OPERATIONAL EVALUATION AND MODEL RESPONSE COMPARISON OF CAMX AND CMAQ FOR OZONE AND PM2.5

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1. INTRODUCTION

State Implementation Plans (SIP) for the 8-hr ozone and PM2.5 National Ambient Air Quality Standards (NAAQS) include assessing the impacts of emission control scenarios with 3-D Eulerian photochemical transport models. Several photochemical models, including the Comprehensive Air Quality Model with Extensions (CAMx4) and the Community Multiscale Air Quality Model (CMAQ), treat the physical processes and chemistry that form ozone and PM2.5. Model performance is typically evaluated on an operational basis, which assesses how appropriately the modeling system responds to emissions adjustments. Since the modeled attainment demonstration includes modeling the relative change between current and future year emissions it is important to have confidence that the model will predict ozone and PM2.5 concentrations appropriately when emissions change (US EPA, 2007). One way to increase confidence in appropriate model response is to demonstrate consistency in response among multiple modeling systems.

States will submit SIPs using either or both of these photochemical models to support modeled attainment demonstrations for ozone and annual PM2.5 NAAQS. It is important to understand how each model compares to observations and how similarly each model responds to emissions adjustments when given the same inputs. The response of each modeling system for ozone and PM2.5 may be different given differences in model formulation.

Relative response factors (RRF) for 8-hr ozone were estimated using the summer of 2002 as a baseline period and emissions projected to 2020 as a future year scenario (Strum et al, 2008). Annual PM2.5 relative response factors were estimated using an annual 2002 baseline period and annual projected 2020 emissions scenario. The RRF is defined as the future year concentration divided by the base year concentration. The 2020 future year scenario has much less nitrogen oxides (NO_X) emissions due to reductions in point and mobile sources and less sulfur dioxide (SO_2) emissions due to reductions in point source emissions due to changed in fuel sulfur content (Figure 1). Total VOC emissions are dominated by regional biogenics, but still have reductions in the projected future year due in part to decreases in mobile source emissions.

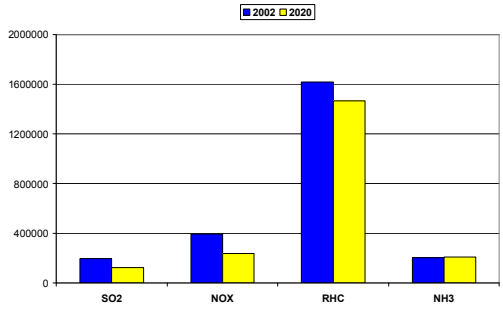

Figure 1. Daily domain total (TPD) emissions for NO_X , SO_2, RHC, and NH3

The operation model performance for each modeling system is compared for ozone and speciated PM2.5. The estimated relative response factors and projected future year concentrations using the standard EPA attainment test are also compared.

2. METHODS

The Comprehensive Air Quality Model with Extensions (CAMx) version 4.50 is a three-dimensional Eularian “one-atmosphere” photochemical transport model. CAMx uses state of the science routines to model ozone and particulate matter formation and removal processes (Nobel et al., 2002; Chen et al., 2003; Baker and Scheff, 2007). CAMx is applied with ISORROPIA inorganic chemistry (Nenes et al., 1998), a semi-

volatile equilibrium scheme to partition condensable organic gases between gas and particle phase (Strader et al., 1999), regional acid deposition model (RADM) aqueous phase chemistry (Chang et al., 1987), and Carbon Bond 05 (CB05) gas-phase chemistry module (ENVIRON, 2008).

The Community Multi-scale Air Quality (CMAQ) model v4.6 is also a state of the science three-dimensional Eularian "one-atmosphere" photochemical transport model (Aiyyer et al, 2007; Byun and Schere, 2006). CMAQ is applied with the AERO4 aerosol module, which includes the ISORROPIA inorganic chemistry (Nenes et al., 1998) and a secondary organic aerosol module based on published research by Odum and Griffin (Odum et al, 1997; Griffin et al, 1999). The CMAQ model is applied with RADM aqueous phase chemistry (Chang et al., 1987) and the CB05 gas-phase chemistry module.

