Preliminary Results on the Development of a Variable-Grid-Resolution Air Quality Model

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1. INTRODUCTION

Many physical and chemical processes in the atmosphere have non-uniform variation in space. Besides the fine vertical resolution, high horizontal resolution is desirable for better modeling of many atmospheric processes. To economize on computer resources, many researchers in the past have explored the viability of using variable horizontal grid-resolution (time independent) in atmospheric models. During the early 1970s, regional meteorological models (e.g., Anthes, 1970) were used to test the concept of variable horizontal resolution. Since then, many researchers (e.g., Skamarock, 1989; Gravel and Stainforth, 1992; Yessad and Benard, 1996; Hardiker, 1997; Fox-Rabinovitz et al., 1997; Allen et al., 2000) studied various aspects of variable-grid-resolution modeling. In general, these studies found that variable resolution grid does not introduce significant noise at grid interfaces; truncation error is smaller compared to process and/or forcing representation error; grid placement is flexible; smooth changes in grid-resolution produces superior results; avoids several numerical simulations that are fundamental in the grid nesting; addresses two-way nesting problems naturally; and finally it is computationally economical.

In air quality modeling, variable horizontal resolution grids have previously been used mostly in global transport models (e.g., Allen et al., 2000). Recently, efforts have been devoted towards implementing variable resolution adaptive grids in regional air quality models; these applications are still in the developmental stage (e.g., Srivastava et al., 2000; Tomlin et al., 1997). The other types of regional air quality models employ nonuniformly stretched grids (e.g., Mathur et al., 1992) to effectively represent sub-grid scale emission source clusters and these grids are static (time independent). There are few studies stressing the importance of grid refinement (e.g., Moussiopolous, 1994; Jakobs, 1994; Sillman et al., 1990; Sunderam et al., 1990) and their ability to capture small-scale phenomena and their impacts on localized air pollution. Along these lines, Peters et al. (1995) provides a detailed review on the need for an efficient grid system for air quality modeling.

Development of a **v**ariable-**g**rid-resolution (VGR) air quality modeling system requires specification of meteorological and emission sources data for the VGR domain, and transport algorithms that can handle variable horizontal grid lengths. Generation of meteorological data from a host model that uses a similar variable resolution grid requires the development of a new meteorological model itself. Alternatively, one could use data from a traditional nested grid meteorological model and interpolate data (either from a single domain or from multiple nested domains) to the nodes of the non-uniform variable grid. Once this dynamical aspect is addressed, emission sources processing can then be done easily for the time independent predefined grid structures. This process is similar to that used for nested grid models.

The VGR modeling approach is an attractive method because it will enables one to place a high-resolution grid over the regions of interest while avoiding problems associated with the interface condition and feedback methodology associated with nested grid approach. Also, it is economical compared to the nested grid approach. Also, VGR approach allows the well-represented plumes over high-resolution regions to naturally propagate to coarse resolution regions without any loss of solution accuracy.

Our primary objectives are to: (1) develop a VGR modeling system, (2) study its functionality, (3) evaluate its performance against uniform nested-grid modeling system, (4) analyze the impact of improved representation of emission sources and transport processes in simulating regional ozone distributions during a summer period, and finally, (5) study its viability as a research as well as an operational model. In this article, we present results from the initial testing and applications of a VGR air quality model.

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2. DESCRIPTION OF VGR MODEL

The Multiscale Air Quality SImulation Platform (MAQSIP) (Mathur et al., 2003; Odman and Ingram, 1996) is used as the host model to develop the variable-grid-resolution air quality model. The VGR model is configured such that it can be applied for uniform grids (i.e., traditional grids) or for variable grids. Various modeling components used in the development of the VGR model are briefly described in the following subsection.

Variable grid generation: The first step in the VGR model application is the development of a variable resolution horizontal grid. Our grid generation algorithm follows the general methodology suggested by Fox-Rabinovitz et al., (1997). This method results in grid lengths in x- and y-directions such that they change smoothly according to geometric progression. Thus, a grid-resolution having a ratio of, for example, 1:9 (shown in Figure 2) can be achieved in a single domain. We emphasize that this type of selection of grid configuration is completely arbitrary; thus it provides flexibility to configure modeling domain of varying horizontal resolution.

Numerical Aspects: Since the grid-resolution can vary (for example, from 4 to 36 km) in the horizontal space, we calculate the advection time step based on the 3-D grid resolution and 3-D wind fields using the CFL (Courant-Friedrichs-Lewy) criteria.

