2.3 A PHOTOCHEMICAL MODEL COMPARISON STUDY: CAMx AND CMAQ PERFORMANCE IN CENTRAL CALIFORNIA

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1. INTRODUCTION

During the comprehensive field monitoring campaign of the 2000 Central California Ozone Study (CCOS) (Fujita et al., 1999), several ozone episodes were captured. One of the captured episodes (July 31-August 2, 2000) was selected for modeling. During this episode, ozone exceeded the federal 1-hour standard in the San Francisco Bay Area, Sacramento, and the San Joaquin Valley. The Bay Area Air Quality Management District (BAAQMD) has been collaborating with the National Oceanic and Atmospheric Administration (NOAA), California Air Resources Board (CARB), and other agencies, to simulate this episode using the Comprehensive Air quality Model with eXtensions (CAMx) (Environ, 2004). A prognostic mesoscale meteorological model (MM5) (Grell et al., 1995) was used to generate meteorological inputs for CAMx. Wilczak et al. (2004) and Soong et al. (2004) investigated the performance of MM5 and CAMx, respectively, for this episode. Here, we employ another air quality model, the Community Multiscale Air Quality (CMAQ) model (U.S. EPA, 1999), to simulate the same episode. Our goals for this paper are to compare CAMx with CMAQ predictions of ozone and its precursors in the study domain, and to evaluate CMAQ model performance with observations.

2. OZONE EPISODE AND MODEL SETUP

2.1 *CCOS Domain*

The CCOS field study domain poses a complex terrain setting. From west to east, it consists of the Pacific Ocean; the Coast Ranges; the Central Valley, which includes Sacramento, Fresno, and Bakersfield; and the Sierra Nevada (Figure 1a). The Coast Ranges are about 0.6-1.2 km and the Sierra Nevada 2-4 km in elevation. The Central Valley is about 80-120 km wide in the east-west direction and 800 km long in the north-south direction. Mountains in the north and the south surround the valley. There are several gaps in the Coast Ranges that allow airflow between the Pacific Ocean and the Central Valley. A major gap is located in the San Francisco Bay Area.

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2.2 *Characteristics of Captured Ozone Episode*

The 2000-CCOS field study captured an extended ozone episode during July 31-August 2, 2000. The maximum ozone concentration was 126 ppb in the Bay Area on July 31, 133 ppb in Sacramento on August 1, and 151 ppb in the San Joaquin Valley on August 2. Soong et al. (2004) provided a more complete listing of observed ozone at selected stations during this episode.

Figure 1b shows the observed ozone in the CCOS domain at 4 pm (PST), July 31, 2000. At this time, there was an ozone exceedance at Livermore in the Bay Area, while at surrounding stations, peak ozone remained less than 85 ppb. It is common to see this type of episode in the Bay Area. While this type of single site episode is common in the Bay Area, it poses a challenge to simulating episodes in this region. Figure 1b also shows that ozone was relatively low in Sacramento, and there were higher values in the San Joaquin Valley at this time.

2.3 *Model Setup*

We configured the study domain for CMAQ to match that for CAMx. The model domain covers the CCOS field study domain horizontally, with 185 x 185 (4 x 4 km^2) grids. Twenty vertically expanding layers were employed in CMAQ. These layers were interlaced from the 50 vertical layers in MM5, with ~25 m resolution in the lowest two layers and ~1 km resolution in the middle troposphere. The SAPRC99 chemical mechanism (Carter, 2000) was used. A day-specific emission inventory was prepared by CARB, and boundary conditions and initial conditions were produced at BAAQMD based on aircraft measurements. Temperatures, pressures, humidity, and horizontal winds were generated from the MM5 run with the Eta PBL scheme and 5-layer soil model without FDDA (Wilczak et al., 2004). Major differences between CMAQ and CAMx are the methods of calculating photolysis rates, chemical integration, vertical transport, horizontal diffusion, and dry deposition. Simulation started on July 29. Detailed model evaluation and comparison were made on July 31 because ozone exceeded the federal 1-hour standard on that day in the Bay Area.

