fundamental property and limitation of grid models is their inability to resolve spatial features smaller than twice the grid cell size used in the simulation. However, for meteorology, each typical model domain uses grid sizes ranging from one to hundreds of kilometers and contains within-grid cell (hereinafter, within-grid) areal variability due to land-use, land-cover and terrain complexities at much finer scales. (Problematic are the methodology(s) devised to treat within-grid fractional land use. In the case of complex terrain, one cannot well extrapolate either the systematic biases due to the meteorology model terrain smoothing methodology or the effects of the sub-grid terrain variability itself.) For typical regional-to-urban scale air pollution modeling, in addition to sub-grid scale modeling issues associated with fine scale land-use and complex terrain features, the usual practice is to amalgamate and disperse into each cell, all the within-grid emission sources, thus producing inherent, but generally unresolved SGV. This problem is ameliorated, but never eliminated entirely, by employing successively finer scale grid sizes (Odman and Russell, 1991; Jang et al., 1995; Gego et al.,

2005), or by specific within-grid model treatments for some of the major point sources, (e.g., Karamchandani et al., 2002). Recently, it has been pointed out that significant spatial and temporal variability can arise even from coupled chemical and turbulent interactions (Herwehe, 2000). On the other hand, siting guidance for locating monitors cannot fully satisfy the representativeness criteria requirement except for idealized horizontally homogeneous, fully dispersed, uniform source distribution situations. The circumstance in which the monitors and grid model outputs are really expected to be completely comparable is conceptually fortuitous, especially in urban areas, as illustrated schematically in Fig. 1. In Fig. 1a for any given cell, there is a cell mean, and some distribution representing the concentration SGV. Fig. 1b is a hypothetical but typical problem facing monitoring deployment; in this situation, the monitor is located far away and upwind of a busy polluted roadside.

An opportunity to explore these considerations is provided as a result of modeling studies using the US EPA CMAQ modeling system (Byun and Ching, 1999) for simulating airborne toxics and other air pollutants at neighborhood scales (Ching et al., 2004a, b, c). Their implementation employed nests of grids for model simulations run at increasingly smaller grid sizes from 36 km, down to 1.3 (or 1) km. These results will serve to illustrate three aspects of grid modeling relevant to model evaluation considerations including: (a) grid resolution, (b) characteristics of and contributions to SGV, and (c) comparison between model simulations at a given grid size from model's run at the prescribed grid size to aggregated results from finer grid sizes. In (a), we show fine-scale features not apparent in coarse grid simulations to become evident as grid sizes become smaller. In (b), we investigate the characteristic features of the SGV distributions of concentration values and comment on their dependence on the within-grid spatial distributions of sources as well as on the nature and extent of turbulence-induced chemistry processes. In (c), we demonstrate that aggregation of model outputs from fine-scale modeling differs, in general, from the results of coarser, native grid simulations of equivalent size. The areas with largest differences are usually co-located with areas containing a significant number of pollutant sources. We suggest that these differences occur because the coarse grid simulations inherently lack model treatments for sources and processes acting at their sub-grid scales.

