COMPARISON OF TWO ANNUAL $PM_{2.5}$ MODELING RESULTS FOR THE SOUTH COAST AIR BASIN

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ABSTRACT

Two air quality models, CAMx and CMAQ, were applied to simulate year 2005 annual $PM_{2.5}$ concentrations in the South Coast Air Basin (Basin) of Los Angeles. Identical input files; emissions, meteorological data, and boundary and initial conditions, were prepared to compare the two modeling results. Speciated $PM_{2.5}$ data measured for the Multiple Air Toxics Exposure Study III (MATES III) during 2005 (Ospital, 2008) were used to evaluate the performance of the CAMx and CMAQ annual modeling results. The two models generally produced similar results. CAMx predicted better than CMAQ for organic carbon, others and $PM_{2.5}$ mass while CMAQ predicted better than CAMx for secondary ammonium, nitrate, and sulfate at every location except the coastal locations of Long Beach and Wilmington. In general, both models tend to overpredict ammonium, nitrate, organic carbon, others, and $PM_{2.5}$ mass.

1. INTRODUCTION

In December 2004, the USEPA designated the Basin as a serious nonattainment area for the $PM_{2.5}$ standards. The nonattainment status became effective on April 5, 2005, and the Basin is required to meet the federal $PM_{2.5}$ standards by April 2015. The Clean Air Act required a $PM_{2.5}$ attainment demonstration plan be submitted no later than April 5, 2008. In response to the CAA, the South Coast Air Quality Management District (District) submitted, as part of the 2007 Air Quality Management Plan (AQMP) (SCAQMD, 2007), a $PM_{2.5}$ State Implementation Plan (SIP) to attain the federal $PM_{2.5}$ standards. CAMx model was selected as the primary modeling platform for the $PM_{2.5}$ and ozone attainment demonstrations presented in the 2007 AQMP. While both CAMx and CMAQ can simulate ozone and $PM_{2.5}$ together in a "one-atmosphere" approach, and recently the CMAQ model is used more widely in the modeling community, familiarity with CAMx emissions processing and overall speed of model simulation focused the District model selection to CAMx. In this paper, the CMAQ model was applied to the same input files used in the CAMx model run and the two simulation results are compared and discussed.

CAMx and CMAQ model performances were evaluated with MATES III $PM_{2.5}$ data for six major chemical components (ammonium, nitrate, sulfate, organic carbon, elemental carbon, and others) and $PM_{2.5}$ mass. A category called "Others" is defined as the difference between the sum of the species and the total $PM_{2.5}$ mass measured on the filter.

2. MODEL INPUT FILES

As shown in Figure 1, the modeling domain is 65 by 40 grid cells of 5km squared grid, and 8 vertical layers. The top of the modeling domain is set to a constant 5,000 m above the ground level for CAMx and 15,674m (10,000 Pa) for CMAQ. The origin of the modeling domain for CAMx is 275 km easting and 3,670 km northing in UTM coordinates and for CMAQ is -130 km and -150 km in Lambert-Conformal coordinates.

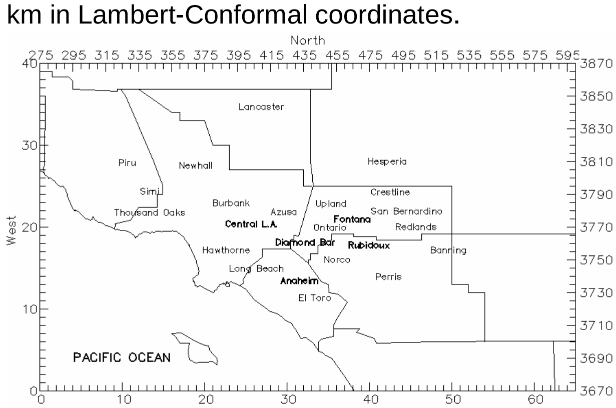

Figure 1. Modeling domain and monitoring stations.

Year 2005 daily emissions are generated using monthly temperature and humidity corrected emissions for a weekday, Saturday and Sunday. Temperature corrected monthly biogenic

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emissions inventory was developed by the California Air Resources Board.