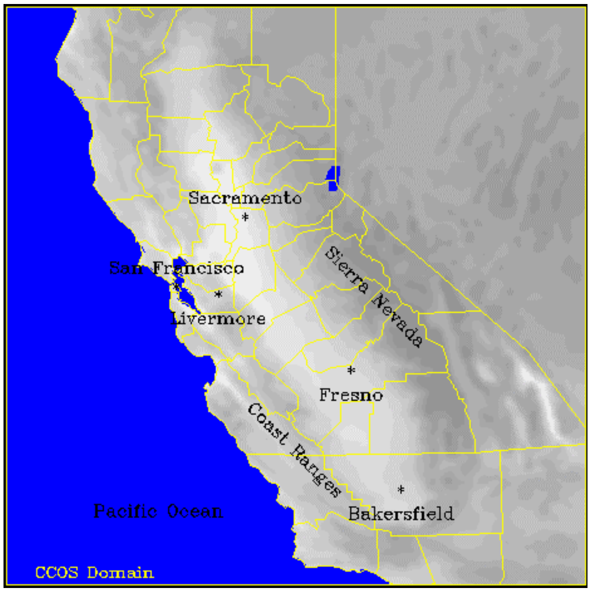

Figure 1a. The Central California Ozone Study (CCOS) domain. The blue regions represent water and the yellow lines mark county boundaries or coastlines. The surface elevation is higher in regions with darker shading.

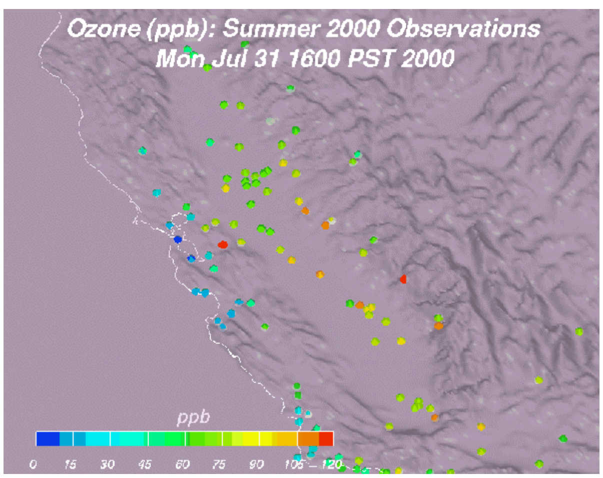

Figure 1b. Observed ozone mixing ratio (ppb) in the CCOS domain at 4 pm (PST), July 31, 2000.

3. CAMx VS. CMAQ COMPARISON

To compare CAMx and CMAQ, this section shows the temporal and spatial distributions of modeled values of ozone, NO_X, CO, and carbonyls in the lowest layers of both models. Figures 2-5 show the diurnal variation of hourly averaged mixing ratios over the lowest level of the entire model domain on July 31, 2000. Figure 2 shows that the domain-averaged surface ozone is higher in CAMx than CMAQ at all hours except between 8-10 am (PST). Surface NO_X in CAMx is higher during the daytime (6 am-5 pm, PST) and lower during the nighttime than CMAQ (Figure 3). Surface CO in CAMx is significantly higher than CMAQ during the entire day, especially during midday (Figure 4). Since CO is relatively inert and may serve as a tracer for transport, Figure 4 suggests that CMAQ has stronger vertical transport than CAMx. The large surplus of ozone in CAMx, compared to CMAQ, built up during 11 am -2 pm (PST) (Figure 2) and is consistent with the large, concurrent consumption of carbonyls, as shown in Figure 5. Figures 2-5 suggest that the two models have fundamental differences in their vertical distribution of both ozone and its precursors.

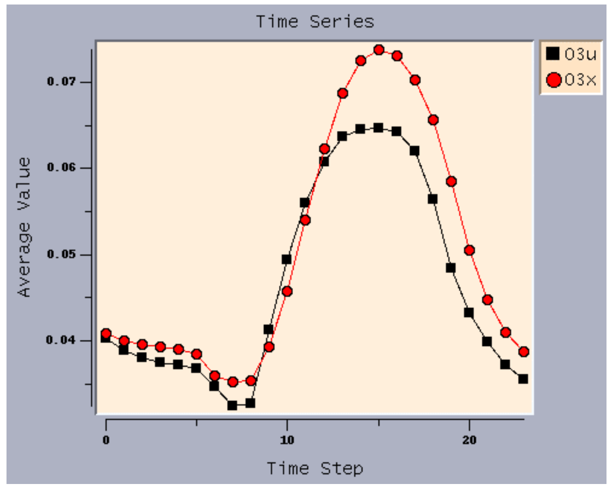

Figure 2. Time series plot of hourly averaged O_3 mixing ratios (ppm) in the lowest layer of CAMx (red) vs. CMAQ (black) averaged over the model domain on July 31, 2000. Time steps correspond to hours 0-23, PDT.

