PARTICULATE MATTER MULTI-MODEL PERFORMANCE EVALUATION

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1. INTRODUCTION

Photochemical grid models have been used extensively in the past to aid in the development of emission control strategies to demonstrate compliance with the ozone standard. More recently the development of "one-atmosphere" air quality models that treat ozone, particulate matter (PM) and other air quality issue within the same platform have gained increasing use.

Five Regional Planning Organizations (RPOs), which consist of States, Federal and Local Agencies, Tribes and Stakeholders, have been formed in the United States (US) to address the requirements of the Regional Haze Rule (RHR) and the regional components of the 8-hour ozone and fine particulate standards. The RHR goal is to achieve natural visibility conditions at Federally mandated Class I areas, which include National Parks and Wilderness Areas. One-atmosphere models are used to project visibility improvements and identify emission control strategies to improve visibility. Three one-atmosphere air quality models are being used by the RPOs to assess visibility impairment at Class I areas:

- Models-3 Community Multi-scale Air Quality (CMAQ) modeling system. (EPA, 1999)
- Comprehensive Air-quality Model with Extensions. (ENVIRON, 2004)
- Regional Model for Simulating Aerosol and Deposition. (ICF, 2002)

The choice of the air quality model depends on various criteria including: scientific credibility, model performance, ease of use, computational requirements, and potential acceptance by EPA in the visibility State Implementation Plans (SIPs) due in 2007/2008. Several of the RPOs have embarked on multi-model evaluation studies to assess the ability of the models to simulate particulate matter (PM), ozone and visibility. This paper discusses such efforts by three of the RPOs:

- Western Regional Air Partnership (WRAP) evaluation of the CMAQ, REMSAD and CAMx models for 1996 and the western US. (Morris and Koo, 2004)
- Visibility Improvements States and Tribal Association Southeast (VISTAS) evaluation of the CMAQ and CAMx models. (Morris et al., 2004)
- Central Regional Air Partnership (CENRAP) evaluation of the CMAQ and CAMx models. (Tonnesen and Morris, 2004)

2.0 WRAP CMAQ, REMSAD AND CAMx MODEL INTERCOMPARISON

WRAP performed regional haze modeling of the western United States (US) and the 1996 year using the CMAQ model to develop the modeling components of the Section 309 SIP for several of the WRAP states. (WRAP, 2003) After the completion of the Section 309 SIP modeling, WRAP extended the CMAQ modeling databases to REMSAD and CAMx.

2.1 Development of CMAQ to CAMx/REMSAD Processors

CMAQ-to-CAMx and CMAQ-to-REMSAD processors were developed to convert the CMAQ emissions, initial concentrations (IC) and boundary conditions (BC) to the file formats and species used by CAMx and REMSAD. CMAQ calculates plume rise external to the air quality model and uses three-dimensional emission inputs in the I/O API format, whereas both CAMx and REMSAD use a two-dimensional surface emissions plus a point source input file and plume rise is calculated

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internally in the two models. The emissions conversion processors perform the following:

- Converts the CMAQ emissions from the I/O API format to Fortran binary format used by CAMx and REMSAD.
- Maps the CMAQ species to those used by CAMx and REMSAD.
- Writes out a surface layer two-dimensional and a point source file that includes the grid cell location (i,j,k) of all non-zero emitted grid cells above the surface.

As a majority of the grid cells above the surface layer have zero emissions, the resultant CAMx and REMSAD emission inputs are a fraction of the size of the CMAQ emission inputs. The IC and BC processors are similar converting the CMAQ IC/BC files from I/O API to Fortran binary and mapping the CMAQ species to those used by CAMx and REMSAD. One note is that CAMx includes separate species for fine and coarse crustal material (dust) that is not separately speciated in CMAQ, so this feature of CAMx could not be evoked in the WRAP 1996 annual modeling.

Hourly meteorological inputs for the CMAQ, REMSAD and CAMx models for the western US 36 km WRAP domain were generated from the raw MM5 output using each model's meteorological processor, namely MCIP, MM5REMSAD and MM5CAMx, respectively.

