11.1 DEVELOPMENT OF A MODELING SYSTEM FOR PRESCRIBED BURN EMISSIONS AND AIR QUALITY IMPACTS

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1. BACKGROUND

The complexity of physical processes and reaction kinetics associated with air pollution makes its understanding highly dependent on computer models. Different approaches exist to modeling air pollution: dispersion, photochemical, and receptor models. Each has a different applicability according to scale, chemical species of interest, and computational resources. The complete transport and transformation progression of specific air pollution incidents is perhaps best observed under photochemical models. Additionally, photochemical models provide an opportunity to forecast the air quality resultant from specified emission scenarios, providing an important decision making tool.

However, the limitations of gridded photochemical models become increasingly apparent as we attempt to lower resolution. Escalating calculation requirements typically restrict these models to grid resolutions of a few kilometers. The assumption of complete mixing and absence of fine-scale specific phenomena may lead to inaccurate results and artificial dilution. Features of air pollution transport and chemistry at lower scales are difficult to observe. Furthermore, the sensitivity of pollutant concentrations to grid resolution has been acknowledged (Arunachalam et al. 2006; Russell; Dennis 2000; Shrestha et al. 2009) and the multiscale nature of air pollution modeling has been identified as an issue that must be addressed (Dabberdt et al. 2004).

Frequently, air pollution episodes occur at scales smaller than those suitable for photochemical models. Moreover, some air pollution incidents involve both characteristics best observed at lower, local scales and at larger, regional scales downwind. Refinement of air pollution models necessitates that the issues of scale applicability be addressed. Simulations that better represent air pollution behavior at small scales and its transition into larger ones will produce the most accurate predictions. Therefore, we believe that it is necessary to take air quality models to unprecedented levels of resolution and prove that finer-scale gridded photochemical air pollution models can produce more accurate results than existing gridded models at an acceptable computational cost.

Enhanced photochemical model resolution will be explored using the adaptive grid approach. Adaptive versions of meteorological and air pollution models using the dynamic solution adaptive grid algorithm have been produced or are currently under development (Xiao et al. 2005). We developed an adaptive grid version of the Community Multiscale Air Quality Modeling System (CMAQ) that can effectively adapt grid distribution to pollutant concentrations. The resultant model is tested by simulation of a real air pollution episode and performance is compared to that of existing fixed grid models.

2. MODELING SYSTEM DESCRIPTION

2.1 Background Science

Initial development of an adaptive grid air quality model was founded on the dynamic solution adaptive grid algorithm (DSAGA) (Srivastava et al. 2000). In the first application of DSAGA to air quality modeling, dispersion of a power plant plume was simulated to observe the adaptive grid algorithm's effect on ozone concentrations (Srivastava et al. 2001). The initial results of this application indicated that results equivalently accurate to those produced by a static grid could be obtained using an adaptive algorithm with much higher computational efficiency. Subsequently, an adaptive grid photochemical model was developed and successfully applied to ozone air quality simulations (Odman et al. 2002). However, inclusion of the adaptive grid algorithm into photochemical models with nonlinear chemistry brought upon a significant computational burden due to the short time step required by smaller grid scales. Subsequently, a variable time step algorithm that allows each grid cell to have a unique time step was developed (Odman; Hu 2007).

We have developed a modified version of CMAQ that includes a dynamic solution adaptive grid algorithm, allowing grid adaptation in response to pollutant concentrations. The algorithm has three main components; a weight function, grid repositioning and solution redistribution. A complete description of the algorithm used for grid refinement can be found in Srivastava., et al., 2000 (Srivastava et al. 2000). The Adaptive Grid version of CMAQ (AG-CMAQ) also includes the variable time step algorithm

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Corresponding author address: Talat M. Odman, Georgia Inst. of Tech., School of Civil and Environmental Eng., Atlanta, GA, 404-894-2783, e-mail: odman@gatech.edu to improve computational efficiency. AG-CMAQ is built on CMAQ Version 4.5 and remains faithful to the “Models-3” concept.

