SENSITIVITY OF PM 2.5 SPECIES TO EMISSIONS IN THE SOUTHEAST

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1. INTRODUCTION

Most of the sensitivity analyses in the past have focused on the effect of NOx and VOC emissions on ambient ozone concentrations. However, less work has been conducted on how fine aerosol particle levels respond to changes in emissions. Thus, we examined the sensitivity of PM 2.5 species to emissions focusing on the eastern United States for July 2001 and January 2002, using Models-3 (CMAQ/MM5/SMOKE).

2. METHODOLOGY

The air quality model contains two domains, one with a 36 km grid and the other with a 12 km grid. The projection of this model is the Lambert conformal conic projection with the central meridian of 97 W and the center of the latitude of 40 N. The standard parallels were 33 N and 45 N (Fig. 1, Table 1). Episodes selected for modeling were July 1-10, 2001 and January 1-10, 2002. These periods correspond to coordinated intensive monitoring by the EPA supersites and others.

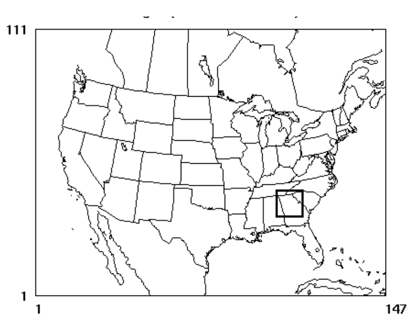

Fig 1. CMAQ model domain. The large rectangle covering the continental United States is the 36 km domain and the small rectangle over the state of Georgia is the 12 km domain.

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Table 1. CMAQ model domain.

	36 km domain	12 km domain
dimension	147 x 111	21 x 18
origin	(-2628, -1980 km)	(1044, -720 km)

2.1 Meteorological Inputs

Meteorological input data for the photochemical modeling runs were processed using NCAR's 5th generation Mesoscale Model (MM5) version 3.5.3 (PSU/NCAR Mesoscale Modeling System, 2003). The physics options selected in MM5 are the simple ice microphysics, Kain-Fritsch cumulus scheme, Rapid Radiative transfer model, Pelim-Chang planetary boundary layer, and the Pleim-Xiu land surface module. Four Dimensional Data Assimilation was performed using the NCEP Eta model outputs for the GCIP project (GCIP NCEP Eta model output , 2003) and NCEP ADP Observational data (NCEP ADP Global Upper Air Observations, NCEP ADP Global Upper Air Observation Subsets, and NCEP ADP Global Surface Observations , 2003) as inputs.

2.2 Emission Inputs

Emissions data were processed using the Sparse Matrix Operator Kernel Emissions (SMOKE). Input emissions for the state of Georgia were developed by Georgia Tech as a part of the Fall Line Air Quality (FAQS) project, using surveys for the state of Georgia, CEM data for major point sources. Emissions for other states were from the 1999 National Emissions Inventory (1999 NEI version 2 for criteria pollutants, 2003).

2.3 Air Quality Model Configuration

Modules selected in CMAQ are SAPRC-99 as the chemical mechanism, a modified Euler backward iterative (MEBI) method for the chemistry solver, the regional acid deposition model (RADM) for clouds, AERO3 for aerosol dynamics, AERO_DEPV2 for the deposition velocities of aerosols, and the piecewise parabolic method (PPM) for horizontal and vertical advection. The minimum vertical eddy coefficient used is 0.3 m^2/sec.

3. EVALUATION

3.1 Meteorological Input

Meteorological input to CMAQ as developed using MM5 was evaluated based on the TDL surface hourly data (TDL U.S. and Canada Surface Hourly Observations, 2003), and results are summarized below (Table 2).

Table 2. The meteorological input evaluation.

Grid size	Episode	Temperature (K)	Specific humidity (g/kg)	Wind speed (m/sec)	Wind direct-ion. (deg)
Mean bias error (MBE)					
36 km	Jul. 2001	-0.333	-0.820	-0.092	11.59
	Jan. 2002	-1.161	0.101	0.135	21.62
12 km	Jul. 2001	0.200	-0.504	0.148	35.7
	Jan. 2002	-1.340	0.051	0.011	8.64
Root mean square error (RMSE)					
36 km	Jul. 2001	1.650	1.806	1.297	58.05
	Jan. 2002	2.053	0.524	1.412	64.60
12 km	Jul. 2001	1.998	1.156	1.410	78.72
	Jan. 2002	2.480	0.396	1.629	54.18

3.2 Air quality model

The air quality model was evaluated based on data from the SouthEastern Aerosol Research and CHaracterization study (SEARCH) (Atmospheric Research and Analysis, 2003) and the Assessment of Spatial Aerosol Composition in Atlanta (ASACA) project (Table 3).