The MM5 meteorological model is used to generate meteorological fields for each day in 2005. The MM5 simulations are initialized from NCEP analyses with a one-day "ramp-up" period and run for 5-day increments without the four-dimensional-data-assimilation (FDDA) option. The same MM5 output files are used to create CAMx and CMAQ meteorological input files.

Initial and monthly boundary condition files are generated from the Western Regional Air Partnership (WRAP) visibility global modeling results in support of the Regional Haze Rule demonstration.

3. MODEL COMPARISON

Although the same input files were used in the simulations, modeling options for the two models were slightly different. Modeling options used for CAMx and CMAQ modeling are summarized in Table 1.

Table 1. Modeling options for CAMx and CMAQ.

	CAMx	CMAQ
Model version	v 4.2	v 4.6
Gas phase chemistry	CB4	CB05
Aqueous chemistry	RADM	RADM
Aerosol chemistry	ISORROPIA	AE4
Secondary organic chem.	SOAP	
Horizontal advection	BOTT	PPM
Vertical advection	BOTT	PPM
Vertical diffusion	Eddy	Eddy
Gas phase chem. solver	CMC	EBI
Aerosol size distribution	2 sec. EFC	3 L-N Modes
Min. vert. diffusivity	0.1 m^2/s	0.1 m^2/s

4. $PM_{2.5}$ AMBIENT DATA

$PM_{2.5}$ sampling was conducted as part of the MATES III program. MATES III is a monitoring and evaluation study to characterize relative Basin carcinogenic risk from exposure to air toxics. Monitoring of toxic air contaminants and speciated $PM_{2.5}$ data were conducted once every 3 days for 24 hours from April 2004 to March 2006 at ten locations in the Basin. At each location, total mass and 43 species were analyzed including ions, organic and elemental carbon, and trace metals. Annual speciated $PM_{2.5}$ data from eight MATES III monitoring sites, including Los Angeles, Anaheim, Burbank, Compton, Fontana, Long Beach, Los Angeles, Rubidoux, and Wilmington, are used in the validation of the model performance. Data from two stations (Huntington Park and Pico Rivera) are not used in the model validation because they have only six months data.

5. MODELING RESULTS AND DISCUSSIONS

The CAMx and CMAQ models were applied to simulate year 2005 annual average $PM_{2.5}$ mass and six major chemical components using the identical emissions, meteorological and boundary conditions described in the preceding section. The $PM_{2.5}$ mass and six chemical components predicted by the two models are compared with the measured $PM_{2.5}$ concentrations.

Two modeling results are summarized side by side in Table 2 that shows commonly used statistics, mean bias, mean error, normalized mean bias and normalized mean error for the six chemical components and $PM_{2.5}$ mass at 8 locations in the Basin.

Model performance is also evaluated by several graphical presentations of error plots, scatter plots and time series plots. Figure 2 presents error plots that show "soccer goal" plots of normalized mean error vs. normalized mean bias for six components and $PM_{2.5}$ mass. Scatter plots provided in Figures 3 through 5 show prediction accuracy between predicted and observed values for each component at three locations (Los Angeles, Rubidoux, and Long Beach). Time series plots (Figures 6 through 8) show differences between predicted concentrations as a continuous solid line and observed concentrations as points for each component at three locations.

As shown in Table 2 and Figures 2 through 8, the CAMx and CMAQ model generally produced almost identical results. However, CAMx predicted better than CMAQ for organic carbon, others and $PM_{2.5}$ mass while CMAQ predicted better than CAMx for secondary ammonium, nitrate, and sulfate at every location except the coastal locations of Long Beach and Wilmington. CMAQ also predicted primary elemental carbon better than CAMx at Fontana, Rubidoux and Wilmington.

In general, both models tend to over-predict ammonium, nitrate, others, and $PM_{2.5}$ mass. Ammonium and nitrate are over-predicted by 1 or 2 $\mu g/m^3$ at most sites for both models. Sulfate is nominally under-predicted for CAMx, however; organic carbon and elemental carbon are well simulated at all stations for both models. Model performance for the others category indicates that an all station average value is over-predicted by 1

Table 1. Summary statistics for CAMX and CMAQ modeling results.

