COMPARISON OF WRF/CAMx AND MM5/CAMx SIMULATIONS FOR AN OZONE EPISODE IN CALIFORNIA

Su-Tzai Soong^{1*}, Philip T. Martien¹, Cristina L. Archer¹, Saffet Tanrikulu¹, Jian-Wen Bao², James M. Wilczak², Sara A. Michelson², Yiqin Jia³ and Chris Emery³

¹ Bay Area Air Quality Management District San Francisco, California 94109

²NOAA/PSD, Boulder, CO 80305

³ ENVIRON International Corporation Novato, California 94945

1. Introduction

Ozone concentrations frequently exceed the federal and California State standards in central California. Over the past twenty years, a number of comprehensive field studies have been conducted to support data analysis and photochemical modeling to better understand the chemical and physical dynamics of ozone formation in the region. One of the modeling systems that has been used extensively relies on the Penn State/NCAR mesoscale model (MM5; Grell et al., 1994) to simulate meteorology and the Comprehensive Air quality Model with extensions (CAMx; Environ 2004) to simulate the photochemical production of ozone. Recently, MM5 was applied to simulate episodic conditions captured during the 2000 Central California Ozone Study (CCOS) and extensively evaluated with the comprehensive meteorological measurements of CCOS at the surface and in aloft layers (Wilczak et al., 2004, hereafter W04). However, NCAR has decided to discontinue future development of MM5 in favor of a new model, the Weather Research and Forecast (WRF) model (Skamarock et al., 2005), thereby prompting our interest in the applications of WRF in central California.

Wilczak et al., in W04, simulated meteorology using MM5 for a multi-day ozone episode (31 July -2 August, 2000) over the CCOS domain. Bao and Michelson (2005, hereafter BM05) also simulated meteorology using WRF over the same period and domain, and they compared the WRF results against the MM5 results.

The purpose of this present study is to compare the CAMx simulations and its ozone performance using the meteorological fields described in W04 and BM05. The results of this study may provide guidance in selecting a meteorological model to prepare inputs to CAMx for upcoming 8-hour attainment demonstration modeling.

As part of this study, we developed a WRF to CAMx model interface (WRFCAMx), which converts the WRF outputs to CAMx-ready meteorological inputs. The resultant fields from WRFCAMx are dynamically consistent, similar to those generated using the previously available MM5 to CAMx interface (MM5CAMx).

2. Ozone observations

During the July-August 2000 episode, ozone exceeded the federal standards in three major regions of the study area: the San Francisco Bay area (SFB), Sacramento area (SAC) and the San Joaquin Valley (SJV). The SFB region includes the cities of San Francisco and Livermore shown in Fig.1; the SAC region includes Sacramento and Sloughhouse; and the SJV region includes Modesto and Turlock in the north, Fresno in the center, and Bakersfield and Edison in the south.

In this paper, we focus on the 1-hour average ozone, as opposed to an 8-hour average ozone. The 1-hour average reveals more temporal variability and greater extremes, and allows for more contrast in model comparisons.

Ozone concentrations first exceeded the 1-hour standard (124 ppb) on July 31 in SFB at Livermore, where ozone peaked at 126 ppb (Table 1). We refer to this day as the SFB exceedance day. On August 1, peak ozone shifted to the SAC region, where ozone reached 133 ppb at Sloughhouse. We refer to this day as the SAC exceedance day. On August 2, peak ozone was observed in SJV, where the 1-hour standard was exceeded at Modesto and Turlock, which both reached 131 ppb, and at Edison, which peaked at 151 ppb. We refer to this day as the SJV exceedance day.

3. The MM5 and WRF simulations

Wilczak et al. (2004) conducted three simulations of meteorology of the July-August 2000 episode with the purpose of improving MM5's performance. All three simulations used a triple-nested domain telescoping down from 36, to 12 and to 4 km grid resolution. The

J1.4

^{*}*Corresponding Author Address*: Su-Tzai Soong, Bay Area Air Quality Management District, 939 Ellis Street, San Francisco, CA 94109; e-mail ssoong@baaqmd.gov.

Table 1. The observed ozone (ppb) from July 31 to August 2, 2000 at stations with 1-hour ozone exceedance.