Table 3. Coordinates of measurement stations.

ID	Longitude	Latitude	State	Source
BHM	-86.82	33.55	AL	SEARCH
CTR	-87.25	32.9	AL	
GFP	-89.05	30.39	MI	
JST	-84.41	33.78	GA	
OAK	-88.93	30.99	MI	
OLF	-87.38	30.55	FL	
PNS	-87.26	30.44	FL	
YRK	-85.05	33.93	GA	
FTM	-84.44	33.70	GA	ASACA
SDK	-84.29	33.69	GA	
TUC	-84.21	33.85	GA	

Performance of both CMAQ 4.2.2 and 4.3 was evaluated. Daily PM 2.5 species and hourly PM 2.5 total mass were evaluated for July 2001 and January 2002. Hourly gas phase species were evaluated for July 2001 (Table 3, Figs 2 and 3). Performance for simulating organic carbon and the nitrate was improved significantly from the CMAQ 4.2.2 to CMAQ 4.3.

Table 3. Performance of hourly ozone concentrations for July 1-10, 2001.

O3	MBE (ppb)	MNB (%)	MGE (ppb)	MNGE (%)
Version 4.2.2	5.38	13.7	24.83	44.35
Version 4.3	11.16	21.6	20.24	38.1

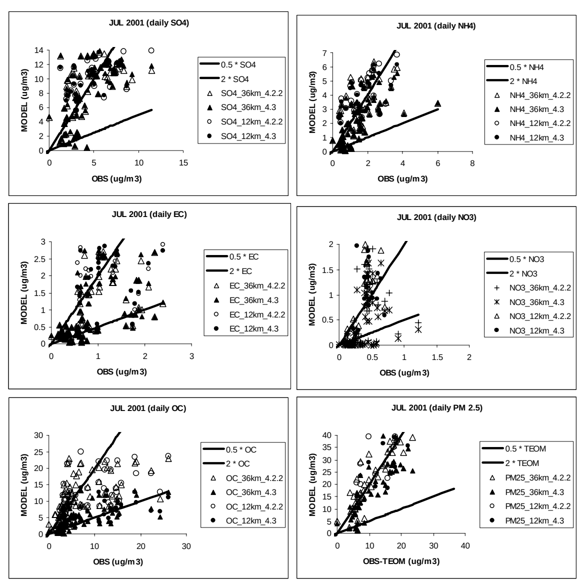

Fig.2 Performance of the CMAQ 4.2.2 and 4.3 for daily PM 2.5 species and total mass.