CMAQ and CAMx are applied for the entire calendar year of 2002 and 2020 with the same initial and boundary concentrations, meteorological model output, pollutant emissions, and land-use information. The largest difference in model formulation is the inclusion of additional heterogeneous reactions that form nitric acid in CMAQ which lead to additional PM2.5 nitrate ion when favorable meteorological conditions exist.

All models are applied with a Lambert projection centered at (-97, 40) and true latitudes at 33 and 45. The CAMx modeling domain consists of 216 cells in the X direction and 240 cells in the Y direction covering the central and eastern United States with 12 km^2 grid cells (Fig. 2). The CMAQ modeling domain is similar to the CAMx domain but extends further west (12 km^2 grid cells), with 279 cells in the X direction and 240 cells in the Y direction. Both models resolve the vertical atmosphere up to approximately 15 km above ground level with 14 layers.

CAMx vertical diffusivity coefficients are based on the CMAQ-like vertical diffusivity algorithm to improve model estimation consistency with CMAQ (ENVIRON, 2008). A sensitivity run using the O'Brien 1970 vertical diffusivity algorithm was performed for July 2002 to compare with the CMAQ-like vertical mixing scheme.

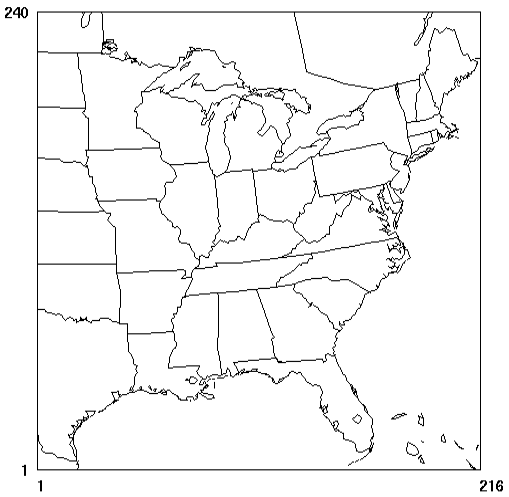

Figure 2. 12 km model domain

The CMAQ-like scheme tends to predict higher mixing heights than the O-Brien 1970 scheme. A landuse-weighted vertical diffusivity coefficient (maximum of 1.0 m^2/s in a completely urban grid cell) is assigned to all grid cells up to approximately 150 meters above ground (model layer 3). This is done to better represent the greater mechanical mixing overnight in urban areas.

Model estimates are compared to observations of ozone and chemically speciated PM2.5 collected during 2002. Ozone data from the AIRS network and speciated PM2.5 data from the IMPROVE and STN networks are used to estimate operational model performance. Metrics used to describe model performance include mean bias, gross error, fractional bias, and fractional error (Boylan et al., 2006). The bias and error metrics describe performance in terms of measured concentration units and the fractional metrics describe performance as a percentage. The best possible performance is when the metrics approach 0. The fractional metrics are bounded by 200%, which is considered very poor performance. All performance metrics include monitors that are common to both the CAMx and CMAQ modeling domains.

Relative response factors are the ratio of the future year predicted concentration divided by the current (or base) year predicted

concentration. These factors are applied to observed design values to estimate a future year design value (FYDV). This future year design value is compared to the National Ambient Air Quality Standards to determine whether a monitor location may show attainment of the Standard in that future year. Relative response factors for 8-hr ozone and annual PM2.5 are estimated using the methods established by the US EPA for modeled attainment demonstrations (US EPA, 2007). The Modeled Attainment Test Software (MATS) software tool was used to calculate both the 8-hr ozone and annual PM2.5 relative response factors (RRF) and projected future year design values (US EPA, 2008).

3. RESULTS & DISCUSSION

3.1 Operational Performance

CMAQ and CAMx 24-hr averaged predictions compared to IMPROVE and STN observations of PM2.5 sulfate ion, nitrate ion, elemental carbon, and organic carbon are shown in Figure 3.