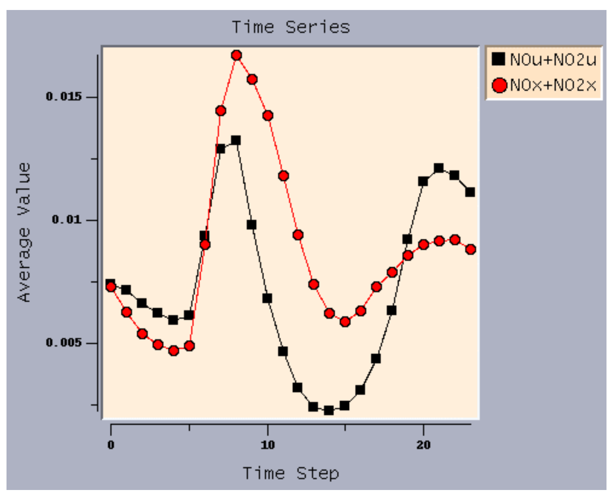

Figure 3. Same as Figure 2, except for NO_X (NO + NO_2).

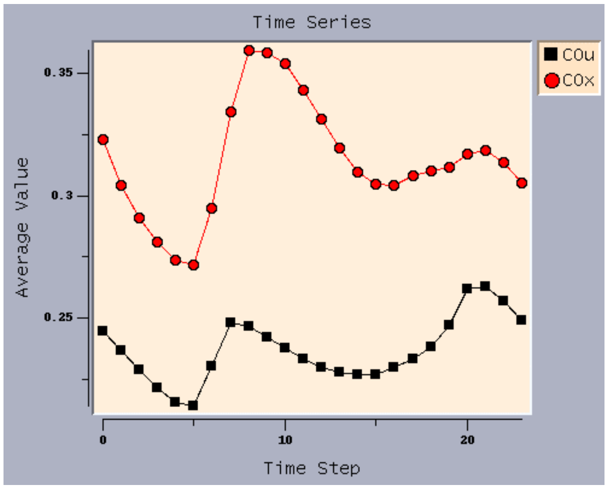

Figure 4. Same as Figure 2, except for CO.

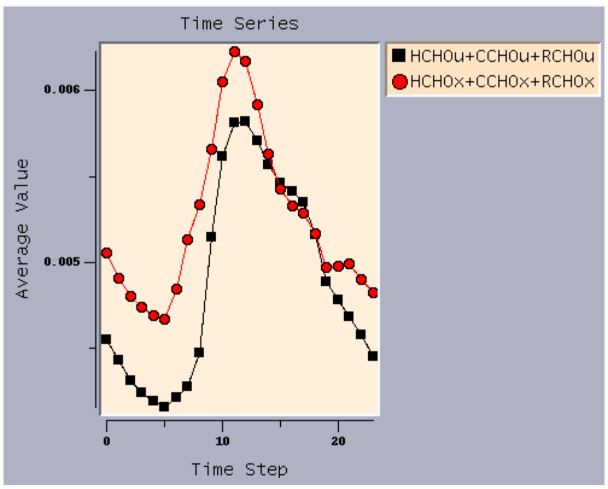

Figure 5. Same as Figure 2, except for total carbonyls.

There are differences in the horizontal distribution of ozone in the lowest model layers (~25 m thick) of CAMx and CMAQ over both the entire CCOS domain (Figures 6-7) and the Bay Area (Figures 8-9) on July 31, 2000. Figures 6-7 show that both models predicted highest ozone in the southeast of the model domain, due to the Manter forest fire in the Sequoia National Forest that burned more than 60,000 acres by July 31, 2000. There was also high ozone in the Bay Area, Sacramento, and the San Joaquin Valley. CAMx predicted larger areas of ozone that exceeded the federal 1-hour standard than CMAQ, while CMAQ predicted higher peak ozone than CAMx in areas influenced by the forest fire.

Table 1 lists the peak ozone in models and observations in the Bay Area, Sacramento, and the San Joaquin Valley on July 31, 2000. Note that the CAMx prediction of peak ozone in the Bay Area was close to the observed peak value. However, CAMx overpredicted peak values in Sacramento and the San Joaquin Valley. On the other hand, CMAQ underpredicted ozone in the Bay Area but performed better than CAMx in Sacramento and the San Joaquin Valley.