The grid adaptation is restricted to the horizontal plane. A 2-D weight function, consisting of the Laplacian of the ground-level PM2.5 concentration field, determines where grid nodes are to be clustered for a more accurate solution. The concentrations are then interpolated to the new grid positions. Owing to the equivalence of interpolation to numerical advection, a higher order advection scheme is used for interpolation. Emissions and meteorological data are also processed to the new grid.

The grid becomes non-uniform after adaptation but, for easy computation of the solution, a coordinate transformation reestablishes the uniform grid. The Jacobian of the coordinate transformation from the physical (x, y, z) space to the computational space is calculated as

$$J = \frac{1}{m^2}\frac{\partial z}{\partial \sigma}\left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial x}{\partial \eta}\right)$$

The governing equation of the CMAQ model is modified as

$$\frac{\partial (Jc_n)}{\partial t} + \frac{\partial (Jv^{\xi} c_n)}{\partial \xi} + \frac{\partial (Jv^{\eta} c_n)}{\partial \eta} + \frac{\partial (Jv^{\sigma} c_n)}{\partial \sigma} + \frac{\partial}{\partial \xi}\left(JK^{\xi\xi}\frac{\partial c_n}{\partial \xi}\right) + \frac{\partial}{\partial \eta}\left(JK^{\eta\eta}\frac{\partial c_n}{\partial \eta}\right) + \frac{\partial}{\partial \sigma}\left(JK^{\sigma\sigma}\frac{\partial c_n}{\partial \sigma}\right) = JR_n + JS_n$$

where the superscripts denote contravariant components of the velocity vector and diffusivity tensor. Since the grid is uniform in the computational space, the same numerical solution algorithms used in CMAQ can be used directly.

2.1 Code Verification

Verification of the developed AG-CMAQ code was carried out considering two simulation scenarios. In an initial test, results from a standard CMAQ simulation were compared to those obtained from AG-CMAQ without activating any grid adaptation. Successful verification would prove both sets of results to be the same. The results from an application of AG-CMAQ without adaptation were practically the same to those from standard CMAQ, except for very small and random differences. An exception are the differences in biogenic organic and nitrate aerosol concentrations, which are small (<0.1 µg m3), but follow a pattern.

A second verification test was carried out to observe performance with grid adaptation. In this test, simulations of a prescribed forest fire plume with standard CMAQ and AG-CMAQ using fine particulate matter (PM2.5) concentration as the refinement variable were compared. Prescribed forest fires are an ideal application of adaptive grid air quality modeling and are discussed in further detail in the following section. Emissions data and model inputs correspond to a prescribed burn performed at Ft. Benning Georgia in April 9, 2008. The results from AG-CMAQ were as expected. Grid resolution was increased in the regions of highest PM2.5 concentration. In the area of highest resolution, cell size was reduced down to approximately 100 m x 100 m from the initial fixed grid dimensions of 1.3 km x 1.3 km. A reduction in the artificial dispersion of plume features typical of photochemical models was also evident from the simulation.

3. CASE STUDY

3.1 Prescribed Burns

Forest fires can grow into major air quality incidents affecting large populations. In the Southeastern U.S., planned fires, or prescribed burns, are successfully applied as a wildfire prevention and habitat restoration strategy. However, pollutants emitted from prescribed burns may be transported and react to form other pollutants, contributing to poor air quality in urban areas. In the Southeastern U.S. planned forest fires are an important source of primary fine particulate matter and gaseous pollutants. One study found that in this region forest fires account for approximately 20% of fine particulate matter emissions, 8% of carbon monoxide emissions, and 6% of organic compound emissions (Lee et al. 2005). Forest fires have also been identified as the main cause for recent increases in fine particulate matter levels and visibility reduction in the United States. Additionally, primary emissions can also produce secondary pollutants, such as ozone, further downwind.

Planned forest fires are commonly used in Georgia and have proved to be effective in accomplishing different land management objectives. Over 1 million acres are subjected to prescribed burns each year in the state at different locations (Lee et al. 2005). For instance, at Department of Defense lands in Fort Benning, Georgia, the location selected for field measurements in this study, approximately 30,000 acres are burned each year. However the impacts of these practices on air quality have also been considerable. In the Columbus, GA Metropolitan Area near Fort Benning concern about high particulate matter and ozone levels has lead to complaints and threats of legal action against land managers. The air quality effects can also impact large urban areas and be experienced at considerable downwind distances.