CAMx Results

	Mean Obs	Mean Pred	Mean Bias	Mean Error	Norm Mean Bias	Norm Mean Error
Ammonium						
All station	2.60	4.19	1.59	2.32	0.61	0.90
Anaheim	2.23	3.71	1.48	2.00	0.66	0.90
Burbank	2.77	3.38	0.61	1.79	0.22	0.65
Compton	2.32	4.65	2.33	2.68	1.00	1.16
Fontana	2.95	3.97	1.02	2.29	0.34	0.78
N Long Bea	2.33	4.15	1.82	2.42	0.78	1.04
Los Angele	2.76	4.60	1.83	2.40	0.66	0.87
Rubidoux	3.20	4.74	1.54	2.34	0.48	0.73
Wilmington	2.13	3.89	1.77	2.41	0.83	1.13
Nitrate						
All station	5.35	7.67	2.31	3.98	0.43	0.74
Anaheim	4.55	7.10	2.55	3.50	0.56	0.77
Burbank	5.85	6.49	0.64	3.44	0.11	0.59
Compton	4.46	7.93	3.47	4.12	0.78	0.92
Fontana	6.76	7.65	0.90	4.38	0.13	0.65
N Long Bea	4.04	6.52	2.48	3.38	0.61	0.84
Los Angele	5.81	8.86	3.05	4.39	0.52	0.76
Rubidoux	7.67	9.68	2.01	4.81	0.26	0.63
Wilmington	3.37	5.51	2.14	2.87	0.63	0.85
Sulfate						
All station	3.73	3.29	-0.44	2.03	-0.12	0.55
Anaheim	3.55	2.75	-0.80	1.77	-0.23	0.50
Burbank	3.63	2.21	-1.42	1.92	-0.39	0.53
Compton	3.96	4.09	0.13	2.53	0.03	0.64
Fontana	3.27	2.61	-0.66	1.63	-0.20	0.50
N Long Bea	4.36	4.34	-0.02	2.18	0.00	0.50
Los Angele	3.78	3.17	-0.61	1.94	-0.16	0.51
Rubidoux	3.11	2.65	-0.46	1.59	-0.15	0.51
Wilmington	4.70	4.90	0.20	2.97	0.04	0.63
Organic Carbon						
All station	4.71	4.83	0.12	1.81	0.03	0.38
Anaheim	4.15	4.87	0.71	1.57	0.17	0.38
Burbank	4.73	4.10	-0.63	1.57	-0.13	0.33
Compton	4.20	5.65	1.44	1.80	0.34	0.43
Fontana	4.75	3.98	-0.77	1.71	-0.16	0.36
N Long Bea	4.19	4.88	0.69	1.81	0.17	0.43
Los Angele	4.75	6.03	1.28	1.81	0.27	0.38
Rubidoux	3.99	4.41	0.42	1.34	0.10	0.33
Wilmington	4.35	4.38	0.03	1.55	0.01	0.36
Elemental Carbon						
All station	1.87	1.66	-0.21	0.82	-0.11	0.44
Anaheim	1.43	1.36	-0.08	0.66	-0.05	0.46
Burbank	2.08	1.25	-0.83	1.00	-0.40	0.48
Compton	1.79	2.04	0.24	0.78	0.13	0.44
Fontana	2.17	1.33	-0.84	1.02	-0.39	0.47
N Long Bea	1.44	2.22	0.78	0.91	0.54	0.63
Los Angele	1.97	1.94	-0.02	0.68	-0.01	0.34
Rubidoux	1.71	1.17	-0.54	0.76	-0.32	0.44
Wilmington	2.07	1.93	-0.14	0.80	-0.07	0.39
Others						
All station	3.62	4.73	1.11	2.87	0.31	0.79
Anaheim	3.49	4.82	1.33	2.59	0.38	0.74
Burbank	4.79	3.12	-1.67	2.83	-0.35	0.59
Compton	3.59	5.23	1.65	3.07	0.46	0.86
Fontana	3.15	4.25	1.10	2.22	0.35	0.70
N Long Bea	3.40	5.77	2.36	3.36	0.69	0.99
Los Angele	3.47	4.82	1.35	2.87	0.39	0.83
Rubidoux	3.55	4.78	1.22	2.45	0.34	0.69
Wilmington	3.72	5.46	1.75	3.73	0.47	1.00
PM2.5 Mass						
All station	19.62	26.14	6.52	10.49	0.33	0.53
Anaheim	17.63	24.45	6.81	8.84	0.39	0.50
Burbank	21.94	20.72	-1.22	8.76	-0.06	0.40
Compton	18.83	29.22	10.39	12.24	0.55	0.65
Fontana	21.44	23.42	1.98	9.29	0.09	0.43
N Long Bea	17.43	27.84	10.41	11.22	0.60	0.64
Los Angele	19.15	29.38	10.23	12.47	0.53	0.65
Rubidoux	21.85	27.05	5.21	10.32	0.24	0.47
Wilmington	18.35	25.33	6.98	10.02	0.38	0.55