Day	7/31/2000						
Hour	12	13	14	15	16	17	18
SF Bay Area							
Livermore - Old	68	88	116	123	126	73	53
Sacramento							
Sloughhouse		100	92	87	78	74	66
San Joaquin							
Edison	115	110	106	94	81	74	38
Turlock	75	91	104	105	96	88	64
Modesto -14th	74	87	94	90	84	81	60

Day	8/1/2000						
Hour	12	13	14	15	16	17	18
SF Bay Area							
Livermore - Old	73	86	92	81	68	65	52
Sacramento							
Sloughhouse	88	112	133	126	119	112	95
San Joaquin							
Edison	113	109	93	102	102	96	83
Turlock	100	101	97	104	86	85	73
Modesto -14th	80	84	99	87	94	91	70

Day	8/2/2000						
Hour	12	13	14	15	16	17	18
SF Bay Area							
Livermore - Old	88	93	98	84	69	57	49
Sacramento							
Sloughhouse	98	102	101	103	98	66	77
San Joaquin							
Edison	129	151	139	121	76	51	45
Turlock	98	95	114	117	116	131	106
Modesto -14th	90	94	95	113	131	128	85

area covered with the 4 km domain is the same as the CCOS field study domain as shown in Fig. 1.

The differences among these three simulations included differences in the use of soil and land surface parameters and in the use of Four Dimensional Data Assimilation (FDDA). Run 1 of W04 used the 5-layer soil model without FDDA; run 2 used the Noah land surface model without FDDA; and run 3 used the Noah land surface model with FDDA. The results of runs 2 and 3 were similar, but run 3 clearly performed the best.

Bao and Michelson (2005) simulated meteorology of the same CCOS period with WRF. The settings of WRF were similar to MM5's settings. To be consistent, they compared the results of WRF against the run 2 of MM5 (without FDDA) rather than run 3 because the version of WRF used in BM05 did not have an FDDA option.

In this study, we applied CAMx with the best performing meteorology from both models. Therefore, we used the results of WRF and run 3 of MM5 to generate the meteorological fields for the CAMx simulations.

Since the details of the MM5 simulations were given in W04 and the details of the WRF simulation will be presented at this conference by Michelson and Bao (2006), here we only briefly summarize the highlights of the two simulations relevant to air quality model applications.

- Both the MM5 and the WRF models simulated daytime surface temperatures and their spatial distributions reasonably well in the Central Valley, where the simulated and observed afternoon high temperatures were between 35C and 40C.
- In coastal areas, both models overestimated temperature by about 5C from the coast line to about 30 km inland..
- In the inland areas of the SFB region, the temperatures were underestimated by both models, especially in the valleys.
- The WRF model consistently overestimated nighttime temperatures by about 5C.
- Both models overestimated the wind speed in the SFB and the SAC regions.
- In the Central Valley, both models predicted wind speeds reasonably well.
- Since no FDDA was applied in the WRF simulation, the wind direction produced by WRF in the Central Valley did not agree with observations from time to time, especially in the afternoon hours.

The bias, root mean square error (RMSE) and the correlation coefficient calculated for the MM5 and WRF models for surface temperature and wind are presented in Table 2. These parameters were calculated for the period from July 31 to August 2, 2000. The RMSE of the temperature for MM5 is much larger than the bias, suggesting there is little systematic error. For the WRF model, both RMSE and the bias were large, mostly due to the WRF's overestimate of nighttime temperatures. Despite the WRF's temperature overestimation, both models produced high temperature correlation coefficients.

Both the bias and the RMSE calculated for the WRF winds were larger than those for MM5. This was expected since FDDA was used in the MM5 model. The correlation coefficients of wind for the MM5 were about 0.6. The correlation coefficients of wind for the WRF model were much lower, between about 0.1 and 0.35. As mentioned above, from time to time, the WRF model was unable to reproduce wind direction in

the San Joaquin Valley, which may have contributed to the low correlation coefficients.

Table 2. The bias, root mean square error and the correlation coefficient of the MM5 and WRF simulated surface temperatures and the u and v components of the wind for July 31 to August 2, 2000, in San Francisco Bay (SFB), Sacramento (SAC), central San Joaquin Valley (C SJV) and southern San Joaquin Valley (S SJV) areas.