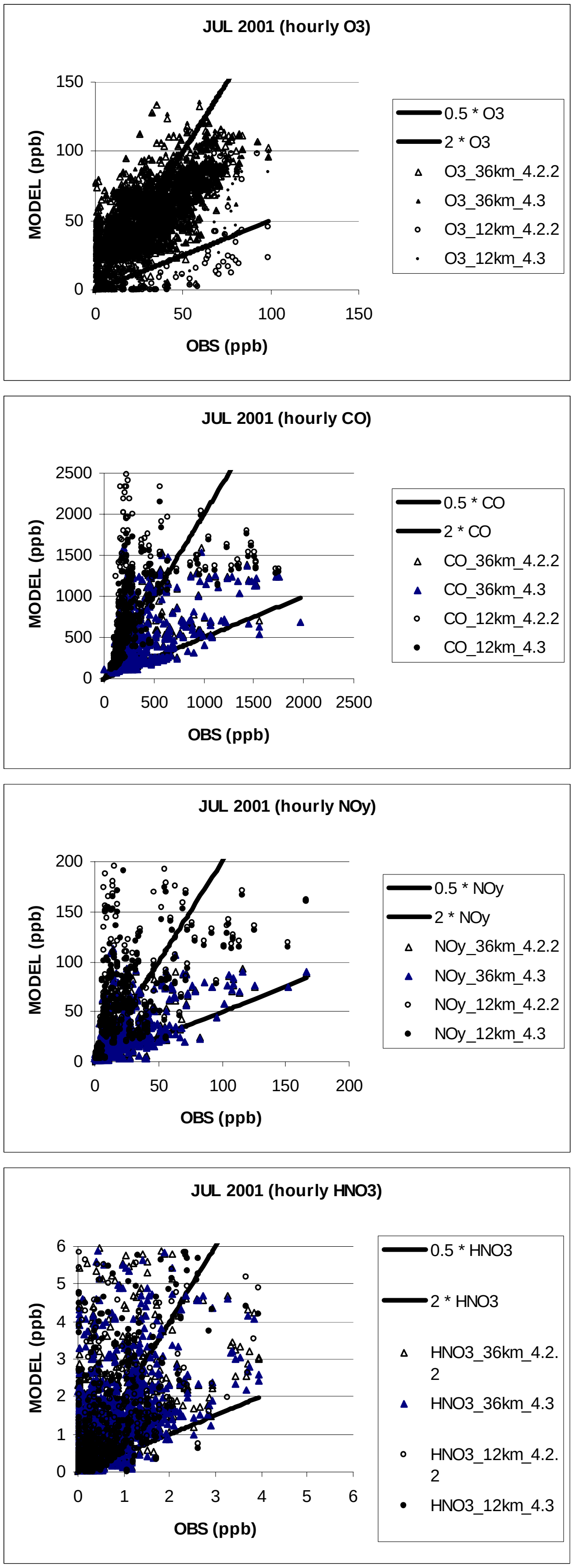

Fig. 3. The performance of the CMAQ 4.2.2 and 4.3 for the hourly gas phase species and PM 2.5 total mass.

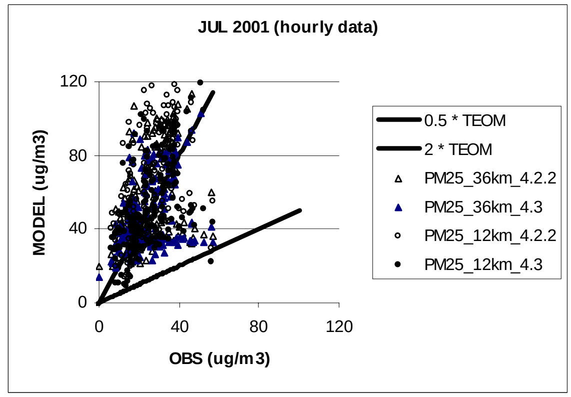

Fig. 3. continued.

4. SENSITIVITY ANALYSIS

Sensitivity analysis was performed using a 20 % reduction of NH_3 and SO_2, and the results are presented below (Table 4, Figs 4 - 6).

Table 4. Sensitivity (%) of PM 2.5 species to a 20 % reduction of NH_3 and SO_2.

	Species	July 2001	January 2002
20 % reduction of NH_3	Sulfate	-1.37	-4.55
	Nitrate	-47.9	-12.96
	Ammonium	-16.8	-10.07
20 % reduction of SO_2	Sulfate	-9.18	-3.96
	Nitrate	88.26	-0.29
	Ammonium	3.45	-1.44
20 % reduction of NH_3 and SO_2	Sulfate	-11.34	-8.32
	Nitrate	-15.41	-8.62
	Ammonium	-11.43	-8.33

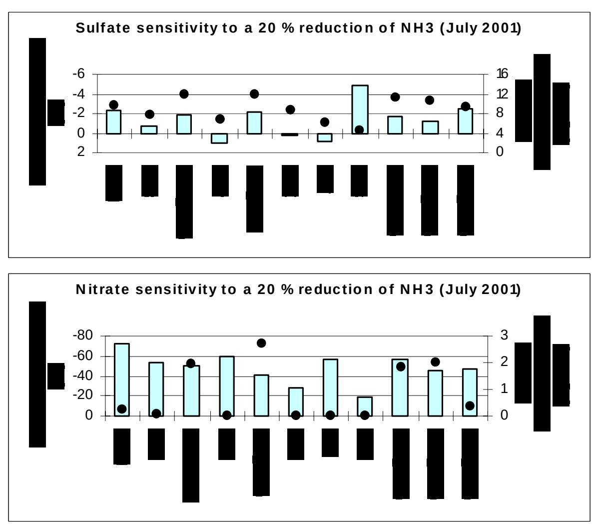

Fig. 4. The sensitivity (bar) of PM 2.5 species and total mass concentration (circle) to a 20 % reduction of NH_3.