Air pollution episodes caused by prescribed burning are excellent examples of highly concentrated events occurring at a lower, local scale with an impact that transitions into a larger, regional scale downwind. Prescribed burn plume development typically occur at scales below those suitable to existing photochemical models due to the limitations of existing photochemical models previously described. In our initial evaluation of AG-CMAQ performance, we analyze the simulation of a large prescribed burn incident affecting a dense urban area as described below.

3.2 Atlanta February 28, 2007 Smoke Incident

In February 28, 2007, air quality in the Atlanta metropolitan area was impacted by heavy smoke caused by prescribed burns. Within hours fine particulate matter levels at monitoring sites throughout the area increased to nearly 150 µg/m3 and ozone levels exhibited increments as large as 30 ppb (Hu et al. 2008). Not surprisingly, an increase in asthma attacks was also observed. Although several prescribed burns were carried out in the region throughout the day, the dramatic increase in pollution levels is mainly attributed to 2 prescribed fires 80 km southeast of Atlanta in the Oconee National Forrest and Piedmont National Wildlife Refuge. In these two prescribed burns about 12 km2 of land were subjected to treatment.

Simulation of air quality resultant from the February 28 Atlanta smoke episode with a fixed grid photochemical model has been previously carried out and is discussed in (Hu et al. 2008). Here the event was re-simulated with the standard and adaptive versions of the CMAQ model using information collected about the 2 major prescribed burns blamed for the event. The vertical distributions of the plumes are input from Daysmoke (Achtemeier 1998) using a "wall" concept developed for the initial attempt to couple Daysmoke with CMAQ.

3.3 AG-CMAQ Simulation and Results

We have simulated the February 28, 2007 Atlanta smoke incident using AG-CMAQ and compared the results to those obtained from the fixed-grid simulation. Model inputs and setup were kept the same as those used for the fixed-grid simulation done at a 4-km horizontal grid resolution for the grid covering Northeastern Georgia. Grid refinement in AG-CMAQ was driven by PM2.5 concentrations. The simulation was initiated at 21Z on February 27th and finalized at 05Z on March 1st. Grid adaptation commenced at 15Z on February 28th consistent with the initial emissions release from the Oconee National Forrest and Piedmont National Wildlife Refuge fires. Figure 1 shows $PM_{2.5}$ concentrations on the modeling domain at 04:45Z on March 1st after full plume development from both the AG-CMAQ and standard CMAQ simulations.

Visual inspection of the modeled PM2.5 concentration fields provides evidence of significant differences between the adaptive grid and fixed grid simulations. The artificial dilution effect generally present in gridded photochemical models appears to decrease when applying an adaptive grid. The smoke plumes drawn with AG-CMAQ appear better defined and pollutant concentrations remain higher near plume cores. Most significantly perhaps, plumes from both ongoing prescribed burns can be distinctly observed when applying an adaptive grid. When using a static grid the plumes cannot be distinguished from each other and appear as a single thicker plume. We believe results from AG-CMAQ better describe local air quality and pollutant dispersion.

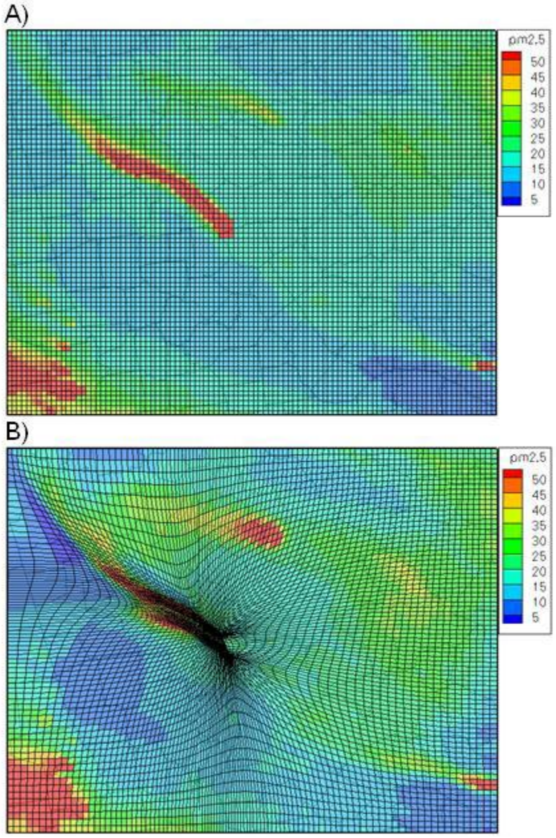

Figure 1. Simulated PM2.5 concentrations (µg/m3) in modeling domain at 04:45 Z on March 1st 2007 using A) fixed grid CMAQ and B) AG-CMAQ.