Area	Temperature							
		MM5		WRF				
	Bias	RMSE	Corr	Bias	RMSE	Corr		
SFB	0.45	2.48	0.93	3.05	3.74	0.93		
SAC	-0.57	1.97	0.98	2.62	3.15	0.93		
C SVJ	-0.30	1.92	0.97	1.32	2.49	0.92		
S SJV	-0.75	2.05	0.95	0.81	2.70	0.89		
		U-Wind						
		MM5			WRF			
	Bias	RMSE	Corr	Bias	RMSE	Corr		
SFB	0.01	1.30	0.45	0.26	1.70	0.27		
SAC	-0.08	1.06	0.62	0.25	1.46	0.36		
C SVJ	0.16	0.99	0.65	0.24	1.51	0.18		
S SJV	0.02	1.10	0.62	0.19	1.40	0.42		
	V-Wind							
	MM5			WRF				
	Bias	RMSE	Corr	Bias	RMSE	Corr		
SFB	0.15	1.16	0.45	-0.24	1.55	0.16		
SAC	-0.06	0.95	0.52	-1.03	1.67	0.17		
C SVJ	-0.12	1.04	0.53	-0.34	1.49	0.24		
S SJV	-0.05	1.01	0.55	-0.02	1.26	0.41		

4. The WRFCAMx program

The hourly outputs of MM5 and WRF need to be processed to provide meteorological inputs to CAMx. An interface program between MM5 and CAMx, MM5CAMx, already exists. As part of this study, we developed an interface between WRF and CAMx. The differences in the structure of MM5 and WRF were considered during this development as highlighted below: the MM5 uses sigma-z vertical coordinates and the Arakawa B grid. The vertical layer thicknesses in MM5 are fixed in time. The Arakawa B grid places the u and v wind components at the corners of a grid square. In contrast, the WRF model uses the sigma-p vertical coordinates and the Arakawa C grid. The vertical layer thicknesses can change in time. The Arakawa C grid places the u and v wind components at the center of the edges of a grid square.

In CAMx, the vertical layer thicknesses may also be time dependent; therefore, the time dependent vertical layer thicknesses obtained from WRF are directly used in CAMx. In addition, CAMx uses the Arakawa C grid; therefore, no wind interpolation is needed from WRF to CAMx. Both MM5CAMx and WRFCAMx include two options for computing vertical diffusivity. One method uses the O'Brien Scheme (O'Brien, 1970); the other uses turbulent kinetic energy (TKE). However, the current standard output of WRF does not include TKE. The WRF model codes need to be modified to include TKE in the output in order to use this second option.

5. CAMx simulations

The July-August 2000 episode was simulated using CAMx with identical emissions and initial and boundary conditions, but two different meteorological inputs: one generated using MM5 and the other using WRF. Here, the CAMx run using MM5's output is referred to as the MM5/CAMx run, while the CAMx run using the WRF's output is called the WRF/CAMx run. The simulated ozone distributions of the MM5/CAMx and WRF/CAMx runs for selected hours on July 31 to August 2 are presented in Figs. 2-7.

For July 31, the SFB exceedance day, the predicted peak ozone distributions from the MM5/CAMx and WRF/CAMx runs were similar. In the San Francisco Bay area, both MM5/CAMx and WRF/CAMx runs predicted peak ozone in the eastern portions of SFB, in Contra Costa and Alameda Counties. The highest observed ozone on this day was at Livermore, slightly to the west of the simulated peak.

On August 1, the SAC exceedance day, the predicted ozone distributions from MM5/CAMx and WRF/CAMx runs were mostly similar in the Central Valley. However, there were some differences in the locations of the predicted peak ozone in and around SAC. The MM5/CAMx run predicted peak ozone east of Sacramento while the WRF/CAMx run predicted it toward the northeast of Sacramento. Further analysis showed that the distribution of peak ozone generated by the MM5/CAMx run was in better agreement with observations. In the SFB region, both runs overpredicted ozone.

On August 2, the SJV exceedance day, the predicted peak ozone distributions from the MM5/CAMx and WRF/CAMx runs were quite different. The WRF/CAMx simulation accurately predicted the peak ozone (131 ppb) near Modesto, as shown in Table 1. The WRF/CAMx run also predicted more ozone than the MM5/CAMx run in the southern SJV near Bakersfield. This is an improvement over the MM5/CAMx run, but the magnitude of the predicted peak was still below the observed peak of 151 ppb at Edison. However, the WRF/CAMx run predicted a large area of high ozone around SFB, which was not observed.