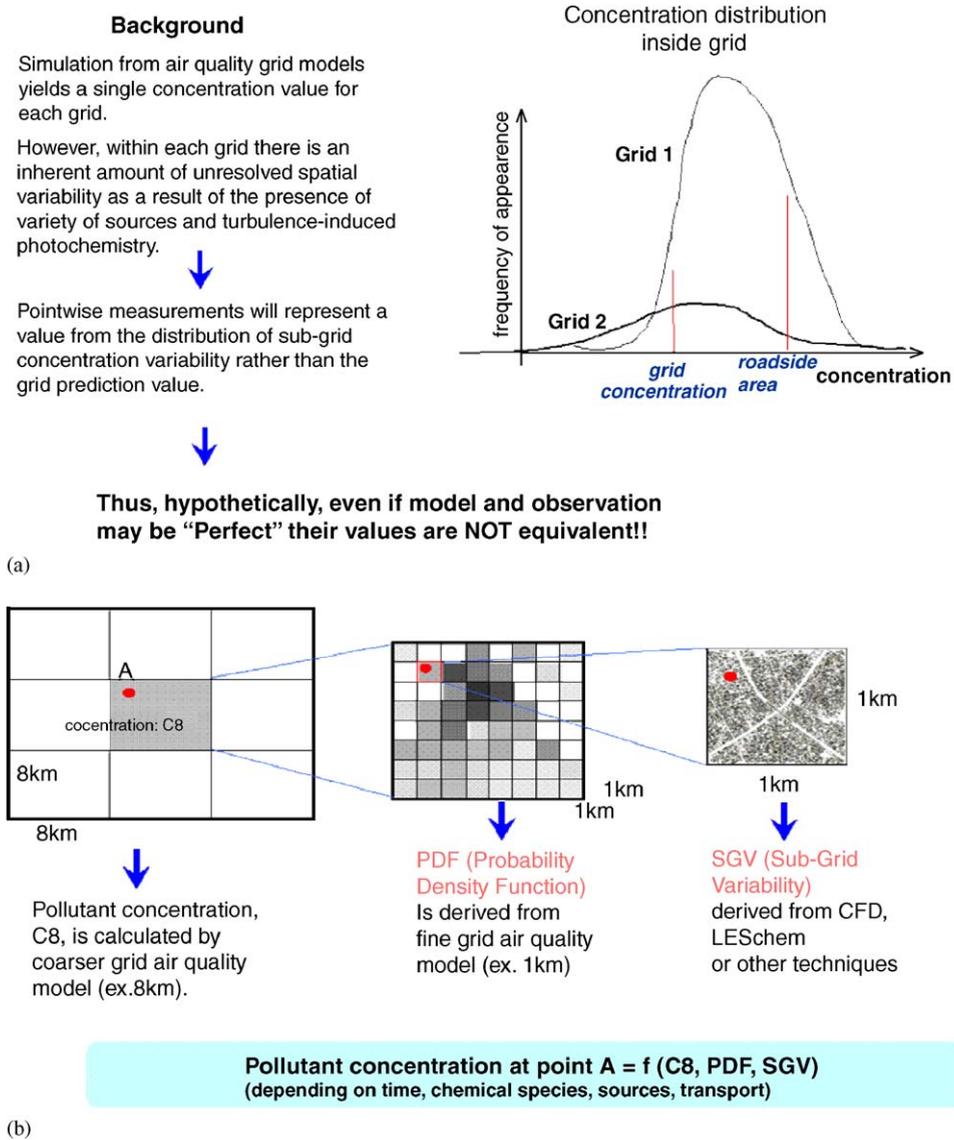


Fig. 1. (a) Schematic indicating concentration variability within each grid cell. (b) Schematic illustrating concentration variability as function of grid size and location in modeling domain relative to observations at a monitoring site location.

As a caveat, we note that there are contributions to SGV at finer grid sizes than the 1.3 or 1 km scale for which we have model results, so the conclusions reached here are based on examples that probably underestimate the full variability.

3. Results and discussion

3.1. Multiscale simulation

The following results are based on the CMAQ (Version 4.2.1) modeling system (for nested model

domains at 36, 12, 4, and 1 km grid sizes that encompass the Houston, Texas and surrounding areas. The simulations were performed for 30 August 2000; the dominant large-scale synoptic pattern was modulated by the land and Galveston Bay breeze circulation. Consequently, the flow field over Houston shifted from a predominantly westerly direction early in the day to a reversal and southeasterly flow in the mid afternoon. The meteorology and emissions for CMAQ runs were from the PSU-NCAR Mesoscale Meteorological model, Version 5 (MM5) and the Sparse Matrix

Operator Kernal Emission (SMOKE) system, respectively.

Modeling performed at fine scales using 1 km grid size provides insights into the sub-grid scale variability for air-quality models run at coarser scales. We recognize that as grid cell size decreases, the model “noise” content increases. At any given point in space and time, modeled values can be highly variable and predictability is reduced because of the influence of stochastic processes (Hogrefe et al., 2000) and errors in the model inputs such as meteorology and emissions (Sax and Isakov, 2003). The emissions outputs from SMOKE were produced using base spatial surrogates set at 1 km grid resolution. Purposefully interpolating from the same source inventory, we ensure the *relative* sensitivity of the model outputs is not compromised as a function of grid size.

Fig. 2a illustrates a simulation for each of the grid resolutions in a common domain for carbon monoxide (CO) at 0700 CDT. The comparisons are shown for the lowest (sigma) layer, which was the same for each of the 4 different grid sizes in this study. Clearly, with each decreasing grid size, finer scale spatial features become apparent. CO is a relatively photochemically inert species, so that the patterns reflect dispersion and transport modeling of the sources. For CO, the mobile contribution is dominant. With the exception of invoking some sort of sub-grid (Karamchandani et al., 2002) treatment, it is important to recognize that within-grid spatial detail of source location and strength are not retained in CMAQ; emissions are dispersed uniformly into and throughout the grid cell identified at the level of source’s plume rise.

Results for photochemically active pollutant species such as for NO_x (NO + NO₂) and ozone, are shown in Figs. 2b and c, respectively. These simulations clearly show finer scale features becoming more pronounced as grid cell size decreases. The NO_x features are much like that of CO, with the mobile sources along the major traffic corridor and at several major industrial sources becoming more distinct with decreasing grid size. Note that the ozone simulations differ considerably as grid size decreases from 12 to 1 km indicating increasingly depressed levels in the ozone in the presence of high NO source areas. While NO_x is a major precursor of ozone, ozone is initially titrated by NO in the near-field. This titration effect is not apparent until the grid resolution is fine enough to resolve the NO_x source patterns. In this study, we see that at coarse

grid spacings of 4 km and larger, the NO_x emissions sufficiently diluted to a level that the titration effect was effectively reduced. At 1 km grid cell size, the spatial pattern of NO_x is discernible and can clearly be identified with its traffic and industrial sources.

