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AN ASSESSMENT OF MODELS-3 PERFORMANCE DURING THE 1999 SOS NASHVILLE STUDY

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1. INTRODUCTION

An evaluation of the integrated Models-3/Community Multiscale Air Quality (CMAQ) modeling system was conducted by the Tennessee Valley Authority. The objectives of this evaluation were to:
(1) Develop model-ready meteorological and emissions inputs for the time period June 29 – July 10, 1999 using NCAR/PSR Mesoscale Model 5 (MM5) and the Sparse Matrix Operator Kernel Emissions (SMOKE).
(2) Simulate air quality for the same time period using the stand-alone version of Models-3/CMAQ for nested coarse and fine grids.
(3) Compare the output from Models-3/CMAQ for ozone (O_3) and speciated $PM_{2.5}$ against observations from monitoring networks and from the 1999 SOS Nashville intensive study in order to evaluate model performance for both grids.

2.0 DEVELOPMENT OF METEOROLOGICAL AND EMISSIONS INPUTS FOR MODELS-3/CMAQ

The PSU/NCAR Mesoscale Modeling System Generation 5 Version 3 (MM5 V3) was used for the meteorological simulation of the Nashville summer 1999 episode. This simulation will be described and evaluated in a separate paper at this workshop, and therefore will not be discussed further in this paper.

The same grids were used for SMOKE and Models-3/CMAQ. The coarse grid was a 160x106 32-km grid covering the lower 48 states of the United States and the fine grid was a 100x100 8-km grid centered on Nashville. Both grids were Lambert conformal with cone latitudes of 30 and 60 degrees; both grids had coordinate system centers of 40 deg N, 100 deg W. The same vertical grid structure, which contained 19 sigma levels and extended to 15700 m, was used for both grids.

Ozone season emissions from the NET96 emissions inventory were used for point, area, and mobile sources. Biogenic emissions were produced using Biogenic Emissions Inventory System version 2 (BEIS2) from 4-km resolution landuse information where feasible and from 36-km resolution landuse information elsewhere. Gridded surrogates were also taken from the 4-km unified grid where feasible, with the 36-km surrogate information used elsewhere. The surrogate and landuse files for the 4-km resolution unified grid were provided by MCNC; the surrogate and landuse files for the 36-km grid were included with SMOKE. MCNC acted as a host site for the surrogate and landuse files for the 4-km resolution unified grid. The RADM speciation profile was used. Hourly point source information for TVA and Southern Company sources 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.

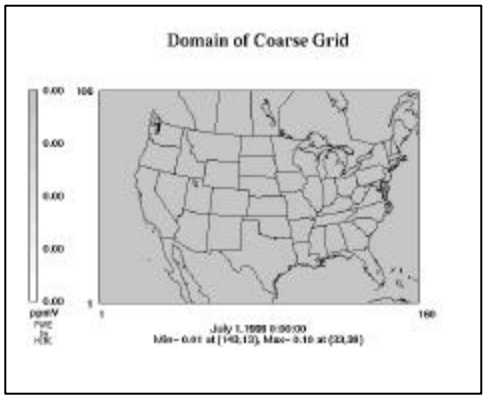

Fig. 1 Domain of coarse grid used for SMOKE and Models-3/CMAQ simulations.

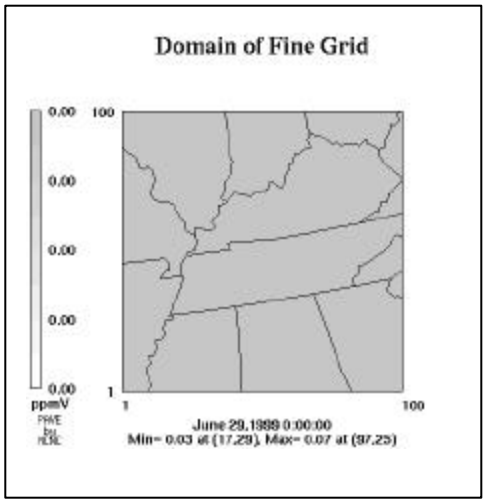

Fig. 2 Domain of fine grid used for SMOKE and Models-3/CMAQ simulations.

The area, mobile, point, and biogenic component files were merged in a separate step to produce the completed emissions files.

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The SMOKE computations were conducted on a Sun Ultra-5_10 Sparc system running SunOS 5.6.