Scatter plots of the observed versus simulated ozone are presented in Figs. 8-15. These figures plot simulated and observed ozone pairs at the location of the observation stations and may not reveal the simulated maximum ozone in a given area. In these figures, the red line represents the 1:1 line, while the green line plots the best linear fit.

For July 31, the SFB exceedance day, the scatter plots shown are for SFB only. Both the MM5/CAMx and WRF/CAMx runs tend to overpredict ozone in the low- and mid-range (below 100 ppb) of the observed ozone. MM5/CAMx provides a slightly better prediction of maximum ozone in a paired comparison. In an unpaired comparison, however, both runs predicted peak ozone close to the observed values.

For August 1, the scatter plots shown are for the SAC region. The scatter plot of the MM5/CAMx run shows uniform scattering around the diagonal line. The simulated and observed peak ozone also fall on the diagonal line, indicating good agreement between simulations and observations. For the WRF/CAMx run, there is an obvious overprediction of ozone at locations with very low observed concentrations. This may be due to the overprediction of nighttime temperatures in WRF, resulting in nighttime unstable air which inhibits the scavenging of ozone by NO. There is also more scatter in the high ozone range, which may be due to an inaccurate simulation of the location of the predicted peak.

For August 2, the scatter plots are presented for the central and southern SJV. For the central SJV, the WRF/CMAx run seems to perform better for predicting peak ozone. Again, both runs overpredicted ozone in the low observed range. The scatter plots for the southern SJV for the MM5/CAMx and WRF/CAMx runs were very similar in this paired comparison. In an unpaired comparison, the WRF/CAMx run generated more ozone in this area, in better agreement with observations.

Figs. 16-19 show the comparison of the unpaired peak performance accuracy (UPPA), the normalized bias and the normalized error between the MM5/CAMx and the WRF/CAMx runs. The 15%, 20% and 35% lines on these figures indicate the EPA performance guidelines for the UPPA, normalized bias, and normalized error, respectively.

In the SFB region, both MM5/CAMx and WRF/CAMx predicted peak ozone within a few ppb of the observed maximum on July 31. The WRF/CAMx run produced smaller normalized bias and error than the MM5/CAMx run. The MM5/CAMx actually failed the EPA limit on the normalized bias. On August 1 and 2, when the observed ozone was low in the SFB area, the MM5/CAMx performance was better than that of WRF/CAMx.

In the SAC region, both models produced good UPPA statistics on all three days. For August 1, WRF/CAMx did slightly better for all three performance measures. The performance of the two models for the other two days is comparable, but the WRF/CAMx did not meet the normalized bias guideline on August 2.

In the central SJV, both models produced statistics that marginally met most performance guidelines. However, for the southern SJV area, both models performed poorly on August 2. This case may be hard to predict since the area of peak observed ozone was apparently limited to one localized region near Edison.

6. Conclusions

In this study, the performance of the MM5 and WRF models was evaluated for an ozone episode in central California from July 31 to August 2, 2000. Both models simulated the wind and daytime temperatures quite well. In the SFB region, both models overestimated the temperature along the coast by about 5C and underestimated it in the Bay Area inland valleys by 3-5C. One shortcoming of the WRF model is the overprediction of the nighttime temperatures, which were about 5C too warm in most areas.

Two CAMx simulations were performed using identical emissions, and initial and boundary conditions. One of them used meteorological output from MM5 and the other from WRF. The MM5CAMx program already exists to convert MM5's output to the CAMx-ready meteorological input. A WRFCAMx program was developed to generate CAMx-ready meteorological inputs from the WRF outputs. Both MM5/CAMx and WRF/CAMx runs performed similarly for the ozone prediction in the SFB area on July 31. The simulated peak ozone near Livermore was close to the observed value.

The MM5/CAMx performed well in simulating ozone in the Sacramento area on August 1. However, the WRF/CAMx did better on each of three statistical measures: UPPA, the normalized bias and the normalized error. Since the area of high ozone simulated by WRF/CAMx for this day was slightly to the northeast of the observed location near Sacramento, it degraded the performance, as determined from paired scatter plot comparisons.