The implication of grid size-dependent simulation is as follows: Hypothetically, if one sampled any and all pollutants somewhere across any one of the 36 km grid cells, one would obtain one data point of each of the species. For each such 36 km simulation, there are correspondingly 9 data points for the 12 km grid size, 81 for the 4 km grid size and 1296 for the 1 km grid size simulations. Typical ambient monitoring networks for environmental measurements are relatively far less dense than that required for evaluating the results of fine-scale modeling. However, it can be clearly seen that sampling at a single point can best represent the value of the grid in closest proximity to it, and that this value may differ greatly from the mean value of the cell of coarser size, especially if it is located in an area in which SGV pollutant concentrations features are characteristically large.

3.2. Implications to model evaluation from fine-scale modeling results

In the previous section, we illustrated the presence of inherent within-grid variability for coarse grid simulations based on the results of finer scale modeling. We now examine the *hypothetical* situation in which information about their SGV concentration distributions is available for comparing the gridded model outputs with ambient data. Given such a priori existence of SGV distribution at any model grid, a single-point measurement can only be, but one member of that distribution. Without other information, we cannot even say whether the measurement represents the most probable range of values of the distribution. It will definitely be biased towards the values in nearest proximity to the site, but such values could be anywhere in the distribution. If the observed value falls within the range of the SGV distribution, this does not necessarily imply that the model estimates are accurate; other acceptance or rejection criteria or evaluation diagnostics should be applied (Fine et al., 2003). However, the potential for model failure is the situation for which the observed value is outside some arbitrary evaluation criteria such as the ratio of the standard deviation to the mean of the distribution, or coefficient of variation (COV),