CMAQ Results

	Mean Obs	Mean Pred	Mean Bias	Mean Error	Norm Mean Bias	Norm Mean Error
Ammonium						
All station	2.60	3.89	1.29	2.13	0.50	0.82
Anaheim	2.23	3.44	1.21	1.83	0.54	0.82
Burbank	2.77	2.78	0.01	1.66	0.00	0.60
Compton	2.32	4.13	1.81	2.34	0.78	1.01
Fontana	2.95	3.60	0.65	1.98	0.22	0.67
N Long Bea	2.33	4.22	1.90	2.37	0.82	1.02
Los Angele	2.76	4.26	1.50	2.22	0.54	0.80
Rubidoux	3.20	4.43	1.23	2.21	0.39	0.69
Wilmington	2.13	4.04	1.91	2.37	0.90	1.11
Nitrate						
All station	5.35	7.40	2.05	3.84	0.38	0.72
Anaheim	4.55	7.03	2.48	3.57	0.55	0.78
Burbank	5.85	5.57	-0.29	3.30	-0.05	0.56
Compton	4.46	7.30	2.84	3.63	0.64	0.81
Fontana	6.76	7.43	0.68	4.19	0.10	0.62
N Long Bea	4.04	6.52	2.49	3.05	0.62	0.75
Los Angele	5.81	8.38	2.57	4.20	0.44	0.72
Rubidoux	7.67	9.80	2.13	4.91	0.28	0.64
Wilmington	3.37	5.98	2.61	3.13	0.78	0.93
Sulfate						
All station	3.73	4.07	0.34	2.11	0.09	0.57
Anaheim	3.55	3.34	-0.21	1.60	-0.06	0.45
Burbank	3.63	2.54	-1.09	1.74	-0.30	0.48
Compton	3.96	4.92	0.96	2.79	0.24	0.71
Fontana	3.27	3.21	-0.06	1.52	-0.02	0.47
N Long Bea	4.36	5.56	1.20	2.75	0.28	0.63
Los Angele	3.78	4.29	0.51	2.12	0.14	0.56
Rubidoux	3.11	3.34	0.23	1.38	0.07	0.44
Wilmington	4.70	5.82	1.11	3.27	0.24	0.70
Organic Carbon						
All station	4.71	5.07	0.36	2.02	0.08	0.43
Anaheim	4.15	5.21	1.05	1.80	0.25	0.43
Burbank	4.73	3.68	-1.06	1.73	-0.22	0.37
Compton	4.20	6.06	1.86	2.15	0.44	0.51
Fontana	4.75	4.00	-0.76	1.89	-0.16	0.40
N Long Bea	4.19	4.93	0.73	1.85	0.18	0.44
Los Angele	4.75	7.06	2.31	2.64	0.49	0.56
Rubidoux	3.99	4.48	0.50	1.43	0.12	0.36
Wilmington	4.35	4.64	0.29	1.69	0.07	0.39
Elemental Carbon						
All station	1.87	1.81	-0.06	0.82	-0.03	0.44
Anaheim	1.43	1.52	0.09	0.63	0.06	0.44
Burbank	2.08	1.20	-0.88	1.03	-0.42	0.49
Compton	1.79	2.25	0.45	0.84	0.25	0.47
Fontana	2.17	1.39	-0.78	0.99	-0.36	0.46
N Long Bea	1.44	2.26	0.82	0.95	0.57	0.66
Los Angele	1.97	2.33	0.37	0.70	0.19	0.35
Rubidoux	1.71	1.27	-0.44	0.68	-0.26	0.40
Wilmington	2.07	2.14	0.08	0.84	0.04	0.40
Others						
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Burbank	4.79	2.95	-1.84	2.94	-0.38	0.61
Compton	3.59	5.83	2.25	3.52	0.63	0.98
Fontana	3.15	4.51	1.36	2.45	0.43	0.78
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Burbank	21.94	18.77	-3.17	9.19	-0.14	0.42
Compton	18.83	30.09	11.26	13.31	0.60	0.71
Fontana	21.44	23.70	2.26	9.13	0.11	0.43
N Long Bea	17.43	29.47	12.03	12.87	0.69	0.74
Los Angele	19.15	32.32	13.18	14.68	0.69	0.77
Rubidoux	21.85	28.15	6.30	10.91	0.29	0.50
Wilmington	18.35	27.76	9.41	11.58	0.51	0.63