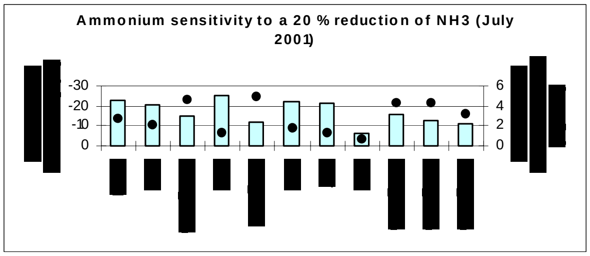

Fig. 4. continued.

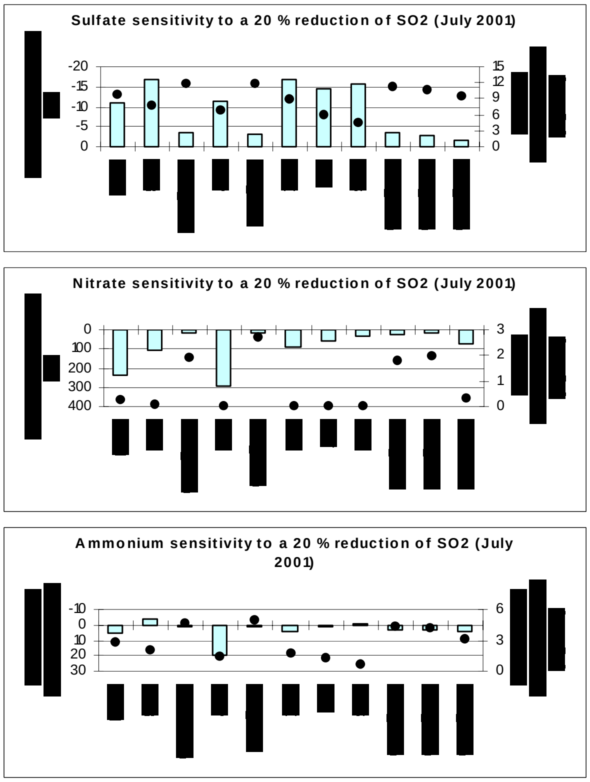

Fig. 5. The sensitivity (bar) of PM 2.5 species and total mass concentrations (circle) to a 20 % reduction of SO_2.

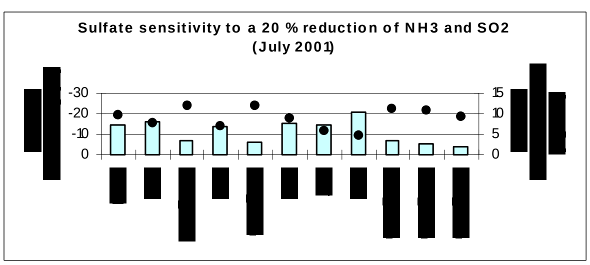

Fig. 6. The sensitivity (bar) of PM 2.5 species and total mass concentrations (circle) to a 20 % reduction of NH_3 and SO_2.

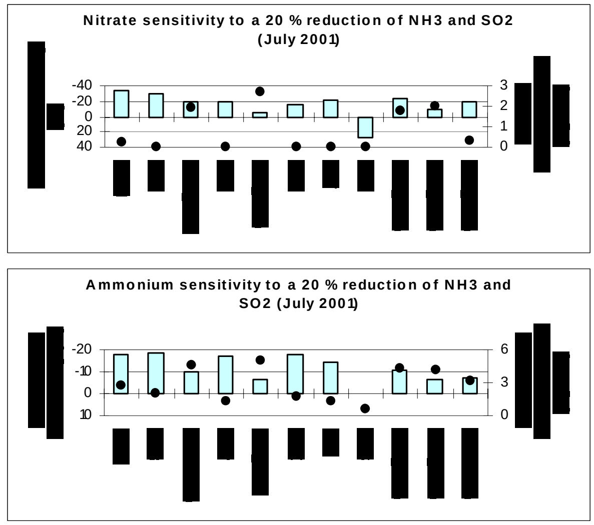

Fig. 6. continued.

5. CONCLUSION

The PM 2.5 and gas phase species were simulated using the CMAQ 4.2.2 and 4.3. The result showed that the performance of CMAQ 4.3 improved markedly, especially for nitrate and organic carbon. The sensitivity of PM 2.5 species were examined using CMAQ 4.3. The reduction of both NH_3 and SO_2 emissions were shown to be effective reducing for the PM 2.5. Future research will include the sensitivity of emissions for different geographic locations.

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