Bias and error metrics are shown in Table 1 along with the coefficient of determination (r^2) and coefficient of variation (CV). The N represents the number of 24-hr samples of that specie used in the analysis over all monitor locations in the modeling domain with valid samples during 2002.

Table 1. CAMx and CMAQ performance metrics by PM2.5 specie

		CAMx			
specie	N	Bias	Error	r^2	CV
$SO4^-$	15,104	0.27	1.50	0.56	58
$NO3^=$	13,929	0.02	0.90	0.46	95
OCM	10,157	-0.31	1.34	0.12	92
EC	14,620	0.26	0.40	0.24	75
$NH4^+$	14,885	0.17	0.68	0.47	58

		CMAQ			
specie	N	Bias	Error	r^2	CV
$SO4^-$	15,104	-0.23	1.23	0.70	48
$NO3^=$	13,929	0.40	1.02	0.53	88
OCM	10,157	-0.83	1.43	0.10	93
EC	14,620	0.19	0.38	0.24	74
$NH4^+$	14,885	0.19	0.63	0.57	52

PM2.5 nitrate ion has a slightly larger over-prediction bias in CMAQ, although the predicted error and strength of relationship is very similar between models. PM2.5 sulfate ion is slightly over-predicted in CAMx and slightly under-predicted in CMAQ. There is a weaker relationship between sulfate predictions and observations with the CAMx modeling system based on r^2 and CV. A visual examination of the entire distribution of sulfate prediction-observation pairs for CAMx and CMAQ indicate that even though the performance metrics differ there is little discernable difference in prediction skill.

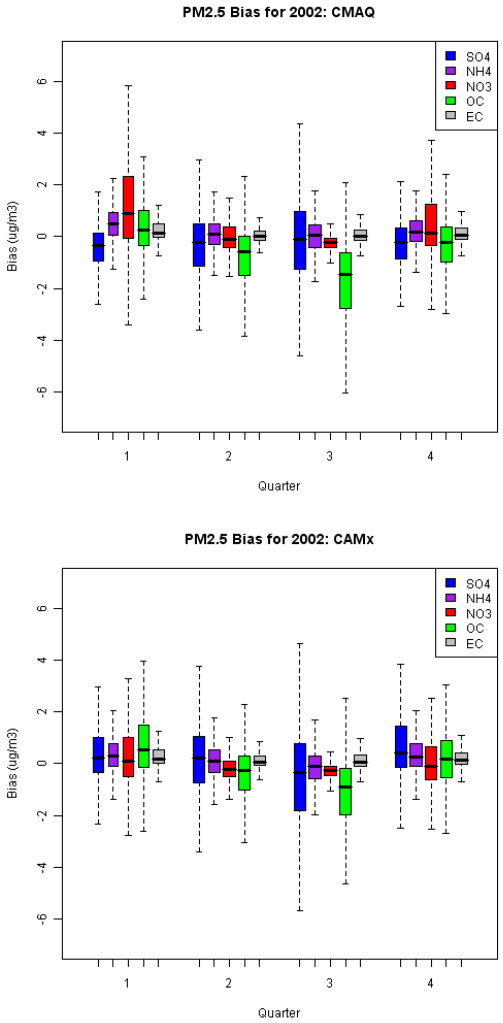

Figure 3. CMAQ (top) and CAMx (bottom) 24-hr average bias for chemically speciated PM2.5

Model estimates for 8-hr maximum ozone are compared to 8-hr ozone observations in Figure 4. This figure includes all valid daily 8-hr ozone maximum observations at

stations in the modeling domain for each day between May and September 2002.

