An Evaluation of Models-3 Determination of $PM_{2.5}$ During the 1999 SOS Nashville Study

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Summary

Until recently, only limited amounts of speciated $PM_{2.5}$ data have been available to evaluate the performance of aerosol models. During the 1999 Nashville Southern Oxidants Study (SOS) field study, ground-level speciated $PM_{2.5}$ data were collected with a time resolution of 24 hours or less. A 10-day CMAQ simulation (July 1-10, 1999) was compared with the daily speciated $PM_{2.5}$ observations and the performance of CMAQ (Models-3 Community Model for Air Quality) was evaluated. The CMAQ simulation was conducted using grids nested at 32 and 8 km, emissions processed with SMOKE (Sparse Matrix Operator Kernel Emissions) and meteorological data processed from MM5 V3 (Mesoscale Modeling System Generation 5 Version 3).

Method – The CMAQ simulation was conducted using grids nested at 32 and 8 km. The 32 km (coarse) grid had dimensions of 160x106x19 cells. It covered the entire contiguous 48 states plus portions of Canada and Mexico. The vertical grid structure for CMAQ had 19 layers, with the layer thickness increasing with height. The layer thickness ranged from 15.2 m for layer 1 to 6000 m for layer 19. The 8 km (fine) grid had dimensions of 100x100x19 cells. It was centered on the states of Tennessee and Kentucky and included portions of the states of Arkansas, Mississippi, Alabama, Georgia, South Carolina, North Carolina, Virginia, West Virginia, Ohio, Indiana, Illinois and Missouri. The vertical grid structure was the same as that used for the coarse grid. Three ramp up days were used for the coarse grid and two ramp up days for the fine grid. Clean air conditions were used for the coarse grid boundary and initial conditions. RADM2 chemistry with extensions for the four-product isoprene mechanism, aerosol formation and aqueous chemistry was used. A fast solver recently developed by the Environmental Protection Agency (EPA) was used. The Piecewise Parabolic Method advective scheme was used. Model runs were conducted on a Compaq alpha computer system using version 4.1 of stand alone Models-3.

The Sparse Matrix Operator Kernel Emissions (SMOKE) system was used to prepare emissions files for the period 29 June 1999 – 10 July 1999 for the coarse and fine grids. Ozone season emissions from the NET96 emissions inventory were used for point, area, and mobile sources, except that VMT data were used for the 8 km mobile sources and point sources except as noted below. Biogenic emissions were produced from 4 km resolution land use information from the unified grid where coverage permitted, with 36 km resolution land use adapted and used elsewhere. Gridded surrogates were also taken from the unified grid where feasible, with the 36 km surrogate information used elsewhere. Some re-gridding was required in both cases.

The unified grid was made up of 702x603 4-km cells. The surrogate and land use files for this grid were not distributed with SMOKE, but were made available for downloading by MCNC in the capacity of serving as a contact point for emissions modeling information. The 36 km grid was made up of 132x90 cells. The surrogate and land use files for this grid were included with SMOKE. Profiles and cross reference data used were generally the ones supplied with SMOKE, with only minor changes. The RADM speciation profiles were used.

The point, biogenic, and 8 km mobile processing required meteorology, and it was produced by running MM5 output through the MCIP processor. Electric utility hourly point source emissions data supplied by Southern Company and the Tennessee Valley Authority were substituted when available. Emissions from the EDGAR global inventory were used to fill in for regions not covered by the NET96 emissions inventory, but this was accomplished outside of SMOKE.

The PSU/NCAR MM5 V3 was used for the meteorological simulation of the Nashville summer 1999 episode. The simulation was done over a twelve-day period, from 00 UTC of June 29 through 00 UTC of July 11. The model was configured with a coarse 32 km resolution domain covering the continental United States and a nested 8-km resolution domain centering at Nashville. There were 31 sigma layers in the vertical. The NCEP/NCAR Global Reanalysis and the NCEP Global Surface and Upper Air Observations data were used for model initialization and boundary condition as well as surface nudging. Model physics included the Kain-Fritsch cumulus parameterization, Reisner's mixed-phase moisture, NCEP's MRF PBL, and Rapid Radiative Transfer Model longwave radiation schemes. In addition, the OSU/Eta Land-Surface scheme was used for predicting soil moisture and temperature.

Results - Data for ozone and NO_X collected by the Tennessee Valley Authority (TVA) and the National Oceanic and Atmospheric Administration (NOAA) during the SOS 1999 study at three sites in the Nashville area (Downtown, Dickson and Cornelia Fort) were used to evaluate the model performance for these species in the vicinity of Nashville.

Two organizations (NOAA and Aerosol Dynamics, Inc.) provided sulfate and nitrate data collected with high time resolution (one to several hours) at the Cornelia Fort site during the SOS 1999 study. These data were compared against the results for these species in the corresponding grid cell to assess how well CMAQ reproduced the observed trends with time.

Southern Company provided particle data collected at its SEARCH network sites. TVA provided particle data collected at its Tennessee Valley $PM_{2.5}$ Partnership Network sites. Particle data were also acquired from the AIRS, CASTNET and IMPROVE networks. Model performance for sulfate, nitrate, organics and $PM_{2.5}$ over a wider geographic area was evaluated using these data.