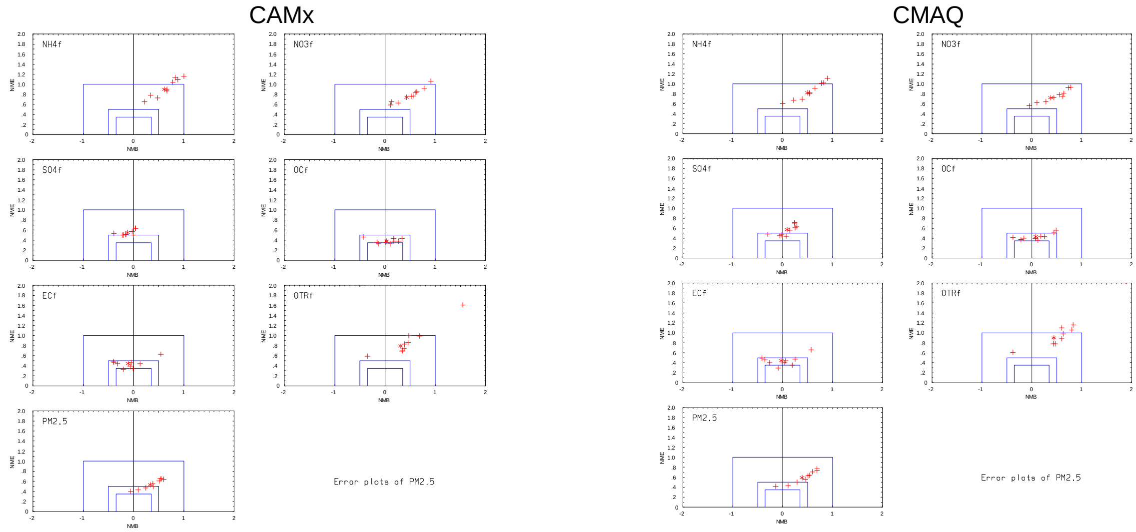

Figure 2. Error plots for CAMx and CMAQ modeling results.