2.2 CMAQ, REMSAD and CAMx Model Evaluation

The CMAQ, REMSAD and CAMx models were exercised for the 1996 year and western US and evaluated against speciated PM measurements from the IMPROVE and CASTNet networks and gaseous species (e.g., ozone) from the AQS network. CMAQ uses a modal approach with three modes to represent PM size distribution where all secondary PM is assumed to be fine. REMSAD has two sections and also assumes all secondary PM are fine. CAMx has two options for representing PM size distribution, Mechanism 4 (M4) that has coarse and fine modes with all secondary PM assume to be fine and a full sectional approach that allows secondary PM to grow to the coarse mode. For the 1996 application CAMx was operated in both the two-section (CAMx_M4) and multi-section with four sections (CAMx_4sec) approaches. Table 1 summarizes the science configurations in the four models used in the 1996 modeling.

Figure 1 displays the sulfate (SO4), nitrate (NO3) and organic carbon (OC) model performance using the IMPROVE measurements in terms of fractional bias for the 1996 year and January and July 1996. The models overestimate sulfate and nitrate in the winter and underestimate it in the summer. Although CAMx_4sec has the highest annual average sulfate bias, it has the lowest monthly bias. All three models estimate nitrate poorly. Organic Carbon is underestimated by all three models.

Table 1. Science algorithms selected for annual 1996 modeling.

	CMAQ	**REMSAD**	**CAMx_M4**	**CAMx_4sec**
Gas-phase	CB4	Micro-CB4	CB4	CB4
Inorganic	ISORROPIA	MARS-A	ISORROPIA	ISORROPIA
Organic	SORGAM	Odum et al. (1997) Griffin et al. (1999)	SOAP	SOAP
Aqueous	RADM	Martin (1984)	RADM	RADM
Size	3 modes	Fine/Coarse	Fine/Coarse	4 sections

3.0 VISTAS PHASE I MODELING USING CMAQ AND CAMx

VISTAS Phase I modeling applied the CMAQ and CAMx models for the July 1999 and July 2001 episodes using a 36 km continental US and 12 km southeastern US modeling domains. Model inputs were developed for CMAQ, which was subjected to a series of sensitivity tests to identify the optimal model configuration for simulating PM in the southeastern US. Figures 2 and 3 summarize the CMAQ and CAMx fractional bias and error performance statistics in the southeast US using the IMPROVE, CASTNet, SEARCH daily, and SEARCH hourly speciated PM concentrations and NADP wet deposition networks. Both models simulate sulfate in the southeastern US very well, albeit with an overestimation bias, with the CAMx overestimation being more severe than CMAQ's. Both models severely underestimate nitrate during the two summer episodes (not shown), a trait seen in the WRAP 1996 western US modeling. Model performance for EC and OC is reasonably good, with CAMx exhibiting better EC and OC model performance than CMAQ that has an underestimation bias.

