AN EVALUATION OF THE 2003 RELEASE OF Models-3 CMAQ

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1.0 INTRODUCTION

The 2003 release of EPA's Community Multiscale Air Quality model was made available during August of this year. As part of this release, an evaluation was performed involving two simulation periods (4 January - 19 February 2002 and 15 June - 16 July, 1999), using two chemical mechanisms (SAPRC and CBIV). For the sake of brevity only the SPARC simulations are presented here. Full evaluation results from the other simulation as well as release notes documenting model changes and updates are available on the website at:
www.epa.gov/asmdnerl/models3/index.html.

2.0 CMAQ CONFIGURATION

The CMAQ configuration evaluated in this abstract uses the SAPRC99 gas-phase chemistry mechanism. The summer simulation was performed using a 32 km resolution grid over the entire U.S. domain with a vertical resolution of 21 layers (set on a sigma coordinate); while the winter simulation used a 36 km resolution grid and 24 vertical layers.

For both simulations, the meteorological fields were derived from MM5, the Fifth-Generation Pennsylvania State University-National Center for Atmospheric Research (NCAR) Mesoscale Model and were processed through MCIP Version 2.2.

Emissions of gas-phase SO_2, CO, NO, NO_2, NH_3, and VOC were based on the 1999 EPA National Emissions Inventory. Primary anthropogenic $PM_{2.5}$ emissions were separated into different species including particle SO_4, NO_3, OC, EC. Emissions of HC, CO, NO_x, and PM from cars, trucks, and motorcycles are based on MOBILE5b, while biogenic emissions were obtained from BEIS 3.11.

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3.0 EVALUATION DATA SETS

3.1 AIRS

Hourly O_3 (ppb) data obtained from EPA's Aerometric Information Retrieval System (AIRS) were used in the evaluation. Over 700 stations were available, mostly in urban areas, resulting in over 500,000 hourly observations. In addition to the hourly data (not presented here), both the maximum 1-hr and maximum 8-hr concentrations were calculated for each station - day over the four week summer evaluation period.

3.2 CASTNet

Weekly average concentrations of SO_4^{2-}, NO_3^-, HNO_3 and NH_4^+ (µg m^{-3}) obtained from the Clean Air Status and Trends Network (CASTNet) were also available for nearly 70, mostly rural stations. Four weekly collection periods coincided with the summer simulation period; while six were available for the winter simulation.

3.3 IMPROVE

Daily average concentrations of SO_4^{2-}, NO_3^-, $PM_{2.5}$, OC and EC (µg m^{-3}) from 50 rural IMPROVE (Interagency Monitoring of PROtected Visual Environments) sites were also used. These data are collected on every third day, (midnight to midnight, local time), limiting the number of days available for comparison to 10 and 15 for the summer and winter simulations, respectively.

3.4 STN

The more recently established STN (Speciated Trends Network) follows the protocol of the IMPROVE network (i.e. every third day collection) with the exception that most of the nearly 60 sites are found in urban areas. Daily average concentrations of SO_4^{2-}, NO_3^-, $PM_{2.5}$, NH_4^+, OC and EC (µg m^3) were available for 15 days during the winter simulation.

4.0 STATISTICS

In addition to scatterplots and boxplots (not shown here), numerous statistical metrics were calculated for each specie, including least squares coefficients, correlations and two measures of bias and error. For bias, the Mean Bias (MB) and Normalized Mean Bias (NMB) were calculated. For error, we calculated the Root Mean Square Error (RMSE) and the Normalized Mean Error (NME). These metrics are provide in Tables 1 and 2 for the summer and winter simulations, respectively.

5.0 RESULTS

5.1 Ozone

Examination of the Tables reveals that CMAQ produces fairly unbiased (NMBs < 10%) and accurate (NMEs ~ 20.0%) simulations of both the max-1 hour and max-8 hour ozone concentrations when compared against the AIRS data. Correlations are also fairly good (between 0.72 and 0.75) indicating that CMAQ is capturing roughly 50% of the variability exhibited by the observations.

5.2 Sulfate

CMAQ performs quite well in simulating SO_4 concentrations. Correlations are high, ranging from 0.90 during the summer (against both CASTNet and IMPROVE sites) to 0.66 in the winter against STN sites. The NMBs are (with one exception) positive and between 9.2 and 38.4%. The lone underprediction occurs against STN data (NMB: -12.0%) and like the lower correlation, may be attributable to the urban nature of the STN. The NMEs range from 25.7% (winter, CASTNet) to 61.9% (summer, IMPROVE).