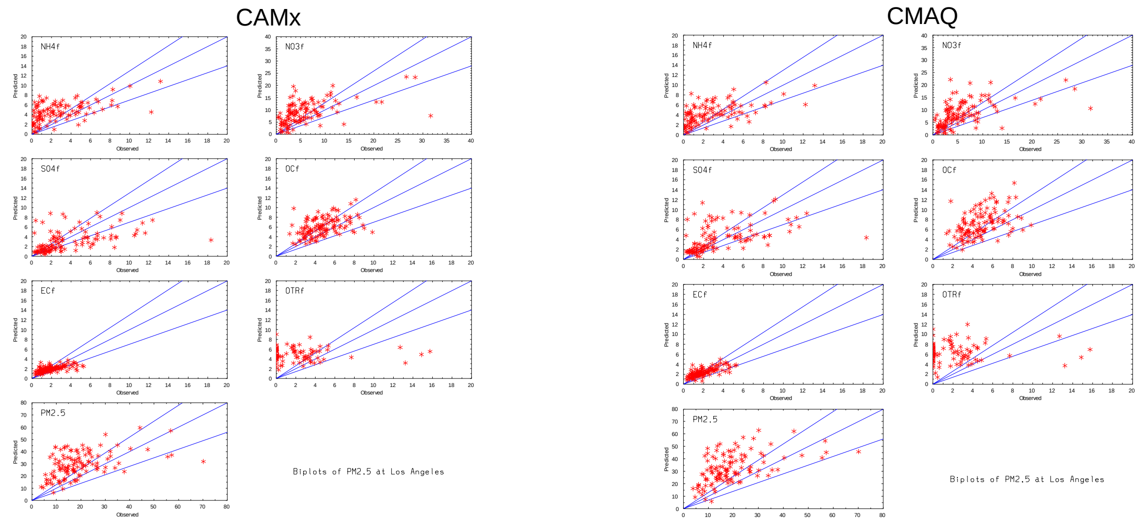

Figure 3. Scatter plots for CAMx and CMAQ at Los Angeles

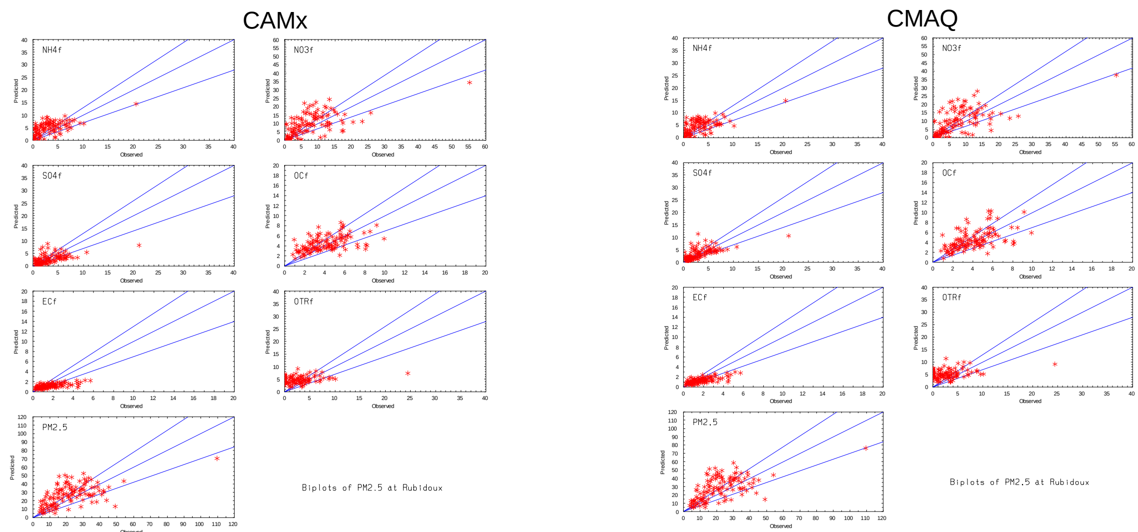

Figure 4. Scatter plots for CAMx and CMAQ at Rubidoux.

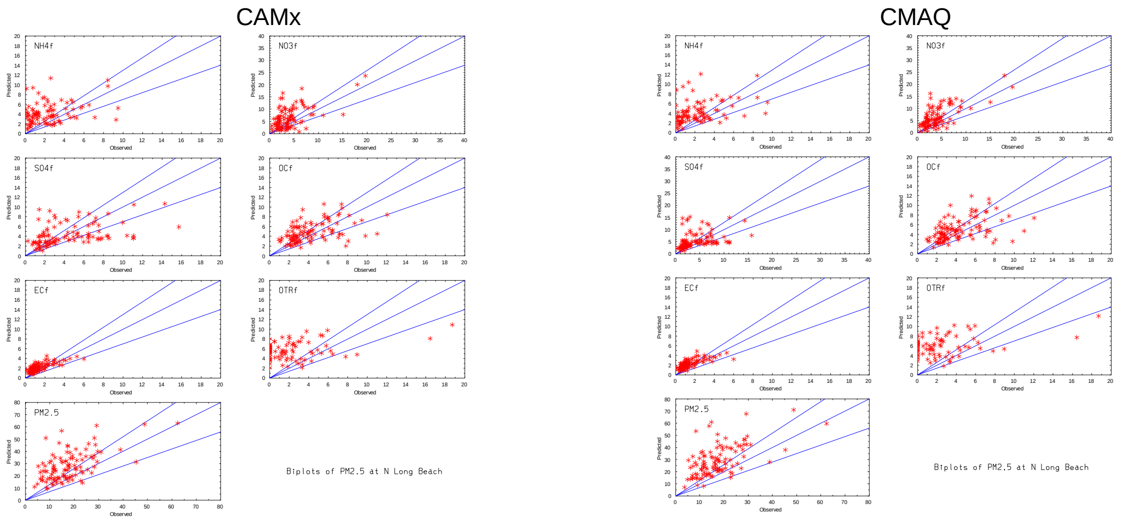

Figure 5. Scatter plots for CAMx and CMAQ at Long Beach.

