Overview of DOE-EPRI-TVA $PM_{2.5}$ Model Study

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Summary

The CMAQ (Community Multiscale Air Quality) model of the EPA Models-3 system is being run for both the 1995 and 1999 SOS Nashville Middle Tennessee Air Quality studies. CMAQ particulate mass estimates for the 1995 period are compared both to available observations and to the Southern Appalachian Mountains Initiative (SAMI) modeling results. For 1999, results are also compared to the more extensive particulate measurements made during the SOS study. This paper describes project objectives, methods, the modeling domain and production of the input data sets. Limited results for the 1999 modeling period are also presented.

Method – Results from CMAQ for the 11-19 July 1995 episode are being compared to results from the URM-1ATM model developed for and applied by SAMI URM-1ATM was developed at the Georgia Institute of Technology to study the relationships between pollutant emissions and atmospheric levels of ozone, aerosols and wet deposition cations and anions. It uses the SAPRC set of chemical reactions and the Reactive Scavenging Model (RSM).

CMAQ inputs are under development that will duplicate inputs used for the URM-1ATM simulation as far as possible. Meteorological data for URM-1ATM were generated using the RAMS model with three domains. The parent grid consisted of an 83x60x35 mesh containing 96-km grid cells. The first nested grid consisted of a 106x90x35 mesh of 24-km cells. The second nested grid consisted of a 100x74x35 mesh containing 12-km grid cells. This grid system was used for RAMS simulations by SAMI. An additional set of outputs from RAMS has been generated using the same grids and input configuration. The new outputs are I/O API (Input/Output Applications Programming Interface) files as required by CMAQ and have been processed through MCIP, the Models-3 meteorological data pre-processor.

The CMAQ grid is a rectangular 12 km grid which approximates the 12 km grid used in the SAMI RAMS simulations. Emissions files for the CMAQ simulation will be generated by re-gridding the emissions files used for URM-1ATM. The URM-1ATM emissions files had been produced using EMS-95. Boundary and initial conditions are based on the boundary and initial conditions used in the SAMI simulations.

Results from the CMAQ simulation are being compared to observations and results produced by the URM-1ATM simulation. Results for O_3, NO_X, sulfate, nitrate, organics and $PM_{2.5}$ are being evaluated to assess the relative performance of the two models.

CMAQ runs are being made 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 surrounding states. 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 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 EPA was used. Model runs were conducted on a Compaq Alpha computer system.

The Sparse Matrix Operator Kernel Emissions (SMOKE) system was used to prepare emissions files for the period 29 June 1999-10 July 1999 for 32- and 8-km 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 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 is made up of 702x603 4 km cells. The surrogate and land use files for this grid are not distributed with SMOKE, but were made by MCNC. The 36-km grid was composed of 132x90 cells. The surrogate and land use files for this grid are included with SMOKE. Profiles and cross reference data used were generally the ones supplied with SMOKE, with only minor changes. RADM2 speciation profiles were used. Electric utility hourly point-source emissions data supplied by Southern Company and the Tennessee Valley Authority were substituted where 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 SMOKE system was developed to work on Sun systems. No executable files were available for the Compaq Alpha. It was not difficult to build executables, but most of them would not run on the Alpha system. A list of problems associated with running SMOKE follows.

- As fixes were made to SMOKE, attempts were made to build and run SMOKE on the Alpha. Eventually all attempts to port SMOKE to the Alpha system were abandoned. Clearly, this software package is not portable to all platforms.
- Originally the intent had been to use VMT data for both grids in order to prepare the mobile files. This idea was abandoned for the 32-km grid because the mobile processors were failing for certain days in regions with large variations in temperature. A fix to SMOKE apparently corrected this problem, but by then it has been discovered that California VMT data were incorrect.
- Early attempts to include hourly point source data failed because this feature of SMOKE was not working for emissions inventory files in IDA format. This problem was fixed in the latest version of SMOKE.
- Newer source code versions of SMOKE were obtained from which executables were built on the Sun system. These executables failed because executables compiled on that system cannot write ASCII records over about 200 bytes long unless the files are opened in a special way. Pre-compiled executable files that were acquired did not have this problem.
- After preparing component files (area, mobile, point, and biogenic), the version of the merge program that merges at the matrix level was run to prepare the combined emissions file. The resulting file was flawed with some regions having no emissions despite significant emissions in the component files. The component files had been overwritten with flawed data, though when they were created one a time they were correct. The solution was to use the merge processor which merges the gridded files. This processor appeared to work, but when an attempt was made to use the resulting emissions file, CMAQ detected that some units were not consistent. The fix for this was to run an extra step to convert the biogenic emissions to moles/second before merging.

The take-home message from this experience is that some components of SMOKE still need refinement before general use by the modeling community.