3.0 MODELS-3/CMAQ SIMULATION

The same grids that had been used in SMOKE were used for Models-3/CMAQ. The standalone version 4.2 of CMAQ was used. The coarse grid simulation ran from June 29, 1999 00Z through July 11, 1999 00Z. The coarse grid was ramped for 3 days and the fine grid was ramped 2 days. Clean air conditions were used for coarse grid initial conditions and coarse grid boundary conditions. Fine grid initial and boundary conditions were calculated from the coarse grid. RADM2 chemistry with 4-product isoprene chemistry was used. The Modified Euler Backward Iterative (MEBI) solver for the RADM2 mechanism and the Piecewise Parabolic Method advective scheme were used. The Models-3/CMAQ simulations were conducted on a Compaq alpha EV5.6 system running OSF1 version 4.0.

4.0 EVALUATION OF PERFORMANCE OF MODELS-3/CMAQ

The performance of Models-3/CMAQ was evaluated for ozone and for speciated $PM_{2.5}$. Data collected in the SOS 1999 Nashville intensive study were used to evaluate model performance in the vicinity of Nashville, and data from several monitoring networks were used to evaluate model performance for both the coarse and fine grids over the geographical extent of the fine grid.

4.1 Observational Data Used for Model Performance Evaluation

During the 1999 Southern Oxidants Study (SOS) intensive study, data were collected at several sites in the Nashville area. Ozone data were collected at the Polk Building, Cornelia Fort and near Dickson, Tennessee. $PM_{2.5}$ data were collected at Cornelia Fort, Hendersonville and Dickson. The Polk Building was located in downtown Nashville and the sampling elevation was 110 meters. Cornelia Fort was located 7.5 km east-northeast of the Polk Building and was within Nashville's urban area. The site near Dickson was a rural site located approximately 50 km west of Nashville. The site at Hendersonville was located approximately 20 km northeast of downtown Nashville. Locations of these sites are shown in Figure 3.

Model performance for O_3 was evaluated using data collected at three sites (Cornelia Fort, Polk Building and Dickson) during the 1999 SOS Nashville intensive study. In addition, data from 145 stations in the AIRS network were used. The AIRS stations were located on the fine grid.

$PM_{2.5}$ data collected at three sites (Cornelia Fort, Dickson and Hendersonville) during the 1999 SOS Nashville intensive study were used to evaluate model performance. In addition, data from several other networks were used. Three stations in the Southeastern Aerosol Research and Characterization (SEARCH) network were used: North Birmingham, Jefferson Street, Atlanta and Yorkville, Ga. The first two of these stations were urban and the last was a rural site. Five stations in the Interagency Monitoring

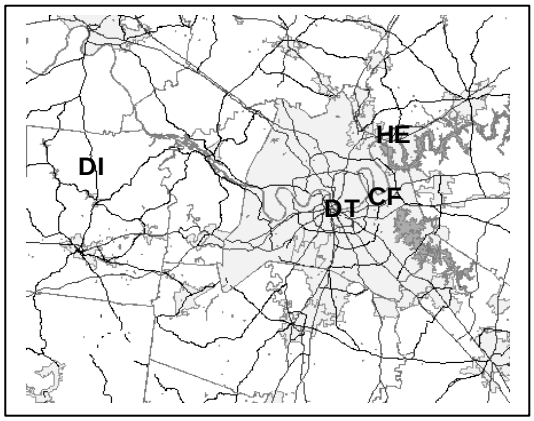

Fig. 3 Locations of monitoring sites during the 1999 SOS Nashville study. The light gray area is Davidson County, the county in which Nashville is located. The four sites were Polk Bldg in downtown Nashville, (DT), Cornelia Fort (CF), Hendersonville (HE) and Dickson (DI).

of Protected Visual Environments (IMPROVE) network were used; these were all rural stations. Total $PM_{2.5}$ data were collected at three sites operated by the Tennessee Valley Authority (Chattanooga, TN; Huntsville, AL, and Lawrence County, TN). Finally, stations from the Clean Air Status and Trends Network (CASTNET) which were located on the fine grid were used.

4.2 Model Performance Evaluation for O_3

Model performance for O_3 at the three sites associated with the Nashville 1999 SOS study was evaluated by comparing the midday maximum O_3 value for each site against the modeled value. This was done for both the single grid cell and for the nearest nine grid cells, and for both the coarse and fine grids. The results are presented in Table 1.