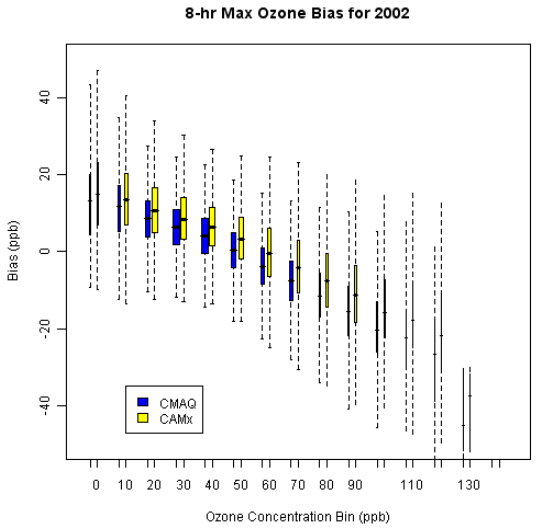

Figure 4. CAMx and CMAQ 8-hr maximum ozone estimates compared to observations.

Ozone performance is shown in Table 2 using the bias and error metrics estimated for various bins of ambient concentrations: less than 65, between 65 and 75, between 75 and 90, and greater than 90 ppb. This separation of ozone by ambient value helps determine how the models perform at concentrations that may be more relevant for regulatory modeling applications.

Table 2. 8-hr ozone metrics (ppb)

		CAMx		CMAQ	
	N	Bias	Error	Bias	Error
obs < 65	87829	7.2	10.1	4.5	7.7
65 => obs < 75	13242	-2.1	9.1	-5.4	8.1
75 => obs < 90	10238	-6.1	10.7	-9.8	11.5
obs > 90	3860	-12.3	14.8	-17.0	17.7

Both modeling systems tend to under-predict the highest ozone measurements and over-predict the lowest measurements. The modeling systems perform best at predicting ozone measurements between 65 to 75 ppb. CAMx tends to predict more ozone than the CMAQ modeling system. Since the same photochemical mechanism (CB05) is used by both models, the differences are most likely due to differences in vertical mixing and photolysis rate attenuation.

3.2 CAMx Vertical Diffusivity Sensitivity Comparison

CAMx model predictions using vertical diffusivity estimates based on O'Brien 1970 (OB70) and CMAQ-like algorithms are compared to observation data for the 12 km July 2002 simulation. The comparison is shown in Table 3 for ozone and for PM2.5 sulfate ion, elemental carbon, and organic carbon. CMAQ estimates are also shown for the same monitors and modeled days.

Table 3. Vertical diffusivity sensitivity simulations compared to observation data

Model & Kv scheme	Specie	N	Bias	Error	r^2
CAMx OB70	$SO4^-$	319	-0.56	1.95	0.86
CAMx CMAQ-like	$SO4^-$	319	-0.65	1.84	0.88
CMAQ	$SO4^-$	319	0.27	1.74	0.89
CAMx OB70	OC	319	-1.90	2.06	0.73
CAMx CMAQ-like	OC	319	-2.17	2.28	0.72
CMAQ	OC	319	-2.55	2.60	0.66
CAMx OB70	EC	319	0.40	0.54	0.40
CAMx CMAQ-like	EC	319	0.32	0.48	0.37
CMAQ	EC	319	0.22	0.42	0.42
CAMx OB70	O3	36478	-11	16	
CAMx CMAQ-like	O3	36478	-15	18	
CMAQ	O3	36478	-15	17	

All three model simulations show similar error (range of 2 ppb) for ozone. The error for PM2.5 sulfate ion has a range of 0.21 ug/m^3 and 0.12 ug/m^3 for elemental carbon. PM2.5 organic carbon error showed the largest range of 0.54 ug/m^3 over the 3 simulations. The model estimates using the O'Brien vertical diffusivity coefficients generally resulted in slightly lower mixing heights and slightly higher estimated concentrations. The similar model performance results for all 3 simulations suggest the vertical mixing schemes result in generally comparable results.

3.3 Model Response Comparison

The relative response factors and projected future year 8-hr ozone design values are shown in Figure 5. The estimates at each monitor location are plotted for each of the models. The variation in relative response factors and future year design values suggest that CAMx and CMAQ respond similarly to emissions adjustments.