Modeled concentrations from both adaptive grid and fixed grid simulations were compared to concentration measurements at several air quality monitoring sites in the Atlanta metropolitan area that experienced a significant increase in PM2.5 concentration during the event. Results for both simulations are plotted along with hourly measurements at the South DeKalb air quality monitoring site in Atlanta in Figure 2. Concentrations resultant from a fixed grid simulation of the smoke incident consistently under-predict peak PM2.5 concentrations at the location of monitoring sites that recorded a significant increase in measured concentrations. Additionally, in some instances modeled concentrations from the fixed grid simulation appear higher than measurements outside the pollution spike and exhibit two distinct concentration peaks.

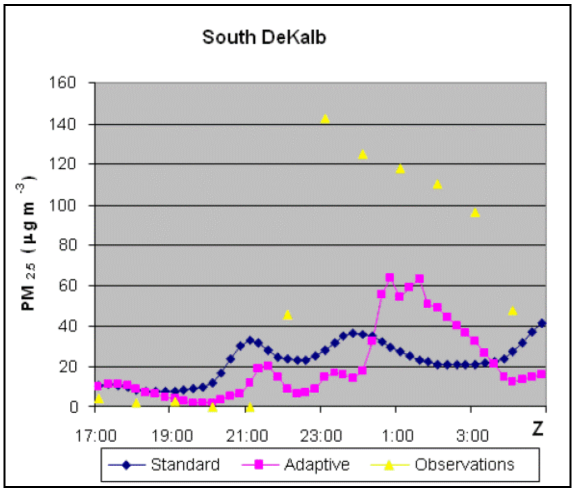

Figure 2. Modeled $PM_{2.5}$ concentrations using standard CMAQ and AG-CMAQ and concentration measurements at the South DeKalb air quality monitoring sites in the Atlanta metropolitan area.

The simulation with AG-CMAQ results in higher concentration peaks compared to the fixed grid simulation and reduces the initial over-prediction of PM2.5 concentrations and significance of the double peak behavior observed with a fixed grid. We believe the differences in simulated concentrations between the fixed grid and adaptive grid simulations reflect the improved replication of plume dynamics and decrease in artificial dilution that can be achieved through grid refinement. However, we believe that underestimation of secondary organic aerosol formation and volatile organic compound emissions are still largely responsible for the differences between modeled results and measurements and that other model characteristics unrelated to grid resolution contribute significantly to the error.

Vertical resolution of the model and the plume height with respect to the boundary layer may be important factors leading to the underestimation in Figure 2. A three-dimensional visualization of the results revealed important clues. Figure 4 is a 3-D version of Figure 1-A after rotation; X and Y are the easting and northing (y) axes, respectively. The elevated plume coming out of the paper bifurcated from the leading part of the plume heading northwest to Atlanta (to the right of the figure) due to wind shear. The trailing part of the plume heading to Atlanta formed after the bifurcation, when the plume height dropped with respect to the boundary layer height. There is no data to verify if the bifurcation really occurred. If it did not, then it is partially responsible for the underestimation in Figure 2. The underestimations may also be due to the overestimation of the plume