Table 1. Peak ozone (ppb) simulated and observed in the Bay Area, Sacramento, and the San Joaquin Valley on July 31, 2000.

Area	Observed Peak	CAMx Peak	CMAQ peak
Bay Area	126	123	114
Sacramento	100	145	90
San Joaquin Valley	115	132	120

For comparison in the Bay Area, Figures 8-9 show that both CAMx and CMAQ predicted high ozone in the eastern part of the Bay Area, though areas with high ozone in CAMx were larger than and further to the east of those in CMAQ. CAMx predicted peak ozone near Livermore, close to the observed location (Figure 8). CMAQ predicted peak ozone at the right time but at a different location (Figure 9).

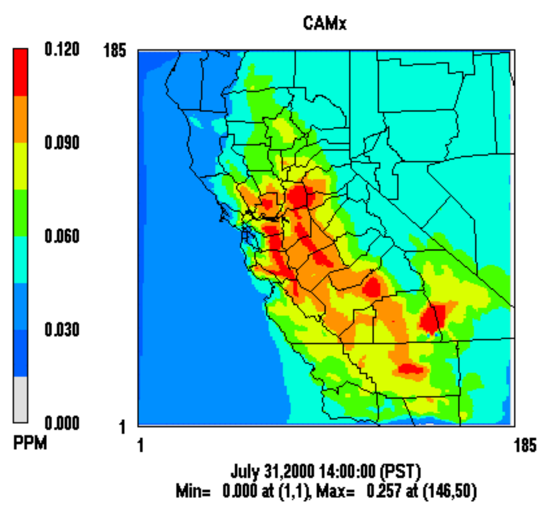

Figure 6. Ozone mixing ratios in the lowest model layer (~ 25 m thick) of CAMx in the CCOS domain at the peak ozone hour on July 31, 2000.

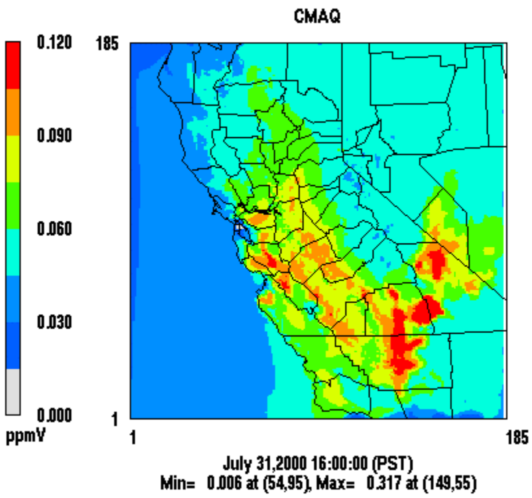

Figure 7. Same as Figure 6, except for CMAQ.

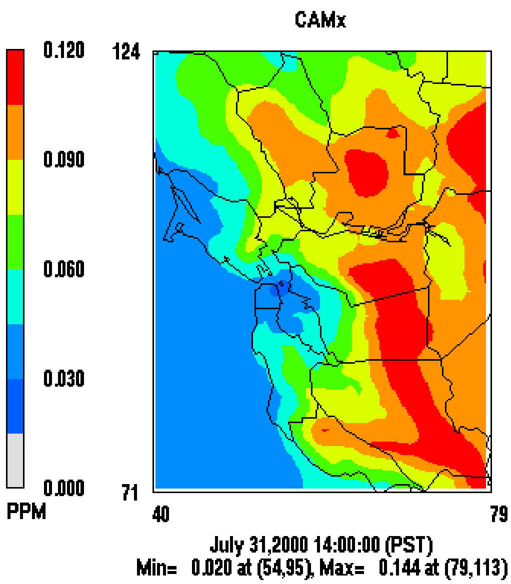

Figure 8. Ozone mixing ratios in the lowest model layer (~ 25 m thick) of CAMx in the Bay Area at the peak ozone hour on July 31, 2000.