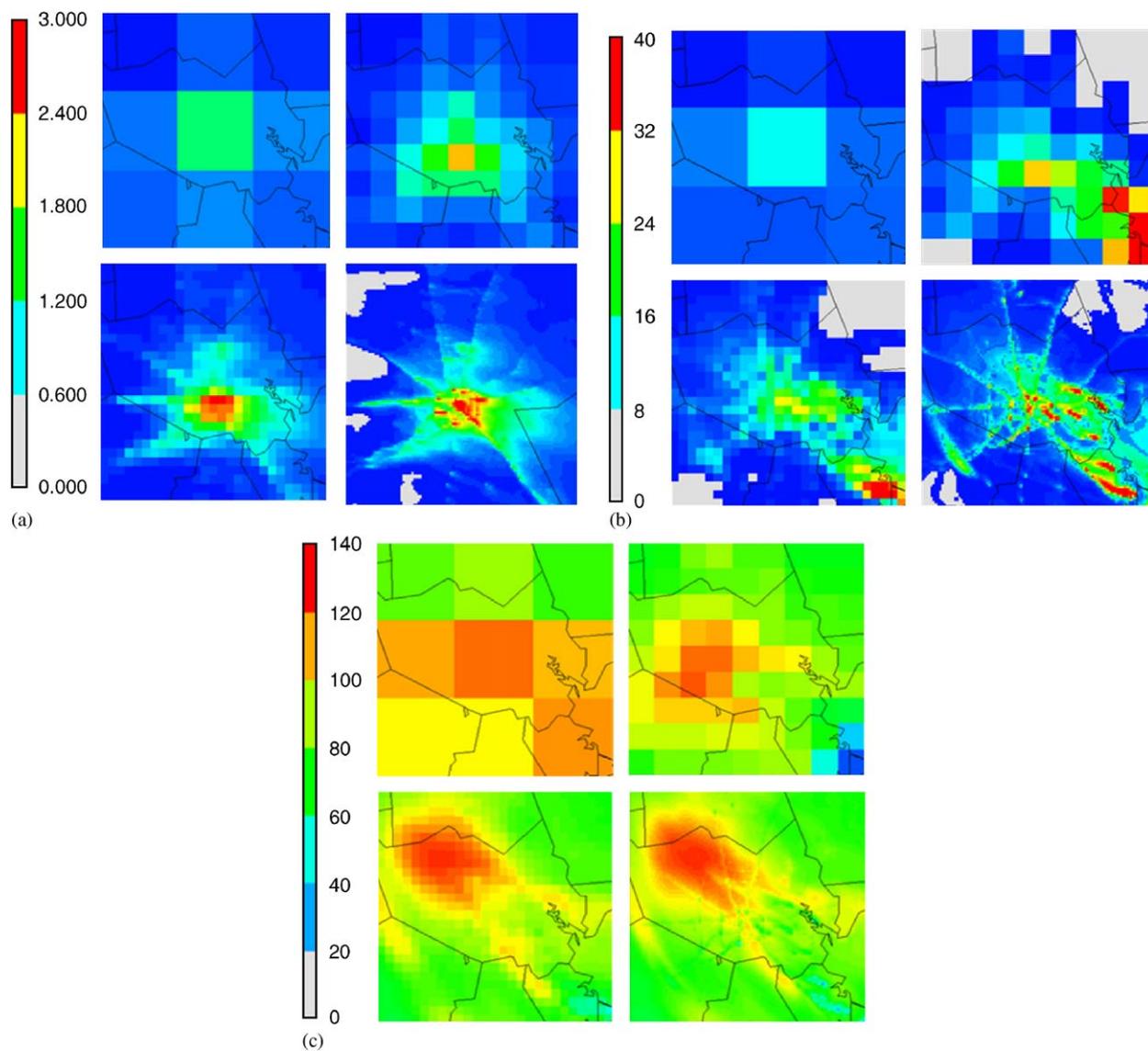


Fig. 2. (a) Results of CO (ppm_v) from CMAQ for 30 August 2000 at 0700 CDT for Houston, Texas' model domain. Panels are: top left is for 36 km; top right is for 12 km, bottom left is for 4 km and bottom right is for 1 km grid size. (b) Results of NO_x (ppb_v) from CMAQ for 30 August 2000 at 1500 CDT for Houston, Texas' model domain. Panels are: top left is for 36 km, top right is for 12 km, bottom left is for 4 km and bottom right is for 1 km grid size. (c) Results of ozone (ppb_v) from CMAQ for 30 August 2000 at 1500 CDT for Houston, Texas' model domain. Panels are: top left is for 36 km; top right is for 12 km, bottom left is for 4 km and bottom right is for 1 km grid size.

or within the 95th percentile value of the SGV distribution. For illustration, we derive COVs for the 12 and 4 km grids using the results of the 1 km simulations. From Fig. 3, we see that the COV for CO is quite variable, spatially, over the urban area, values as large as 0.6 are seen.

It is of interest to understand the characteristics of the distribution of the SGV. For convenience, we utilize results based on a study (Herwehe et al., 2004) that focused on the descriptive characteristics

of sub-grid features. The dataset for that case study utilized a set of CMAQ simulations run at 36 km and nested to 12, 4 and 1.33 km grid sizes for a Philadelphia domain for 14 July 1995. Herwehe et al. derived measures of SGV for the 12 km grids using the results of the fine scale modeling at 1.33 km. Histograms for a subset of the 12 km grids in the Philadelphia area of the modeling domain are shown in Fig. 4. We have arbitrarily chosen the example of acetaldehyde (CH₃CHO), but we could

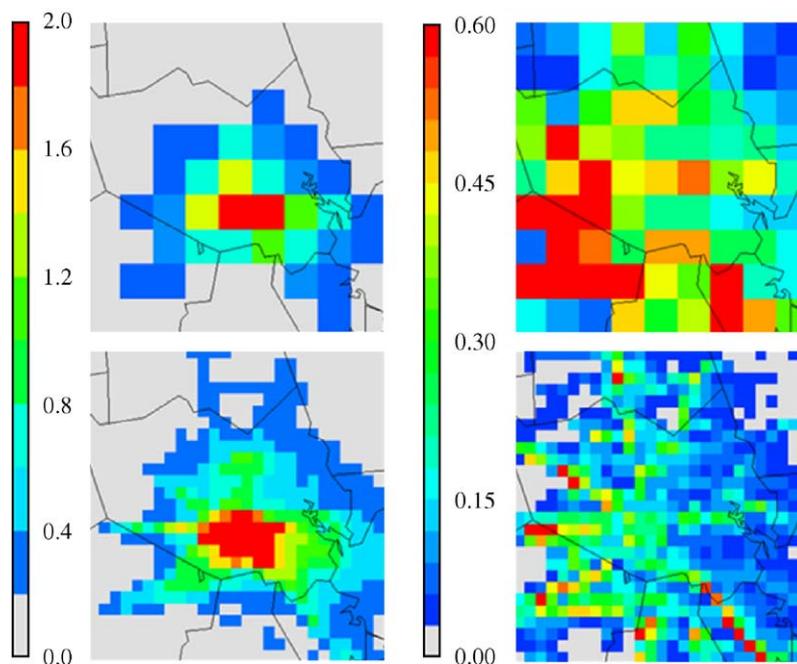


Fig. 3. CO for 30 August 2000 at 0700 CDT using CMAQ for Houston, Texas' modeling domain. Gridded means (ppm_v) aggregated from 1 km simulations are on left-hand side, ratio of standard deviation-to-aggregate mean shown on right-hand side. Top figures are for 12 km, the bottom figures are for 4 km.