Horizontal Advection and Diffusion Schemes: Horizontal advection and diffusion are the two processes that need special attention in a variable grid-resolution model. Since the rest of the processes act either in the vertical direction or are direction independent no modifications are required in the representation of those processes. For this purpose we have used a generalized version of the PPM advection scheme to perform horizontal advection on the variable grids. More details on the PPM advection scheme can be found in Colella and Woodward (1984). To address the horizontal diffusion modeling on the variable grids, we have adapted the vertical diffusion algorithm used in the MAQSIP to perform horizontal diffusion. Since the vertical diffusion algorithm operates on variable-thickness vertical grids, it naturally fits to perform horizontal diffusion on horizontally varying grids.

Mass Balance and Vertical Advection: Meteorological input data to drive the VGR model is obtained from the Mesoscale Model, Version 5 (MM5) simulations. Since the conservation equation for air density is not solved in the MM5, air density is approximated from the ideal gas equation. Usage of this air density data along with the prognostic wind fields from the MM5 in tracer transport calculations often leads to mass-inconsistency which can manifest as an artificial first-order source/sink term (e.g. Kitada et al., 1983; Mathur and Peters, 1991). Two types of simple remedies are available to address the mass balance issues in air quality models. The first method, commonly used in several models, involves advection of density followed by a mass correction step to obtain a "corrected" concentration field. The second approach involves adjustments to the vertical wind component and is based on re-diagnosis of a vertical wind component (given a density and horizontal wind field) that satisfies the discrete form of continuity equation used in the tracer model (Odman and Russell, 2000). We have used the latter methodology in the VGR model simulations.

3. NUMERICAL SIMULATIONS

To test the functionality of the VGR model we performed several idealized tracer transport simulations with known analytical solutions. We then performed 3D air quality simulations using realistic emissions and meteorological inputs. We present preliminary results from one idealized and two realistic applications of VGR model; one for regional-to-urban scale simulations and the other for urban-to-plume scale simulations (Alapaty et al., 2002).

4. PRELIMINARY RESULTS

In the idealized 2-D VGR simulation, a passive scalar puff with an initial conical concentration distribution was subject to diagonal advection on both a uniform and a variable resolution grid. Figures 1-3 present temporal variations in tracer maximum concentration, minimum concentration, and total mass, respectively, for both the uniform grid (labeled as *Ugrid*) and the variable grid (labeled as *Vgrid*) simulations. The maximum concentration provides a measure of the diffusive characteristics of the solution. Examination of the minimum concentration (initially specified as 5 in this test) on the other hand is useful in determining if "ripples" arise from the numerical advection scheme on the variable grid. Though reduced, the maximum concentration of the scalar is much higher in the *Vgrid* than that in the *Ugrid*; the initial decline in peak concentration (upto hour 24) is due to advection on a relatively coarse grid. Note that in the *Vgrid* solution, the numerical diffusion associated with the advection scheme is almost absent during the simulation hours 24-76 when the peak value of puff is resident in the high-resolution region indicating that the spatial gradients are better resolved in the *Vgrid* simulation. Since the grid-resolution is constant and coarse in the *Ugrid*, there is a continuous degradation in the maximum concentration due to the numerical diffusion associated with PPM advection scheme. The steep fall in the maximum concentration of the scalar puff after 170 h of simulation is due to the fact that puff is advected out of the domain in both simulations. Even at this exit time, the maximum concentration in the *Vgrid* is much higher that in the *Ugrid*. This result is analogous to the result that may be obtained using a two-way interaction nested grid models. However, advantage of VGR methodology over the nesting is that interactions between the various modeled scales are naturally built in the VGR formulation.

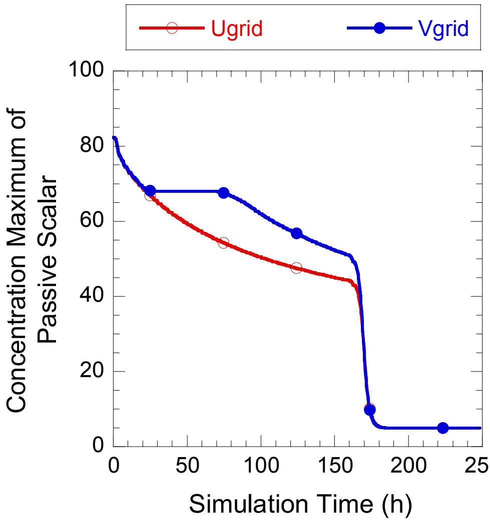

Figure 1. Temporal variation of concentration maximum of a scalar puff in Ugrid and Vgrid simulations.