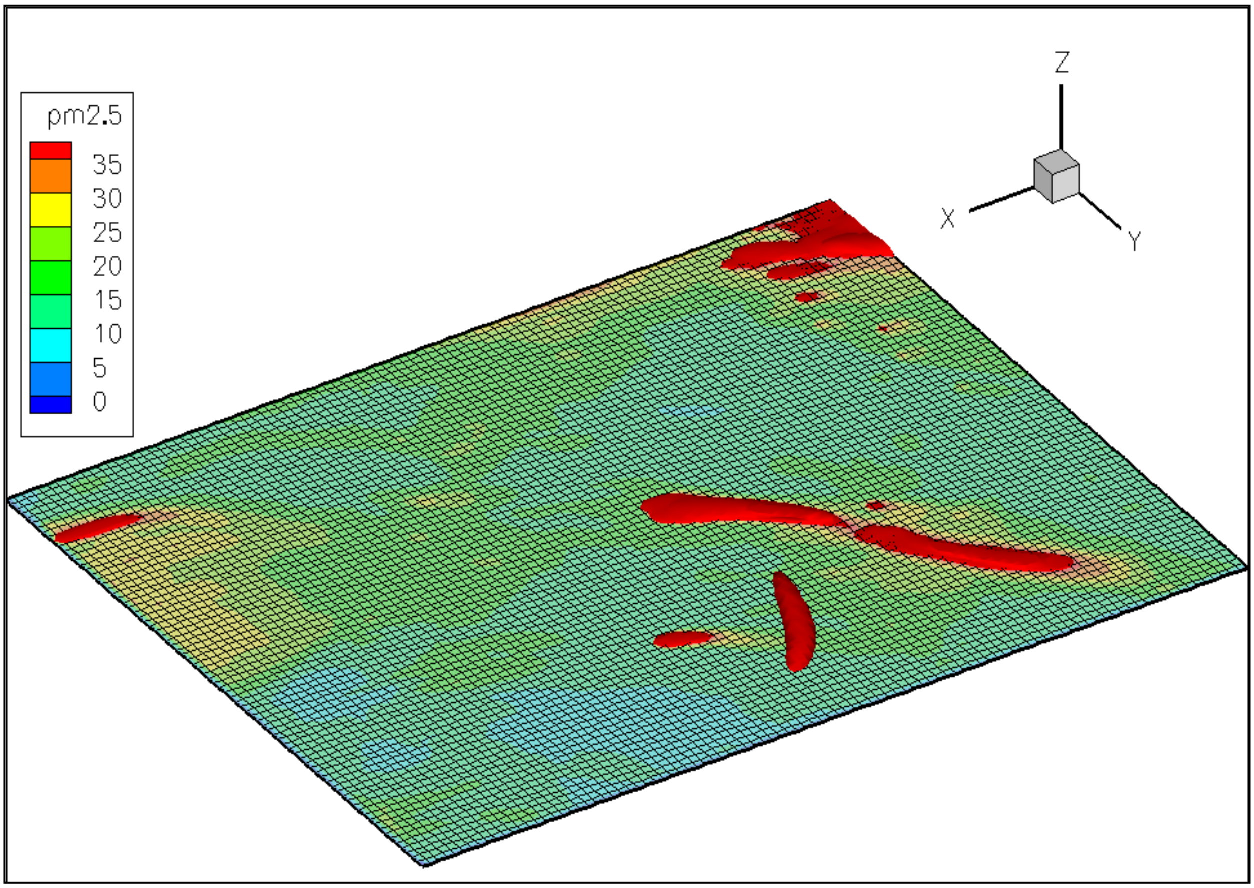

Figure 3. Three-dimensional view of the plumes in Figure 1-A. Note the different orientation of the easting (X) and northing (Y) axes after rotation. The elevated plume coming out of the paper bifurcated from the leading part of the plume heading northwest to Atlanta (to the right) due to wind shear.

height which, together with the coarse model resolution above the boundary layer, may be artificially lofting the plume above the boundary layer and leading to the bifurcation due to wind shear.

Considering these possibilities a new simulation was performed using a different plume height and 34 vertical layers, instead of 13 used in the previous simulation. One of the most sensitive parameters that plume height in Daysmoke is most sensitive to is the initial plume diameter, which depends on the fuel type. The diameter used in earlier simulations was 200m; this time the diameter was reduced to 70m. As a result, the mean plume height reduced from 1200 m to 500m. No bifurcation was observed in the standard CMAQ simulation, and the PM2.5 concentrations in Atlanta increased by more than 50 µg/m3 (Figure 4).