have easily focused on any of the other pollutants simulated by the CMAQ modeling system. Contributions to the ambient acetaldehyde distribution come from both primary sources as well as from photochemical processes. For this species (and while not shown, for all the other pollutants simulated) the characteristics of modality, shape, and spread (range) of the distribution in each grid cell varied both across the modeling domain as well as in time throughout the day. While the variations in the distributions give the appearance of randomness, in certain special instances some order appears (for example, while not shown, for those grids in which ozone titration by NO is pronounced, those distributions show the ozone and NO to be characteristically negatively and positively skewed, respectively, as expected).

In order to further describe the SGV distributions, we employ a specialized statistical analysis tool called CDFware (Herwehe et al., 2004) that determines an appropriate distribution at any given time for each grid cell and estimates the parameters of this distribution. Perusing the results, we found that it took a wide range of functions to describe the gridded SGV across the modeling domain. While no single type of distribution seems to be able to

describe the SGV for all the grids in the modeling domain, the initial screening survey showed about 40% of the grid cells were best described by a Weibull distribution function. This is not surprising, since the Weibull distribution offers considerable curve-fitting flexibility. Fig. 4 also shows the Weibull distribution fit to the histograms for acetaldehyde. The shape of the Weibull distribution can vary widely, depending on the values of the parameters, which govern it. In Fig. 4, the Weibull distribution's parameters allowed for distribution shapes for cells that were severely right-skewed and for cells in which the shape is more or less symmetric. While not evident in Fig. 4, it was able to describe well distributions that were strongly left-skewed, as for example is characteristic of the distributions for O₃. Assuming that acetaldehyde can be described by the Weibull distribution, we next attempted to map the estimates of the shape and location parameters. Unfortunately, we found these parameters to be highly variable in both space and time-of-day across the modeling domain; the practical implication is that no convenient parametric descriptions for the SGV emerged from this study (Herwehe et al., 2004). Nevertheless, the magnitude and distribution of the SGV can be