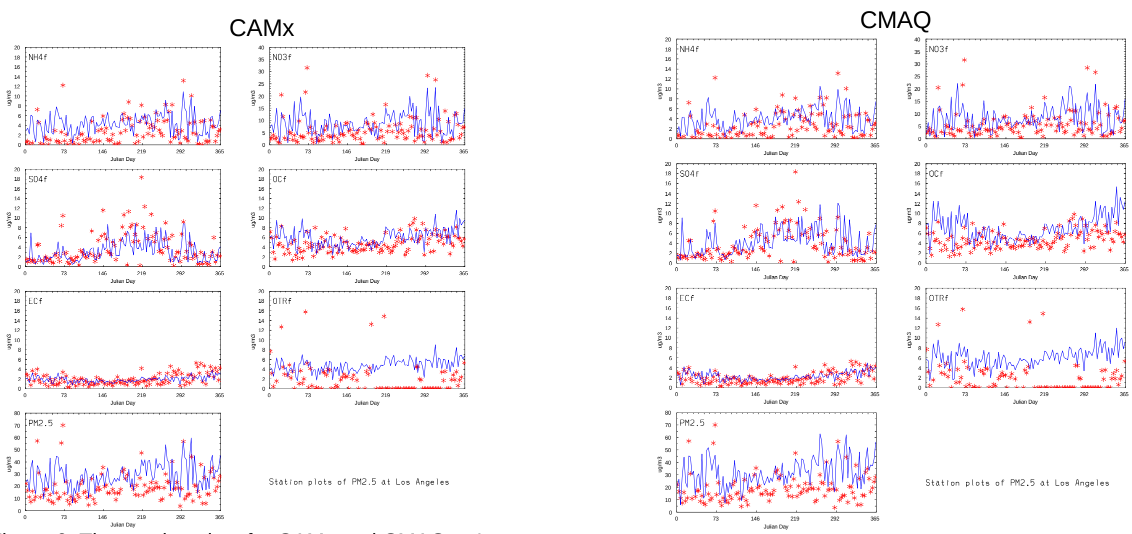

Figure 6. Time series plots for CAMx and CMAQ at Los Angeles.

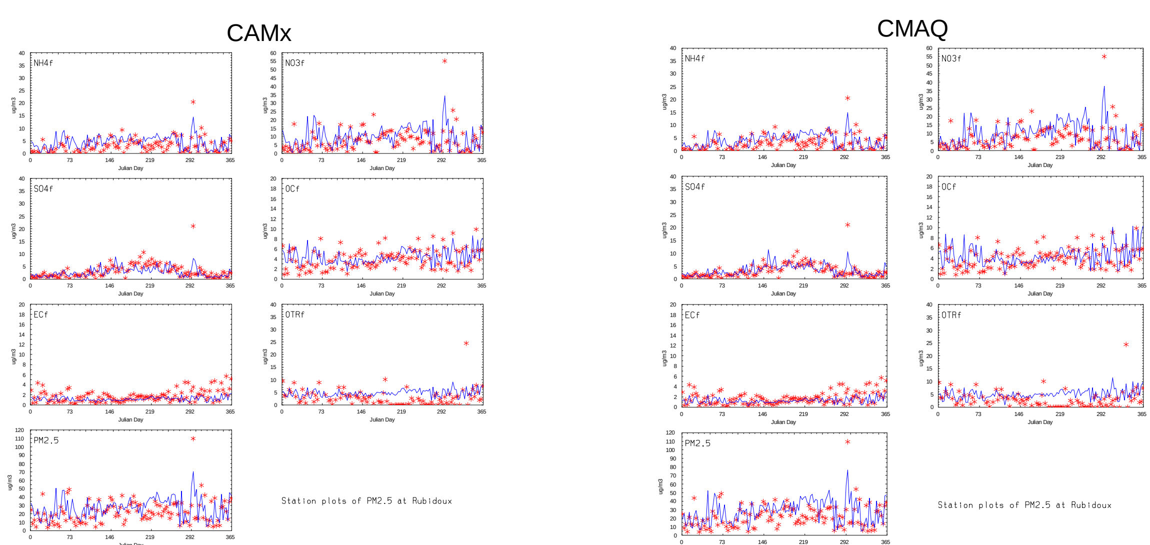

Figure 7. Time series plots for CAMx and CMAQ at Rubidoux.