Station	# Days	Difference (ppb)			
		Coarse Grid		Fine Grid	
		9 cells	1 cell	9 cells	1 cell
CF Urban	9	10.6	16.7	10.6	12.8
Polk Urban	8	10.2	17.7	6.9	8.5
DI Rural	6	29.0	31.8	25.1	24.9

Table 1. Mean differences (modeled – observed) for the daily maximum O_3 concentration at three monitoring sites during the 1999 SOS Nashville intensive study.

The data in Table 1 indicate that the model tended to overpredict O_3 levels. Agreement between the

modeled and observed data was better when the nearest nine cells were used instead of the single cell in which the monitoring site was located. Results from the fine grid usually showed less bias than results obtained from the coarse grid. For the three SOS sites, the model showed greater agreement with observations at the two urban sites than it did at the rural site.

The daily mean bias was calculated using MAPS for the 145 AIRS stations which were located on the fine grid (McNally (1995)). These results are presented in Figure 4. The daily mean bias was typically between 10 and 20 ppb. It was lower for the fine grid than it was for the coarse grid, and appeared to be inversely related to O_3 concentration when the O_3 concentration exceeded 60 ppb.

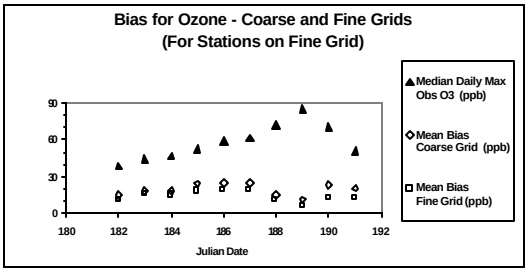

Fig. 4 Daily mean O_3 bias calculated for the coarse and fine grids for 145 AIRS stations located on the fine grid.

4.3 Model Performance Evaluation for $PM_{2.5}$

During the 1999 SOS Nashville intensive study, $PM_{2.5}$ samples were collected at three locations. At Cornelia Fort, particulate sulfate and nitrate data were collected by Aerosol Dynamics, Inc. with 10-minute time resolution using a continuous sampling technique similar to that described in Stolzenburg (2000). The samples were analyzed in-situ by flash vaporization using a method analogous to that of Roberts (1976). Open-faced filter samples were collected by the NOAA Aeronomy Laboratory and analyzed as described in Fehsenfeld (1998). The samples collected by NOAA were not strictly of the $PM_{2.5}$ size fraction. However, since most $SO_4^=$ and NO_3^- should occur in the $PM_{2.5}$ size range, it is reasonable to consider these samples to be surrogates for $PM_{2.5}$ samples. At Hendersonville and Dickson, $PM_{2.5}$ samples were collected by Georgia Institute of Technology for 24 hours using a three-channel Particle Composition Monitor (PCM) as described in Baumann (2002).

Hourly averages were calculated for the $PM_{2.5}$ data collected by ADI. Model results were averaged over the time period corresponding to the sample collection times for the samples collected at Dickson and Hendersonville. A simple criterion was used to evaluate model performance. Performance was considered to be acceptable if the modeled concentration was within the range: observed value/2 to observed value*2. The results from these calculations are shown in Table 2. Model performance was reasonable for $SO_4^=$; typically the criterion was met for about 70-75% of the samples. Performance was poorer for NO_3^-; the criterion was typically met for only 15-20% of the samples

Participant	Site	Sample Duration	N	Percent of cells within + factor of 2			
				Coarse		Fine	
				1 cell	9 cells	1 cell	9 cells
$SO_4^=$							
ADI	CF	Hourly	130	63.1	67.7	67.7	70.8
NOAA	CF	Hourly	46	75.0	79.5	77.3	77.3
GIT	DI/HEN	24 hrs	7	71.4	71.4	57.1	57.1
NO_3^-							
ADI	CF	Hourly	125	14.6	13.1	20.8	20.8
NOAA	CF	Hourly	46	13.3	8.9	17.8	17.8
GIT	DI/HEN	24 hrs	7	28.6	42.9	28.6	28.6

Table 2. Percent of hourly data points for $SO_4^=$ and NO_3^- at the SOS 1999 intensive data collection sites which met the criterion: observed value/2 <= modeled value <= observed value*2.