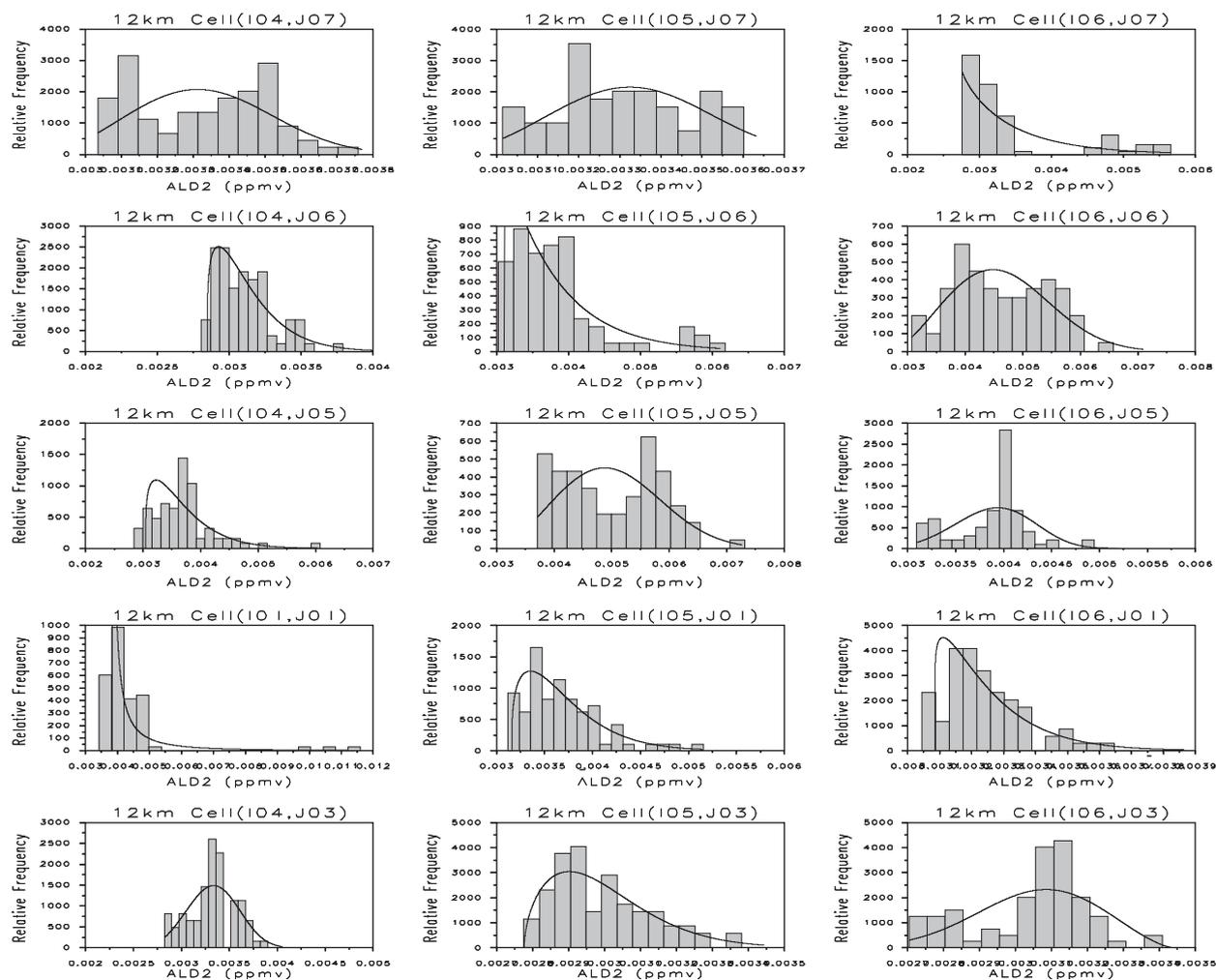


Fig. 4. Acetaldehyde relative histograms (relative frequency versus mixing ratio) are shown with Weibull probability density function fits shown as heavy lines. These distributions show the sub-grid variation of surface acetaldehyde for each $(12\text{ km})^2$ grid cell derived from blocks of 81 km grid values at 15:00 LST from the CMAQ simulation of the Philadelphia area for 14 July 1995. This figure represents a 3×5 -grid cell subset of the 10×10 -cell-domain; the center cell (105, J05) is for central Philadelphia. Plot axes use automatic ranging to clarify sub-grid distribution shape.

quite large for many of the grids in the modeling domain, thus, either broadening the acceptance level of models or requiring additional density of observation sites in monitoring networks.

3.2.1. Contributions to SGV from turbulence-induced photochemistry

Additional SGV exists, in principle, for the relatively fine (1–1.33 km) grid size simulations. These will arise from within grid source contributions as well as from internal-coupled turbulent and photochemistry aleatory interactions. For example, Herwehe (2000) demonstrated that chemical hetero-

genities will arise from the process of photochemical reactions that take place as a consequence of turbulent transport in a polluted atmosphere. Herwehe's LESchem modeling system utilized a large-eddy simulation model of boundary layer turbulence with online-coupled photochemistry, allowing studies to be performed for which chemical reactions occur during mixing motions on turbulent scales. His studies have shown that transient SGV arises, even from relatively simple cases. For example, from Herwehe (2000) as seen in Fig. 5, turbulent motions will transform the properties of a volume of air for an idealized case of steady and uniform surface source (flux) of precursor