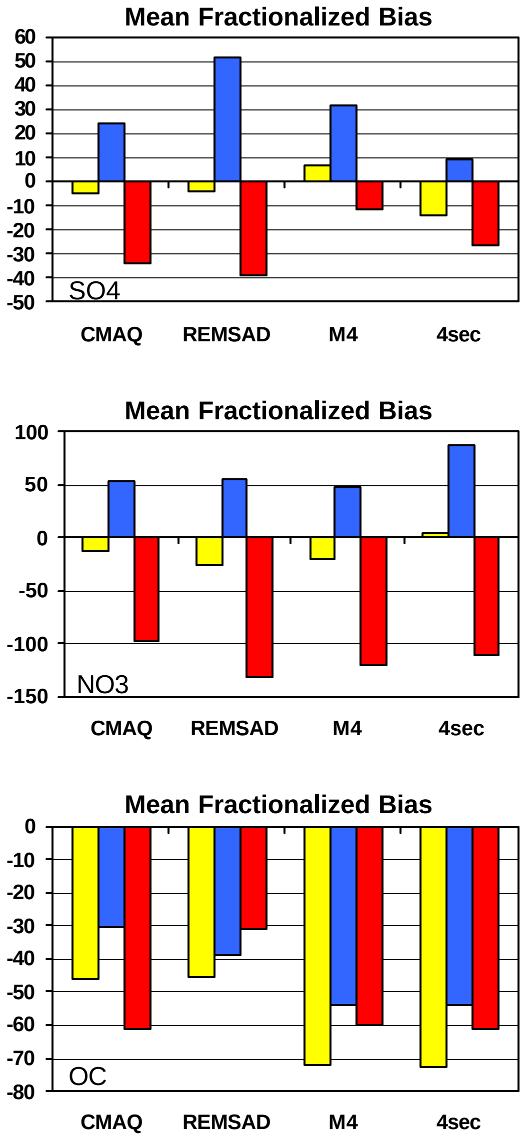

Figure 1. Annually, January and July fractional bias performance measures for sulfate (top), nitrate (middle) and organic carbon (bottom), the CMAQ, REMSAD, CAMx_M4 and CAMx_4sec models, the western US and 1996.

4.0 CENRAP CMAQ AND CAMX COMPARISONS

CENRAP analyzed the VISTAS Phase I modeling results focusing on performance in the Central States that is summarized in Table 2. CAMx exhibits better model performance for ozone than CMAQ with lower fractional bias (-10% versus –29%) and fractional error (25% versus 32%). CMAQ, however, exhibits better model performance for NO2 and SO2. Both models simulate sulfate fairly well, with the CMAQ performance being better than CAMx. Nitrate is severely underestimated by both models. CAMx is simulating the Carbon species (EC and OC) better than CMAQ in the Central States.

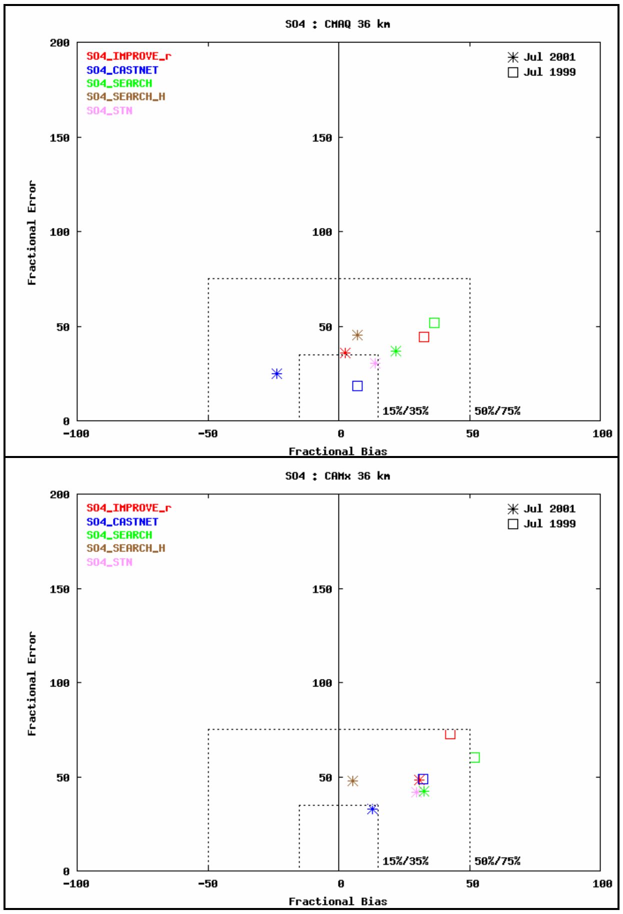

Figure 2. Fractional bias versus error performance statistics for sulfate (SO4) in the Southeastern US and the July 1999 and July 2001 episodes for the CMAQ (top) and CAMx (bottom) 36 km base case simulations.

5.0 CONCLUSIONS

The CMAQ and CAMx photochemical grid models represent two distinct one-atmosphere modeling platforms to address ozone, PM, visibility and other air quality issues. From the early WRAP 1996 to the more recent VISTAS and CENRAP 2001 and 2002 modeling there has been substantial improvement in the CMAQ and CAMx model performance. Both models exhibit good performance for sulfate, with CAMx having an overprediction tendency for the summer episodes that has been addressed in the latest updates to MM5CAMx. Carbon performance is also fairly good, with CAMx exhibiting better performance than CMAQ. Nitrate performance continues to be a problem for both models with a winter under – and summer over–estimation bias. Soil and coarse matter (CM) performance is also problematic and related to emission inputs and grid resolution.