WRF/CAMx did better in SJV on August 2. It produced high ozone near Modesto, in better agreement with observations. Near Bakersfield, both MM5/CAMx and WRF/CAMx underestimated peak ozone but the predicted peak from WRF/CAMx was higher and closer to the observed peak location.

In general, this initial application of the WRF model produced meteorological predictions similar to those produced by MM5. The subsequent CAMx application also produced acceptable ozone statistics. The overall performance of MM5/CAMx and WRF/CAMx is similar, even though no FDDA is used in the WRF model. With the future improvement planned for the WRF model, including the implementation of the FDDA option, the WRF model appears to have good potential to be used in air quality studies in California.

Acknowledgement

We gratefully acknowledge the computer support provided by the Scientific Computing Division of NCAR.

References

Bao, J.-W. and S. A. Michelson: 2005: Comparison of WRF and MM5 simulations for air-quality applications. *15th MM5 Users' Workshop*, NCAR, June 27-30, 2005. P3.2.

ENVIRON, 2004: Comprehensive air quality model with extensions (CAMx), version 4.10s. User's guide, ENVIRON International Corporation, Novato, CA, 120 pp.

Grell, G.A., J. Dudhia and D.R. Stauffer, 1994: A description of the fifth-generation Penn State/NCAR mesoscale model (MM5) NCAR Technical Note, NCAR/TN-398+STR, 122 pp.

Michelson, S. A. and J.-W. Bao, 2006: Comparison of two meteorological community models for air-quality applications. 14th Joint Conference on the Applications of Air Pollution Meteorology with the Air and Waste Management Association, Amer. Meteo. Soc, J2.7

O'Brien, J.J, 1970: A note on the vertical structure of the eddy exchange coefficient in the planetary boundary layer. *J. Atmos. Sci.* 31, 1213-1215.

Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, D. M. Barker, W. Wang, and J. G. Powers, 2005: A description of the advanced research WRF version 2. NCAR/TN-468+STR, 88 pp.

Soong, S.-T., S. Tanrikulu, J. M. Wilczak, J.-W. Bao, P. T. Martien, and S. A. Michelson, 2004: Simulations of an ozone episode during the Central California Ozone Study. Part II: CAMx air quality model simulations. 13th Conference on the Applications of Air Pollution Meteorology, Amer. Meteor. Soc., J2.2.

Wilczak, J. M., J.-W. Bao, S. A. Michelson, S. Tanrikulu, and S.-T. Soong, 2004: Simulations of an ozone episode during the Central California Ozone Study. Part I: MM5 meteorological model simulations. 13th Conference on the Applications of Air Pollution Meteorology, Amer, Meteor. Sco., J.2.1.



Fig 1. Color shaded areas plot the regions referenced in Table 1. Red dots indicate the locations of selected ozone stations.



Fig. 2 The simulated ozone of MM5/CAMx run at 1500 PST July 31, 2000.



Fig. 3 The simulated ozone of WRF/CAMx run at 1500 PST July 31, 2000.



Fig. 4 Same as Fig. 2 but for August 1, 2000.



Fig. 5 Same as Fig. 3 but for August 1, 2000.



Fig. 6 Same as Fig. 2 but for August 2, 2000



Fig. 7 Same as Fig. 3 but for August 2, 2000.



Predicted Ozone [ppb] Fig. 8 The scatter plot of ozone in the SFB region for July 31, 2000 from the MM5/CAMx run.



Fig. 9 The scatter plot of ozone in the SFB region for July 31, 2000 from the WRF/CAMx run.



Fig. 10 The scatter plot of ozone in the SAC region for August 1, 2000 from the MM5/CAMx run.



Fig. 11 The scatter plot of ozone in the SAC region for August 1, 2000 from the WRF/CAMx run.



Fig. 12 The scatter plot of ozone in the central SJV region for August 2, 2000 from the MM5/CAMx run.



Fig. 13 The scatter plot of ozone in the central SJV region for August 2, 2000 from the WRF/CAMx run.











Fig 16. The Unpaired Peak Prediction Accuracy (UPPA), Normalized Bias (N. Bias) and Normalized Error (N. Error) for the San Francisco Bay Area.



Fig. 17. Same as Fig. 16 but for the Sacramento Area.



Fig. 18. Same as Fig. 16 but for the central San Joaquin Valley.



Fig. 19. Same as Fig. 16 but for the southern San Joaquin Valley.