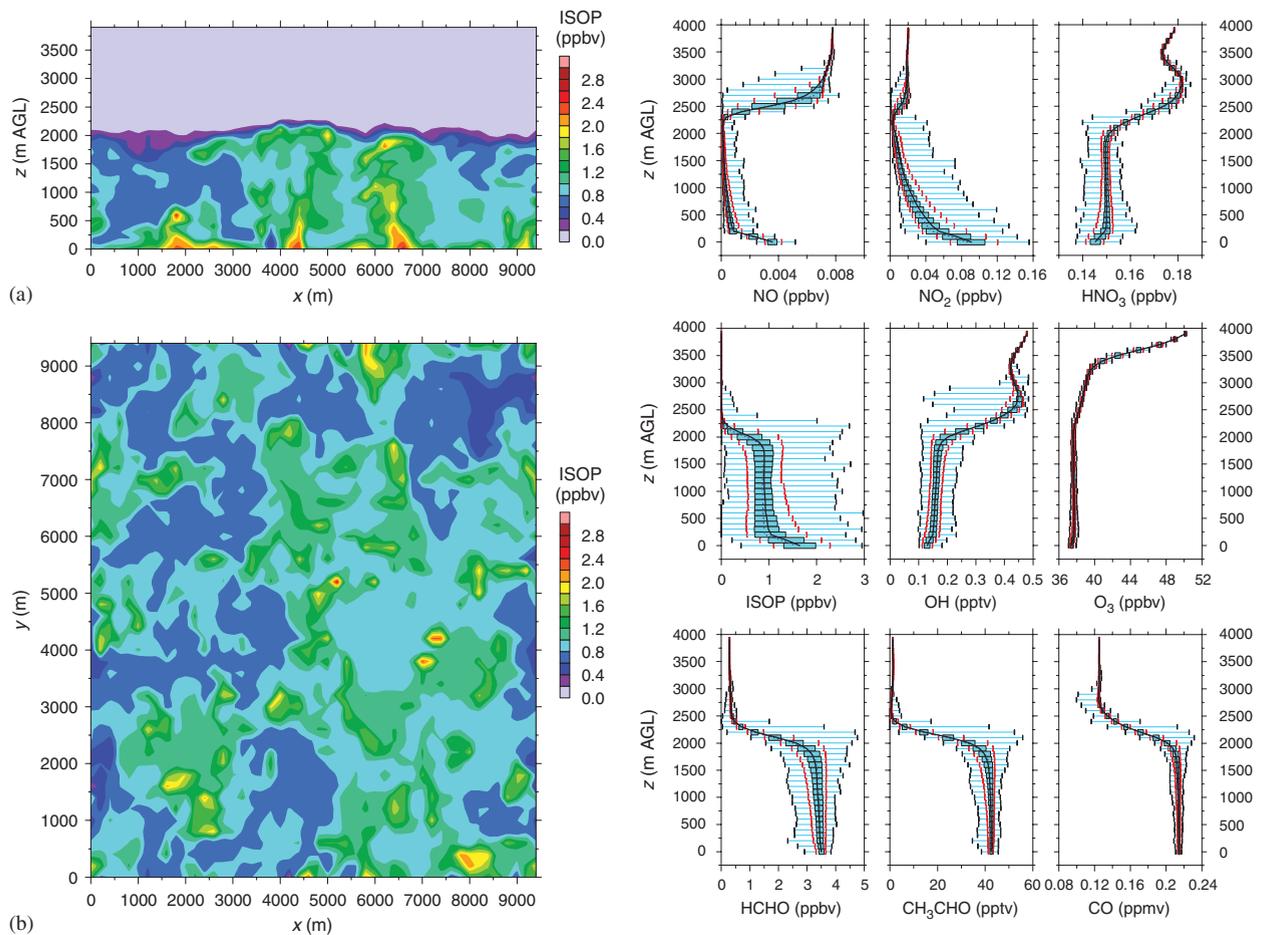


Fig. 5. Top left. Isoprene mixing ratio cross sections are shown from an idealized midday convection simulation (no mean wind) from LESchem model. Bottom left. A vertical slice of isoprene located at $y = 5800$ m is shown in (a) and a horizontal isoprene slice from the middle of the convective boundary layer (CBL) at $z = 1000$ m. Note the complex turbulence-induced structure of the isoprene field despite horizontally homogeneous isoprene surface emissions. Right. Vertical profiles of mixing ratio statistics are shown for selected trace gases from the LESchem simulation. Shown for each grid level are minimum and maximum values (whisker end points), 10th and 90th percentiles (red brackets), 1st and 3rd quartiles (cyan boxes), the median (dashed blue line), and the mean (solid black line).

(isoprene). Stochastic descriptions of variability were produced even for local aleatory states due to turbulence; sampling from this volume yielded a unique set of vertical profiles of concentration fluctuation distributions for each of the various pollutants throughout the mixed layer.

Further results of studies conducted using LESchem with a variety of line and area source configurations showed considerably increased complexity in detail from that in Fig. 5. This verified our anticipation that in the urban atmosphere (where chemical mixtures, the source configurations and the turbulent mixing properties are complicated) the complexity of the SGV distributions across the modeling domain is exacerbated.

3.3. Comparison of coarse grid results versus aggregation of fine-scale model results

The results of nested fine-scale modeling using results from the CMAQ-nested simulations for the Houston case study described above provide an opportunity to investigate the differences between coarse grid simulations and those aggregated using finer grid simulations. These differences thus represent the extent to which the coarse scale simulations are limited by ignoring processes and details at its sub-grid scale (represented by the fine grid results). In the context of model evaluation, these differences should ideally be small to justify ignoring the fine scale concentration features that are unresolved at

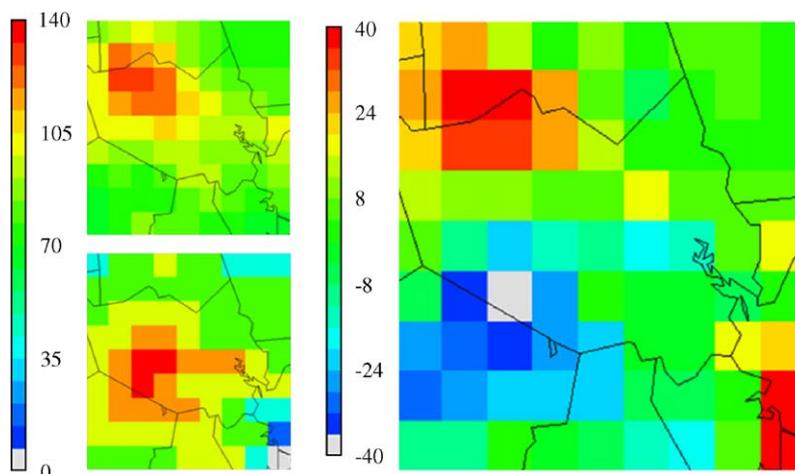


Fig. 6. Comparison of ozone at 12 km grid spacing at 1500 CDT modeled using CMAQ for Houston, Texas model domain for 30 August 2000: top left, ozone aggregated from 1 km grid simulations, bottom left, ozone at native 12 km spacing and at right, the difference between the aggregation mean and the native 12 km simulations.