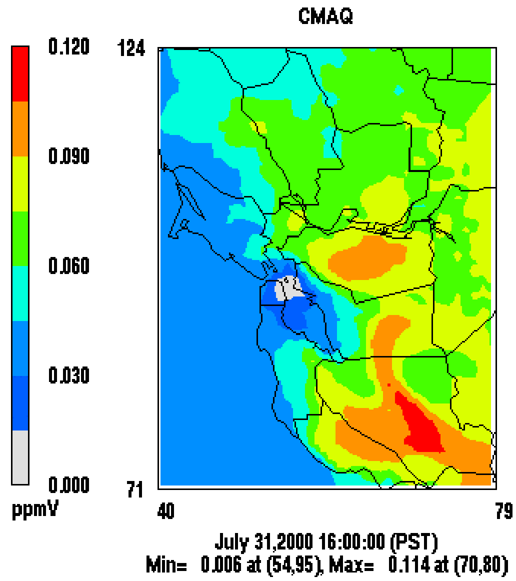

Figure 9. Same as Figure 8, except for CMAQ.

4. CMAQ MODEL EVALUATION

An evaluation of CAMx was presented in Soong et al. (2004) for this modeling period. Here, we focus on the evaluation of CMAQ. We first show scatter plots of ozone and its precursors, predictions versus observations, and then show time series of ozone and its precursors at selected stations. Finally, we show statistical metrics required by the U.S. EPA for model evaluation.

4.1 *Scatter Plots*

Figures 10-12 show the scatter plots of ozone in CMAQ versus observations over the Bay Area, Sacramento, and the San Joaquin Valley on July 31, 2000. Correlation coefficients between observations and CMAQ predictions for ozone in the Bay Area, Sacramento, and the San Joaquin Valley are 0.77, 0.69, and 0.77, respectively. In general, ozone was overpredicted in CMAQ, especially when observed ozone was lower than 40 ppb. When observed ozone was higher than 80 ppb, however, CMAQ underestimated ozone in the Bay Area and Sacramento (Figures 10-11), but did not have an obvious bias in the San Joaquin Valley (Figure 12).

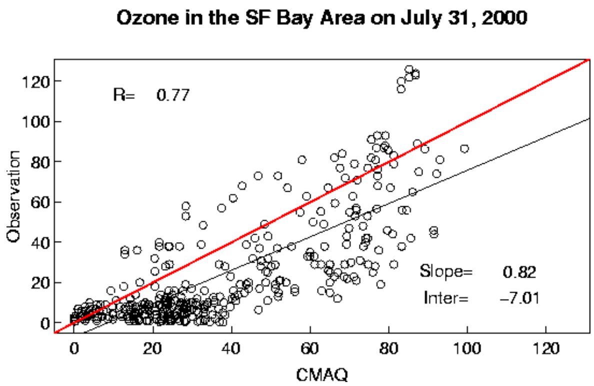

Figure 10. Scatter plot of hourly averaged ozone (ppb) in CMAQ versus observations at 16 stations over the Bay Area on July 31, 2000. The red line represents perfect match between predictions and observations, and the black line is the least squares fit, with slope and intercept shown in the figure. The correlation coefficient (R) is also shown. Observations were collected at ground level, while model values were at ~12 m above the ground.

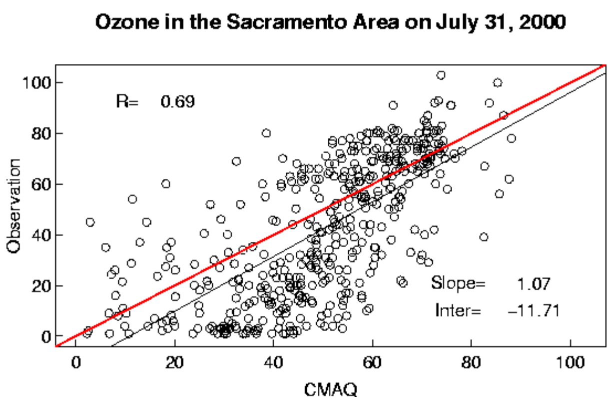

Figure 11. Same as Figure 10, but for Sacramento.

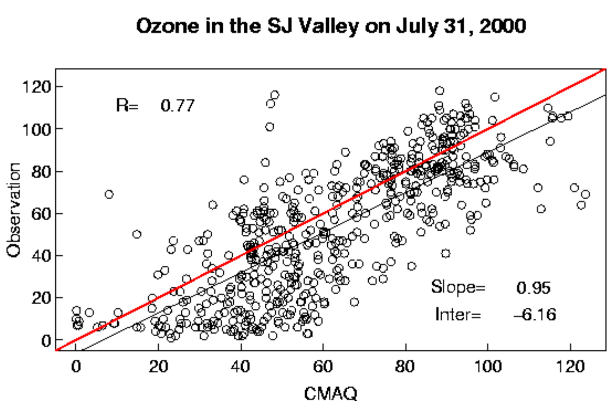

Figure 12. Same as Figure 10, but for the San Joaquin Valley.