Figures 4 and 5 show the modeling domains used in our 3-D VGR model simulations with grid resolutions varying from 36 to 4 km (Fig. 4) and 5 to 0.5 km (Fig. 5). Our preliminary analysis of these two simulations indicated that VGR model is functional and capable of establishing scale-process interactions that are absent in one-way interaction nested grid models. Details of these simulations will be presented at the workshop. Given the similarity in model structure and attributes between the MAQSIP and CMAQ models, it is anticipated that the VGR methodology can be adapted in the CMAQ model.

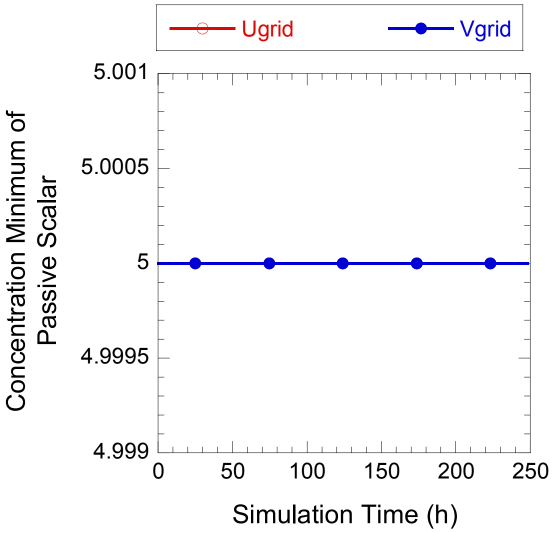

Figure 2. Temporal variation of minimum concentration in the Ugrid and Vgrid simulations

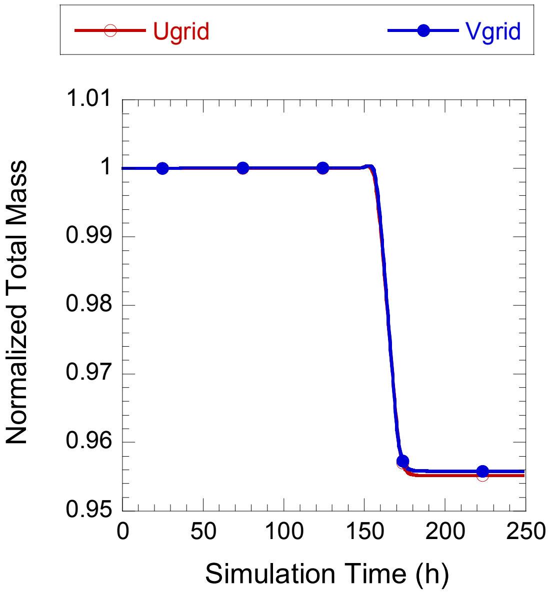

Figure 3. Temporal variation of domain total tracer mass in the Ugrid and Vgrid simulations

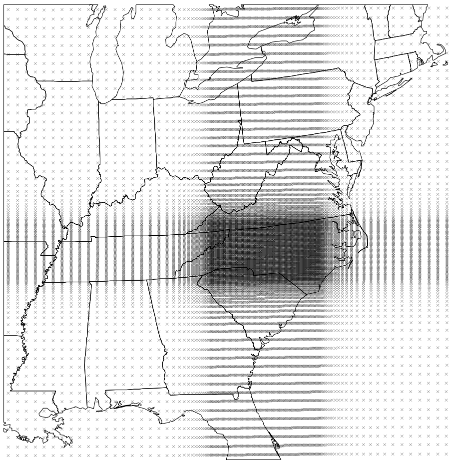

Figure 4. Grid structure used in the regional-to-urban scale VGR simulations. Grid resolution varied from 36 to 4 km with high-resolution grids over NC.

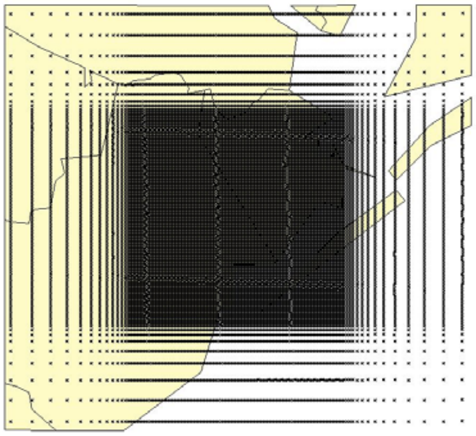

Figure 5. Grid structure used in the urban-to-plume scale VGR simulations. Grid resolution varied from 5000 to 500 m with high-resolution grids over Brazoria County (south of Houston-Galveston region of Texas.

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