5.3 Nitrate

Of all of the species simulated by CMAQ, NO_3 simulations are the worst. Correlations are lower for the winter simulations (0.27: CASTNet, 0.36: IMPROVE) when compared to the summer simulations (0.39: STN, 0.54: IMPROVE, 0.76 (CASTNet). The summer simulation produces negative biases (NMB: -30.8% for CASTNet, -39.1 for IMPROVE), while NMBs for the winter simulation are mixed, ranging from 8.0% for STN to 46.8 for CASTNet. The errors associated with NO_3 simulations are generally the largest produced by CMAQ and range from 66.9% (winter, STN) to 96.5% (winter, IMPROVE).

5.4 Ammonium

Results of NH_4 simulations mirror those of SO_4 in that CMAQ performs quite well and consistently especially when compared against CASTNet observations (correlations: 0.86 summer simulation, 0.85 winter). As seen with SO_4 and probably for the same reason, the CMAQ correlation against the STN is considerably lower (0.41). The NMB against STN data is however small (5.2% for the winter simulation) when compared against CASTNet (40.0% for the winter and 22.7% summer). The NMEs range from 36.5% (summer CASTNet) to 57.7% (winter STN)

5.5 PM$_{2.5}$

The results of the $PM_{2.5}$ simulations are like PM2.5 itself, a composite of the other species. Correlations associated with the more rural IMPROVE network are considerably higher (0.71 summer, 0.68 winter) than those associated with the more urban STN network (0.37 winter). The NMB for the summer simulation is small and negative (-9.8%) against the IMPROVE network, small but positive for the winter simulation against STN and large and positive for the winter simulation against the IMPROVE network. The NME range from 40.3% (summer simulation against IMPROVE) to 57.7% (winter simulation against STN).

5.6 Nitric Acid

The results associated with the HNO_3 evaluation are consistent between the summer and winter simulations. The correlation for the summer simulation is 0.79, while that for the winter is 0.64. The NMBs are positive (49.0, 44.2 for summer, winter respectively) and the NMEs average near 60%.

5.7 Organic Carbon

Results for OC are mixed depending on season and network. The NMB against IMPROVE is small and negative (-1.5%) in the summer yet it is positive and larger in the winter (17.2%). Against the STN data, the winter CMAQ simulation significantly underpredicts (NMB: -50.0%). The NMEs are more consistent - though large, ranging from 60.4 to 70.0%, and the correlations range between 0.32 and 0.56.

5.8 Elemental Carbon

The summer CMAQ simulation of EC is unbiased (NMB: 1.0%) and produces a correlation of 0.69 when compared against IMPROVE data. Conversely, the winter simulation significantly overpredicts EC, resulting in large positive biases (31.0% and 59.1% against IMPROVE and STN respectively) and large errors as well (NME 81.0, 95.0%.

Table 1. Summer 1999 Evaluation statistics

Species	O_3 Max-1	O_3 Max-8	SO_4		NO_3		$PM_{2.5}$	NH_4	HNO_3	OC	EC
Network	AIRS	AIRS	CAS	IMP	CAS	IMP	IMP	CAS	CAS	IMP	IMP
n	23,196	23,196	264	490	264	415	457	264	264	396	396
r	0.72	0.75	0.90	0.90	0.27	0.36	0.71	0.86	0.79	0.32	0.69
MB	2.3	4.3	1.74	0.75	-0.15	-0.11	-0.73	0.31	1.11	-0.02	0.00
NMB (%)	3.8	8.7	38.0	38.4	-30.8	-39.1	-9.8	22.7	49.0	-1.5	1.00
RMSE	14.5	12.8	2.89	2.37	0.57	0.51	4.70	0.70	1.77	1.35	0.24
NME (%)	18.8	20.2	46.4	61.9	75.7	95.0	40.3	36.5	58.7	67.2	52.6

Table 2. Winter 2002 Evaluation statistics

Species	SO_4			NO_3			$PM_{2.5}$		NH_4		HNO_3	OC		EC	
Network	CAS	STN	IMP	CAS	STN	IMP	STN	IMP	CAS	STN	CAS	IMP	STN	IMP	STN
n	407	1149	728	407	1044	688	927	714	407	1149	407	731	1106	731	1148
r	0.83	0.66	0.85	0.76	0.39	0.54	0.37	0.68	0.85	0.41	0.64	0.56	0.47	0.55	0.40
MB	0.15	-0.26	0.29	0.64	-0.27	0.20	0.51	1.49	0.33	0.07	0.55	0.14	-1.64	0.07	0.42
NMB(%)	9.2	-12.0	31.5	46.8	-8.0	28.9	4.1	40.3	40.0	5.2	44.2	17.2	-50.0	31.0	59.1
RMSE	0.60	1.16	0.72	1.36	4.37	1.26	10.45	3.81	0.51	1.46	1.07	0.93	3.32	0.48	1.17

NME (%)	25.7	35.9	53.1	70.4	66.9	96.5	50.0	68.9	47.2	57.7	61.3	70.0	60.4	81.0	95.0