coarse scale. Large differences are evident in some grid cells over several different areas at 12 km grid sizes between the aggregation from 1.33 km to the native 12 km simulations in the case of ozone (Fig. 6). While not shown, the general pattern and magnitude of the difference fields are similar for NO_x , while considerably reduced for the CO simulations. Both positive and negative differences are observed indicating the non-linear outcomes from modeling the processes at different scales between 12 and 1.33 km. Results from this type of analyses suggest the need for improved epistemology of the underlying assumptions of the model parameterizations to the resulting CMAQ outcomes based on grid size.

4. Summary

The underlying principle of this paper is that the fundamental property of air quality models be employed for the purpose of *qualifying* the appraisal or evaluation of model performance. Simply stated, “When comparing model results against observations, it is an important consideration to examine the degree to which the data falls inside or outside of the SGV distribution for the grid.” One cannot simply reject a model if the observations fall within some criterion based on the distribution of the SGV of that grid, even if the difference is large. We then investigated the nature of, the contributions to, and the distributional characteristics of SGV, approaching this subject with illustrations using results of fine

scale air quality and coupled LES and chemistry modeling.

This model evaluation paradigm is an extension of the neighborhood-scale model conceptual framework (Ching et al., 2004a) requiring each grid to have its own signature SGV distribution function. The example results of SGV distributions for different pollutants in urban areas indicate that the shape and characteristics of the SGV distributions varied considerably both across the modeling domain, by species and (while not shown) by averaging times. We have employed a newly developed technique to derive PDFs of the SGV distribution for each grid in the modeling domain. Our initial explorations have indicated that these stochastic distribution functions exhibit cell-to-cell variations on the hourly predictions that reflect both their source distribution characteristics and the photochemistry of the chemical mixtures within cells. For practical considerations and applications where fine scale modeling is unfeasible, it is desirable to obtain stable parameterizations of these SGV PDFs. Further studies will be needed to obtain systematic and generalized stochastic distribution functions for the pollutant SGV distributions as a function of grid size. They will need to be appropriately tailored to the averaging time needed for the specific application. For operational implementations, even PDFs, crudely based on source distribution and dispersion potential might at least provide upper and lower bounds useful as a measure for model evaluation and modeling in general.

However, we know that the SGV determined from the 1.33 and 1 km simulations are underestimated. Investigations are now underway to investigate the additional variability directly from (1) within-grid pollutant source distributions and from (2) those derivable from turbulence-induced photochemistry. For the latter, we foresee such parameterizations to be stochastic and dependent on a number of properties of the pollutant mixture, including (a) the composition of the mixture, (b) the Damköhler number, i.e., the ratio of the time scales of the chemical reactivity to the eddy diffusivity, and (c) the intensity of segregation parameter which is the ratio of the concentration covariance to the product of mean concentrations for two reactants (Herwehe, 2000). They will be needed to apply over a wide variety of atmospheric conditions and for modeling periods ranging from hourly to multi-day simulations. In addition, we have used a “traditional” one-hour time step for coupling the meteorology with the chemistry model. We have performed sensitivity studies that show some (albeit limited) degree of suppression of variability in the resulting modeled concentration fields. Thus, with finer time steps used to couple meteorology and chemistry, the SGV bandwidth would increase somewhat, as pointed out earlier by Grell et al. (2004), however, it does not alter the general conceptual paradigm for utilization in model evaluation.

As another result of this study, we have observed differences between the outputs of model runs at coarse grid sizes from those aggregated to the corresponding grid cell sizes from the finer grid simulations. These differences arise primarily because coarse grid models typically do not model atmospheric processes and dispersion at their sub-grid scales. In the context of model evaluation, it is desirable that these differences be known and characterized, and ideally, minimized.

The conclusions are of a conceptual nature based on fine scale modeling results. It is appreciated that for modeling performed at finer scales, it is important to minimize risk of poor model fidelity; thus, the model physics and input data requirements must be adequately commensurate with the scale. In this regard, it is appreciated that the outcomes of fine scale modeling also need to be evaluated; field experiments using mobile sampling platforms and/or saturation-sampling protocols would be highly desirable. These impressions and conclusions presented in this paper were drawn from a one-day case study period. Results and findings of other model-

ing studies (e.g., Sax and Isakov, 2003) are qualitatively consistent with the results and conclusions of this study.

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