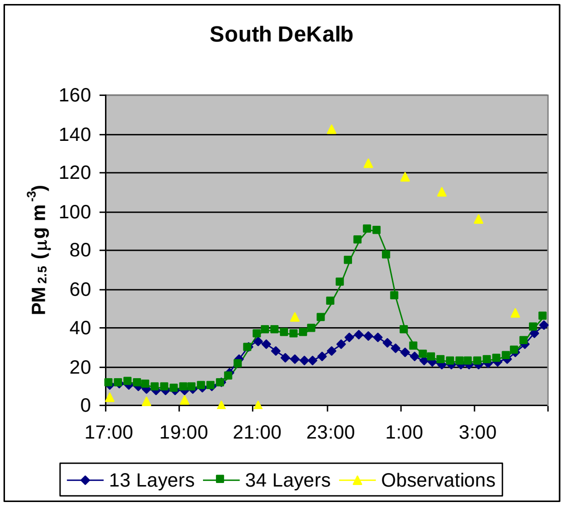

Figure 4. Modeled PM$_{2.5}$ concentrations using standard CMAQ with 13 and 34 layers respectively and observations at the South DeKalb air quality monitoring site in Atlanta.

4. FUTURE WORK

4.1 Coupling Daysmoke with CMAQ (Dynamic coupling)

One of the goals of this project is the development of a suitable coupling technique that can inject Daysmoke particles into the CMAQ grid cells without significant loss of accuracy. For this, we decided to employ a Fourier analysis technique in the following sequence. First, the smoke particle concentrations predicted by Daysmoke are represented as spectra of waves with different frequencies. Then, the waves whose frequencies cannot be supported by the adaptive CMAQ grid are identified. If the amplitudes of those waves are negligible, then the plume is handed over to CMAQ; otherwise the plume is continued to be followed by Daysmoke.

The metric used for assessing the difference between the original and (forward and backward) Fourier transformed distributions is usually a high moment of the concentration. We have been using the square of the concentrations but the third power would be even more discerning. While the difference helps to decide whether to hand over the plume to CMAQ or continue to follow it with Daysmoke, the knowledge of what grid resolution would minimize the difference can be used as a criterion for grid adaptation in AG-CMAQ. Several Daysmoke plumes were analyzed to determine the CMAQ grid resolutions needed at different downwind distances to minimize the loss of information during transfer of the plume from Daysmoke to CMAQ. There seems to be an optimal downwind distance for any given grid resolution at which the transfer results in minimum loss (Figure 5).

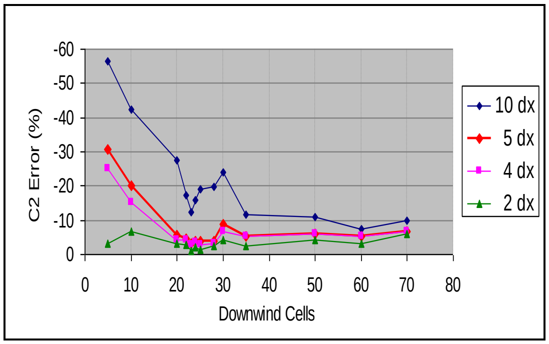

Figure 5. The error in the sum of squared concentrations as a function of downwind distance for different grid resolutions ranging from fine (2 dx) to coarse (10 dx).

4.2 Conclusion

An adaptive grid version of CMAQ, AG-CMAQ, has been developed and rigorously verified. This model is ideal for resolving plumes from particular sources such as power plants, wild land fires, and urban and industrial centers. Application of AG-CMAQ to the study of the air quality impacts of prescribed burns in Southeastern U.S. is under way. The model is providing more detailed simulations of the plume evolution compared to the standard CMAQ at very fine resolution.

Adaptive grid air quality models could benefit from synchronous adaptation in weather prediction models. We will apply the grid refinement methodology in AG-CMAQ to meteorological models and develop weather models that can effectively adapt to air pollutant concentrations. Such adaptation will require continuous input of pollutant concentrations from the air quality model into the meteorological model. Therefore, coupled air quality and meteorological adaptive grid models will be created to operate simultaneously and continuously exchange feedback. Additionally, air quality modeling at finer scales brings about an opportunity, and perhaps a necessity, to research and account for the effects of air pollution on meteorology. The weight of coupling on simulated air pollutant concentrations will be quantified and the nature of relationships between air pollution and weather will be studied.