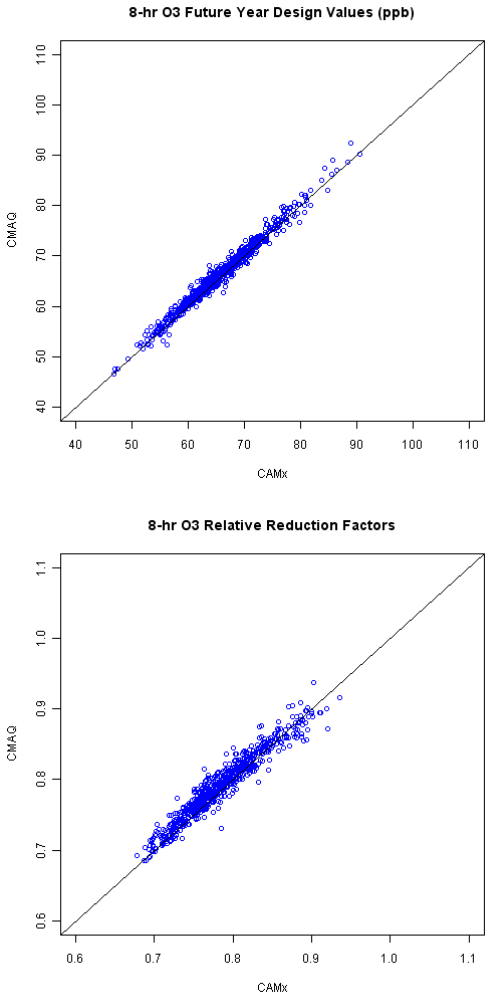

Figure 5. 8-hr ozone future year design values (top) and relative response factors (bottom)

The model-model comparisons for RRFs and future year design values are very consistent for 8-hr ozone. The distribution for RRFs show less association (r^2=.933) compared to the future year design values (r^2=.977). The coefficient of variation is almost identical for both distributions, with the RRFs being 1.49 and the future year design values being 1.52.

The annual PM2.5 future year design values estimated by CAMx and CMAQ are shown in Figure 6.

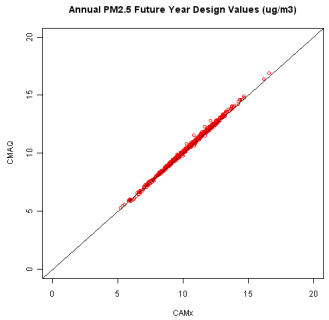

Figure 6. Annual PM2.5 future year design values

Similar to ozone, little variability exists between the annual PM2.5 future year design value estimates of CMAQ and CAMx. The quarterly relative response factors estimated by CAMx and CMAQ are shown in Figure 7 for PM2.5 nitrate, ammonium, sulfate, soil, organic carbon, and elemental carbon.

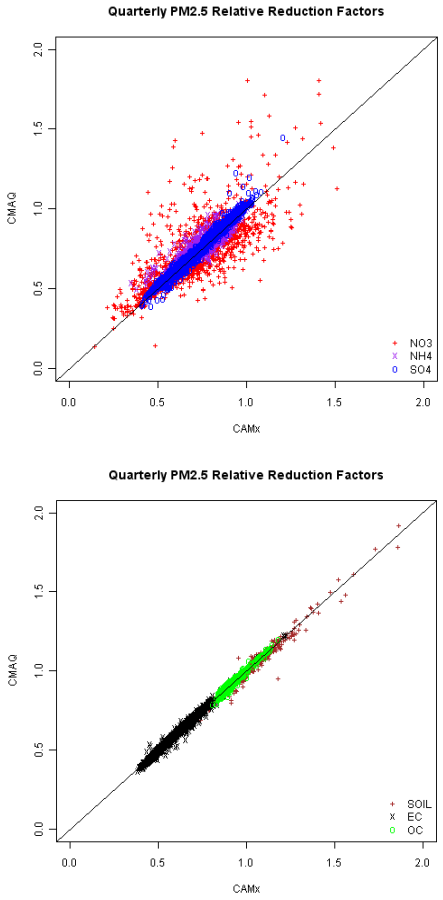

Figure 7. Quarterly PM2.5 RRFs for nitrate, ammonium, sulfate (top) and elemental carbon, organic carbon, and soil (bottom)

There is very little variability between models for estimated RRFs of soil, organic carbon, and elemental carbon. More variability is seen for sulfate and ammonium ions. The most variability is evident in the nitrate ion RRF predictions. Quarterly PM2.5 nitrate ion design values and relative response factors are shown in Figure 8.