The mean concentrations of $PM_{2.5}$ species for sites on the fine grid are present in Figure 5. Agreement of the model results with observations was reasonably good. There were several trends worth noting. The fine grid usually gave poorer agreement for $SO_4^=$ than the coarse grid. The model usually underestimated the total $PM_{2.5}$ compared to observations and the fine grid usually showed poorer agreement for total $PM_{2.5}$ than the coarse grid. With the exception of the observed data at Hendersonville, both observed and predicted EC concentrations were higher at urban

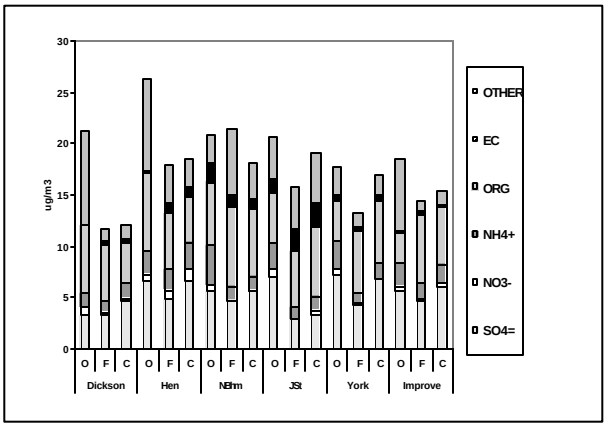

Fig. 5 Mean concentrations of $PM_{2.5}$ species by site. The bars labeled "O" show the observed data; the bars labeled "C" show results for the coarse grid and the bars labeled "F" show results for the fine grid. The bars are stacked in the same order from bottom to top as the legends are.

sites than at rural sites. At the rural sites, but not necessarily at the urban sites, the model

underpredicted the concentration of the OTHER category compared to the observations.

In Table 3, the mean concentrations and biases are presented for the $PM_{2.5}$ species. The results presented in this table demonstrate again the conclusions that the model usually underestimated total $PM_{2.5}$ relative to observation and that $SO_4^=$ was

Particle Speciation Statistics from SEARCH, IMPROVE, TVA and 1999 SOS sites				
Species	N	Mean Obs	Mean Bias	
		(ug/m^3)	(fine)	(coarse)
			(ug/m^3)	(ug/m^3)
Total $PM_{2.5}$	31	19.83	-4.27	-4.46
$SO_4^=$	47	5.84	-1.55	-0.19
NO_3^-	47	0.5	-0.42	-0.25
NH_4^+	44	2.52	-1.28	-1.02
Org	47	4.68	1.53	1.17
EC	47	0.79	0.06	-0.04

Table 3. Mean biases for $PM_{2.5}$ species observed on the coarse and fine grids.

Statistics for $PM_{2.5}$ Species from CASTNET Sites					
	Units	N	Mean Obs	Mean Bias	Mean Bias
				(fine)	(coarse)
$SO_4^=$	ug/m^3	11	5.66	-1.41	-0.68
SO_2	ug/m^3	11	4.33	3.10	2.71
NH_4^+	ug/m^3	11	1.55	-0.04	0.14
NO_3^-	ug/m^3	11	2.79	1.24	1.42

Table 4. Statistics for $PM_{2.5}$ Species at the CASTNET sites.

usually more underpredicted on the fine grid than it was on the coarse grid.

From the data in Table 3, it does not appear that the model performs more accurately for $PM_{2.5}$ species on the fine grid than it does on the coarse grid. In fact, for all the quantities in the table with the exception of total $PM_{2.5}$, the absolute value of the mean bias was larger for the fine grid than it was for the coarse grid.

Statistical results for the CASTNET sites which were located on the fine grid are given in Table 4. The CASTNET samples were collected weekly; therefore the time resolution was not as good as it was for the observations that have already been discussed. The model displayed a negative bias for $SO_4^=$ data and a positive bias for SO_2 and NO_3^- data.

5.0 CONCLUSIONS

A complete suite of software MM5/SMOKE/CMAQ was used to simulate the air quality episode that corresponded to the time period of the 1999 Nashville intensive study. The performance of Models-3/CMAQ was evaluated using observational data from the 1999 SOS intensive study and from several air quality monitoring networks. The model tended to overpredict O_3 maximas unless the observed O_3 concentrations were high. Modeled O_3 values were more accurate on the fine grid than on the coarse grid. Model performance was acceptable for $PM_{2.5}$ speciation, and did not appear to be better on the fine grid than on the coarse grid. Generally the model underpredicted total $PM_{2.5}$ and $SO_4^=$. Results for other $PM_{2.5}$ species were mixed.

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5.1 References

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