Fine-scale air pollution modeling will also be explored through the application of sub-grid dispersion models. Special attention will be given to Advanced Plume Treatment (APT) in CMAQ-AMSTERDAM (Karamchandani et al. 2000) and CALPUFF (Scire et al. 2000). Simulations of air pollution episodes will be carried out on these models and established as benchmarks. A new reactive plume model will be developed from the non-reactive Daysmoke plume model (Achtemeier 1998). A chemistry module will be designed for the model to include reactivity. The model will be evaluated with real data upon completion and performance will be compared to that of other reactive plume models. Finally model coupling will be considered as a method for transitioning between different scales by coupling AG-CMAQ to the dispersion model developed.

7. REFERENCES

Achtemeier, G. L., 1998: Predicting dispersion and deposition of ash from burning cane. *Sugar Cane*, **1,** 17-22.

Arunachalam, S., A. Holland, B. Do, and M. Abraczinskas, 2006: A quantitative assessment of the influence of grid resolution on predictions of future-year air quality in North Carolina, USA. *Atmospheric Environment*, **40,** 5010-5026.

Dabberdt, W. F., and Coauthors, 2004: Meteorological research needs for improved air quality forecasting - Report of the 11th prospectus development team of the US Weather Research Program. *Bulletin of the American Meteorological Society*, **85,** 563-586.

Hu, Y. T., and Coauthors, 2008: Simulation of air quality impacts from prescribed fires on an urban area. *Environmental Science & Technology*, **42,** 3676-3682.

Karamchandani, P., L. Santos, I. Sykes, Y. Zhang, C. Tonne, and C. Seigneur, 2000: Development and evaluation of a state-of-the-science reactive plume model. *Environmental Science & Technology*, **34,** 870-880.

Lee, S., and Coauthors, 2005: Gaseous and particulate emissions from prescribed burning in Georgia. *Environmental Science & Technology*, **39,** 9049-9056.

Odman, M. T., and Y. Hu, 2007: A Variable Time-Step Algorithm for Air Quality Models *Air Pollution Modeling and its Application XVII: Proceedings of the 27th NATO/CCMS International Technical Meeting on Air Pollution Modelling and Its Application held in Banff, Canada, October 24-29, 2004*, C. Borrego, and N. A.-L., Eds., Springer 411-420

Odman, M. T., M. N. Khan, R. K. Srivastava, and D. S. McRae, 2002: Initial Application of the Adaptive Grid Air Pollution Model. *Air Pollution Modeling and its Application XV: Proceedings of the 25th NATO/CCMS International Technical Meeting on Air Pollution Modelling and Its Application held in Louvain-la-Neuve, Belgium, October 15-19, 2001*, B. C., and S. G., Eds., Kluwer Academic/Plenum Publishers, 319-328

Russell, A., and R. Dennis, 2000: NARSTO critical review of photochemical models and modeling. *Atmospheric Environment*, **34,** 2283-2324.

Scire, J. S., D. G. Strimaitis, and R. J. Yamartino, 2000: A User's Guide for the CALPUFF Dispersion Model (Version 5). Earth Tech Inc.

Shrestha, K. L., A. Kondo, A. Kaga, and Y. Inoue, 2009: High-resolution modeling and evaluation of ozone air quality of Osaka using MM5-CMAQ system. *Journal of Environmental Sciences-China*, **21,** 782-789.

Srivastava, R. K., D. S. McRae, and M. T. Odman, 2000: An adaptive grid algorithm for air-quality modeling. *Journal of Computational Physics*, **165,** 437-472.
——, 2001: Simulation of dispersion of a power plant plume using an adaptive grid algorithm. *Atmospheric Environment*, **35,** 4801-4818.

Xiao, X., D. S. McRae, H. A. Hassan, F. H. Ruggiero, and G. Y. Jumper, **2005**: Dynamically Resolved Simulation of Atmospheric Features and Turbulence-Initial Results. *43rd AIAA Aerospace Sciences Meeting and Exhibit*, American Institute of Aeronautics and Astronautics.