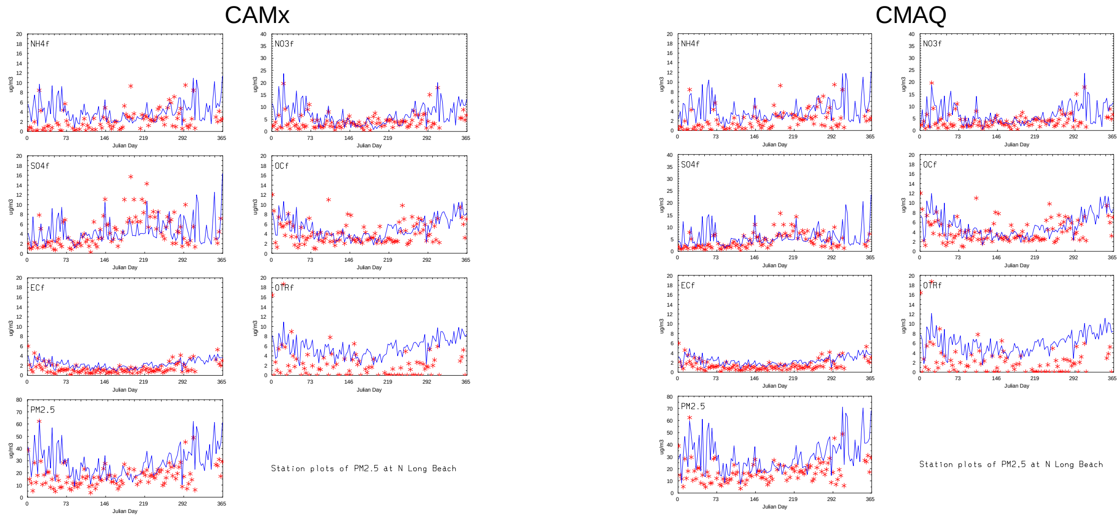

Figure 8. Time series plots for CAMx and CMAQ at Long Beach.

µg/m^3 above the observation for CAMx and 1.6 µg/m^3 for CMAQ. Overall, the over-prediction for ammonium, nitrate and the others resulted in an over-prediction of $PM_{2.5}$ mass for both models.

The performance statistics summarized in Table 2 and Figure 2 show that normalized mean errors are between 50 and 100 percent error for ammonium, nitrate, and others category. Normalized mean errors are near 50 percent for sulfate and between 30 and 50 percent for organic carbon and elemental carbon. Normalized errors for $PM_{2.5}$ mass are between 30 and 75 percent. Percent errors for others category may reflect uncertainties in the fugitive dust emissions inventory. Further efforts need to be focused on improving model performance for all components of $PM_{2.5}$, especially secondary nitrate particles.

6. SUMMARY AND CONCLUSIONS

Two widely used models, CAMx and CMAQ, were applied to the same input files and the simulation results are compared. CAMx and CMAQ models produced similar results. In general, both models tend to over-predict ammonium, nitrate, organic carbon, others, and resulted in an over-prediction of $PM_{2.5}$ mass. CAMx predicted better than CMAQ for organic carbon, others and $PM_{2.5}$ mass while CMAQ predicted better than CAMx for secondary ammonium, nitrate, and sulfate at every location except the coastal locations of Long Beach and Wilmington.

Simulation with CAMx model is about 2 times faster than CMAQ. CAMx modeling on a Xeon computer with one CPU takes ~3 days for a one-year simulation while CMAQ takes ~7 days.

REFERENCES

Ospital J.; Cassmassi J.; Chico T. Multiple Air Toxics Exposure Study in the South Coast Air Basin (MATES III), Draft Final Report; South Coast Air Quality Management District, Diamond Bar, CA. July, 2008.

SCAQMD. 2007 Air Quality Management Plan. Appendix V: Modeling and attainment demonstrations, South Coast Air Quality Management District, Diamond Bar, California, 2007.