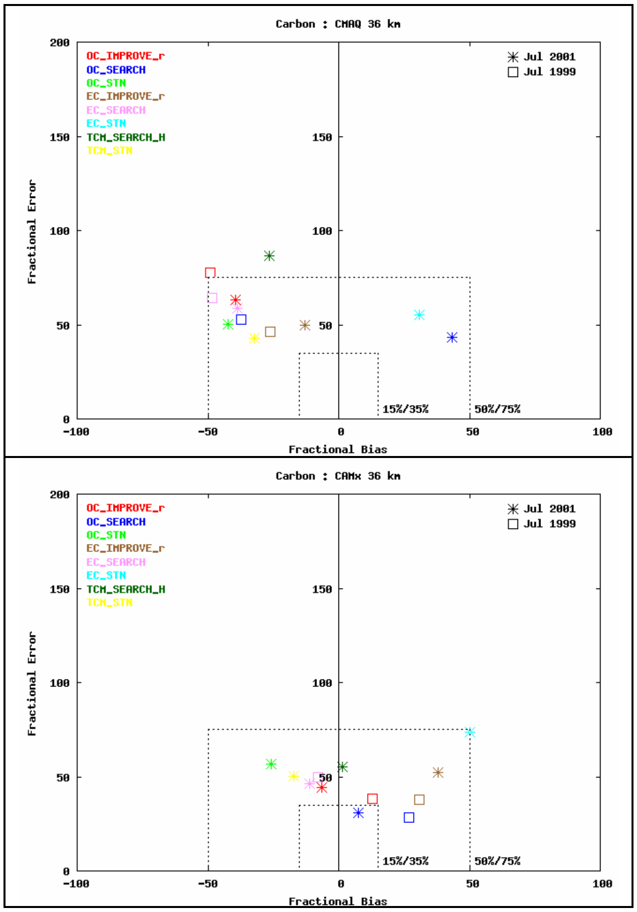

Figure 3. Fractional bias versus error performance statistics for Carbon (EC, OC and TCM) across the various monitoring networks and the July 1999 and July 2001 episodes for the CMAQ (top) and CAMx (bottom) 36 km base case simulations.

6.0 REFERENCES

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ENVIRON, 2004: User's Guide: Comprehensive Air Quality Model with Extensions (CAMx) – Version 4.10s. www.camx.com. August.

Table 2. Summary Fractional Bias (FB) and Fractional Error (FE) performance statistics for the CENRAP states and the July 2001 episode.

Species	Network	Base		CAMx	
		FB(%)	FE (%)	FB(%)	FE (%)
O3	AQS	-28.80	32.00	-10.03	24.86
CO	AQS	-44.15	69.14	NA	
NO2	AQS	17.39	67.98	30.36	67.54
SO2	AQS	9.11	72.77	48.39	72.79
SO4	IMPROVE	7.73	36.93	19.49	45.99
	STN	17.71	28.26	28.23	38.17
	NADP	18.54	65.13	NA	
NO3	IMPROVE	-161.85	161.85	-144.06	161.00
	STN	-83.70	98.65	-21.09	107.51
	NADP	-86.82	95.10	NA	
NH4	IMPROVE	-30.60	41.82	-16.61	49.14
	STN	26.66	36.96	46.63	53.27
	NADP	-28.30	57.42	NA	
OC	IMPROVE	-36.20	62.12	-21.56	45.17
	STN	-57.58	67.42	-31.46	51.79
EC	IMPROVE	-44.77	57.65	-5.74	35.19
	STN	38.75	50.36	52.84	57.96
TCM	STN	-43.77	58.40	-20.67	46.99
CM	IMPROVE	-97.74	103.25	-159.99	160.01
SOIL	IMPROVE	-27.26	76.49	45.94	97.71
	STN	69.63	99.24	115.28	123.31
PM25	IMPROVE	-31.79	41.70	-14.41	40.82
	STN	-9.36	41.94	20.48	45.11
PM10	IMPROVE	-48.86	59.23	-43.88	65.51

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