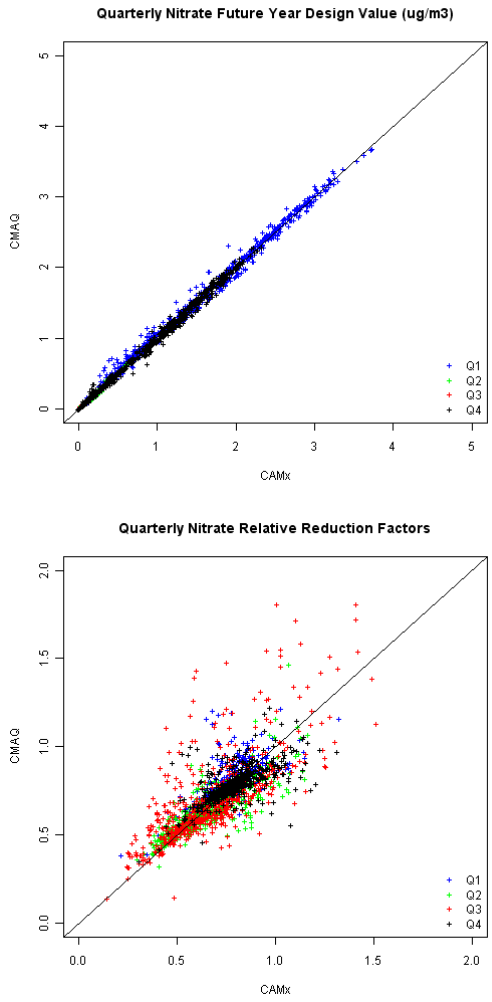

Figure 8. Quarterly PM2.5 nitrate future year design values (top) and relative response factors (bottom)

The results shown in Figure 8 and Table 4 show that the large variability in PM2.5 nitrate RRFs do not translate in large differences in future year design value estimates. Most of the variability in nitrate RRFs occurs in the warmer months when concentrations are very small in the eastern United States, so very small changes to very small concentrations have little impact on estimated future year PM2.5.

Table 4. Relationships between CAMx and CMAQ estimated RRF and FYDV by specie

	RRF		FYDV	
specie	r^2	CV	r^2	CV
$SO4^-$	0.977	2.90	0.985	2.72
$NO3^=$	0.562	15.00	0.997	7.00
$NH4^+$	0.885	3.64	0.992	2.83
OC	0.918	1.13	0.999	1.22
EC	0.988	1.79	0.997	2.00
CRUSTAL	0.975	1.29	0.999	1.29

Most species have very similar CV values for relative response factors and future year design values. The exception again being nitrate, which shows almost a factor of 2 differences in variability about the mean between the RRF and FYDV distributions. The relationships between CMAQ and CAMx predicted RRFs and FYDVs are very strong for all species (all $r^2 > .918$) with the exception of the nitrate and ammonium RRFs which are not as well correlated due to the variability in the small model estimates.

4. CONCLUSION

It is important to develop confidence that CMAQ and CAMx modeling systems will accurately predict ambient concentrations of 8-hr ozone and PM2.5 since they are used to support modeled attainment demonstrations for NAAQS. Appropriate model response to emissions adjustments is also important since modeled attainment demonstrations show the improvement in air quality that results from emission control programs implemented between the current (base) year and future attainment year. Both modeling systems similarly predict 8-hr ozone and daily speciated PM2.5 concentrations. Perhaps more importantly, both modeling systems respond very similarly to changes in emissions pre-cursor species. The relative response factors and future year design values of 8-hr ozone and annual PM2.5 are very similar using both CAMx and CMAQ. This shows that using a difference modeling system should not give a very different predicted future year design value when inputs and key physics options are consistent.

5. REFERENCES

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