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SELECTED RESULTS OF MODELING WITH THE CMAQ PLUME-IN-GRID APPROACH

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1. INTRODUCTION

Important characteristics of pollutant plumes emitted from major point sources are their initially small size and their gradual growth rates downwind due to meteorological processes. However, major point source emissions are instantly mixed into an entire grid cell volumes with the traditional Eulerian air quality grid modeling method, which causes considerable overdilution depending on the model grid cell size. Consequently, plume-in-grid approaches have been developed as an alternative method to more realistically simulate the dynamic processes and chemical evolution of pollutant species within point source plumes. This paper briefly describes the CMAQ plume-in-grid method and provides an overview of model applications for two domains. The presentation will highlight the results of model simulations, which were performed with and without the plume-in-grid approach and will explore the impact on modeled concentrations. Comparisons to observations will also be made.

2. MODEL OVERVIEW

Details of the technical approach and model formulation of the CMAQ Plume-in-Grid (PinG) technique can be found in Gillani and Godowitch (1999). The PinG approach employs a Lagrangian framework to simulate a contiguous pollutant plume with a series of moving plume sections. To capture the large pollutant gradients occurring across a plume emitted from a high emission major point source, the PinG module is composed of an array of adjacent plume cells, which resolve the internal concentration variations within each plume section.

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The key modeling components of the CMAQ PinG approach are the Plume Dynamics Model (PDM) processor program and the Lagrangian reactive plume algorithm (PinG module).

The PDM processor needs meteorological input files generated by the MCIP processor and a stack file containing the physical stack parameters of each point source. PDM generates horizontal and vertical dimensions, grid positions, and other parameters for each plume section released from each point source. The PDM output file is used to drive the PinG module, which executes concurrently with the Chemical Transport Model (CTM). The Sparse Matrix Operator Kernel Emissions (SMOKE) processing system, which has replaced the MEPPS emissions system, provides a stack parameter file and an emissions file for specific major point source to be treated by the PinG method based on user-specified criteria.

The PinG module simulates horizontal and vertical entrainment, horizontal mixing, dry deposition processes, and chemical evolution of gaseous species in each plume cell during the active subgrid simulation period. Since the PinG module is coupled to the CMAQ/CTM, boundary conditions are provided by the CTM grid cell concentrations surrounding each plume section. Additionally, a feedback mechanism exists since when a plume section reaches the model grid cell size, plume section material is transferred to the appropriate CTM grid cell. Additionally, the species concentrations of each active plume cell during the subgrid period are stored in a separate PinG concentration file. After a model simulation, a postprocessor program may be executed to merge the CTM and PinG concentration files in order to account for the subgrid scale active plume concentrations contained in particular grid cells.

The CMAQ PinG was designed to deal with pollutant plumes for the rather coarse grid sizes defined for regional-scale modeling domains. Results of regional modeling applications are particularly valuable for specifiying boundary

conditions for nested finer-grid modeling domains. The CMAQ PinG approach is not suited for modeling applications with fine-grid sizes of urban domains since major point source plumes can be treated in the 4-5 km grid cells in the urban scale domains.

3. MODEL RUNS

Model simulations to be reported at this forum were conducted for two different domains. A large regional modeling domain encompassed the entire eastern half of the U.S. with 87 x 81 horizontal grid cells at a 36 km grid cell size. There were 77 major point sources designated as PinG sources during emissions processing with the criteria that NOx emission rate exceeded 75 tons/day or the SO2 emission was greater than 150 tons/day. All other point sources were subjected to plume rise and their emissions were incorporated into the appropriate vertical layer(s) within the 3-D emissions file for input to the CTM. Another modeling domain consisted of a nested 12 km gridded domain defined on a horizontal grid of 72 x 90, which encompassed the greater Ohio River and Tennessee Valley areas with Nashville, Tennessee at the center of the domain. Using the same emission rate criteria, a set of 45 major point sources was identified for the PinG treatment in this domain. There were 21 vertical layers used in both modeling domains. Model simulations were performed for a 10-day period in July 1995 that included a relatively high pollution episode occurring during an ongoing experimental field study.

The CMAQ/CTM was exercised with the same set of modeling components, except one series was run without the PinG treatment and another modeling series applied the PinG method to the designated major point sources. Both the CTM grid model and PinG module employed the same chemical mechanism and the Gear chemical solver method was applied.

A clean set of initial and boundary values was prescribed for the large, regional 36 km domain. To generate the initial and boundary conditions with the ICON and BCON processors for the 12 km nested modeling domain, the gridded concentration files from the 36 km model simulations were employed since the results were already generated. For the 12 km CTM/PinG simulations, the BCON processor was exercised by using both the 36 km CTM and PinG concentration files to generate the boundary conditions.

4. SUMMARY OF MODEL RESULTS

The results to be summarized herein focus on ozone concentrations generated from the 36 km regional domain simulations. The 2-D concentration fields in layer 1 revealed the largest ozone differences were found in the grid cells where the major point (PinG) sources were located and in areas downwind. Ozone concentrations were generally higher in the CTM/NoPinG results, which was anticipated for this grid resolution. Due to overdilution of the high NOx emissions and instantaneous mixing with VOC's in the large grid cell volumes, rapid photochemical ozone production occurs. In contrast for the CTM/PinG runs, the high NOx emissions were injected into the relatively small subgrid plumes causing rapid titration of plume ozone by the high NO concentrations and a subsequent ozone deficit in the plume. Ozone concentrations gradually recover downwind. For more details about the evolution of concentrations within the subgrid plumes, Godowitch (2001) presents results from selected point sources and compares modeled plume concentrations to observed plume data. The ozone concentrations far downwind of the PinG sources were generally comparable from both sets of simulations, although in some small areas downwind ozone in the CTM/PinG runs was slightly higher.

Comparisons of model and observed hourly ozone concentrations were made to examine the impact on model evaluation performance. The general conclusion is that the CTM/PinG results displayed better agreement and less bias than the CTM/NoPinG results. Ozone tracked closer to observations from the CTM/PinG runs, especially at sites in the region where numerous major point sources treated by PinG were located. Results from model runs for the12 km domain will also be provided. Concentration fields for ozone and other notable species will be shown in the presentation.

REFERENCES

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