Figures 13-16 show scatter plots of NO_X, NMHCs, HCHO, and CO in CMAQ versus observations over the Bay Area on July 31, 2000. Correlation coefficients between observations and CMAQ model for NO_X, NMHCs, HCHO, and CO were low (0.45, 0.32, 0.59, and 0.53, respectively). Ozone precursors (NO_X, NMHCs, and HCHO) as well as CO were under-predicted in CMAQ overall. While the underprediction of ozone precursors has been commonly reported in air quality modeling studies, the causes of this underprediction remain to be investigated.

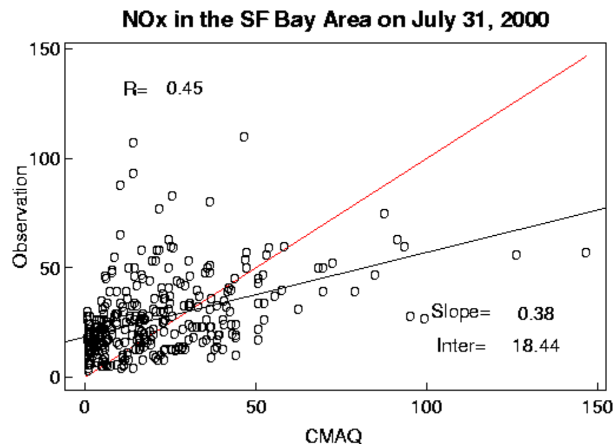

Figure 13. Scatter plot of hourly averaged NO_X (ppb) in CMAQ versus observations at 14 stations over the Bay Area on July 31, 2000. The red line represents perfect match between predictions and observations, and the black line is the least squares fit, with slope and intercept shown in the figure. The correlation coefficient (R) is also shown. Observations were collected at ground level, while model values were at ~12 m above the ground.

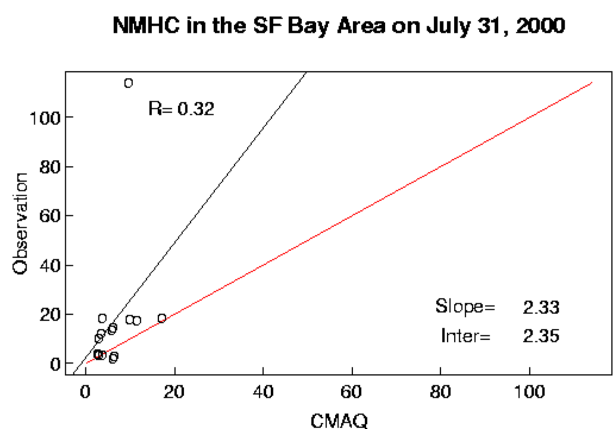

Figure 14. Scatter plot of 3-hour averaged total non-methane hydrocarbons (pphm) in CMAQ versus observations at 4 stations over the Bay Area on July 31, 2000. Notations are the same as in Figure 13.

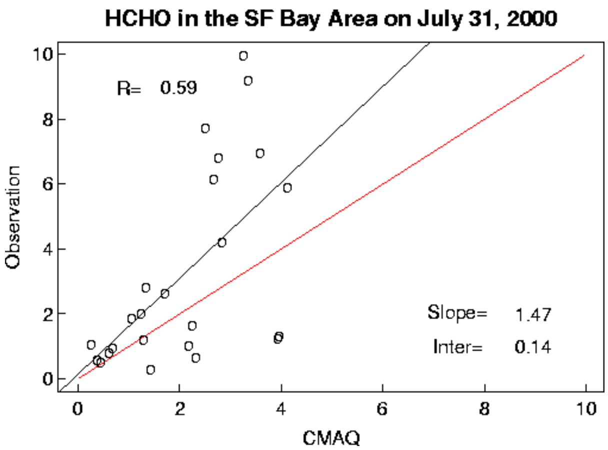

Figure 15. Scatter plot of 3-hour averaged HCHO (ppb) in CMAQ versus observations at 6 stations over the Bay Area on July 31, 2000. Notations are the same as in Figure 13.

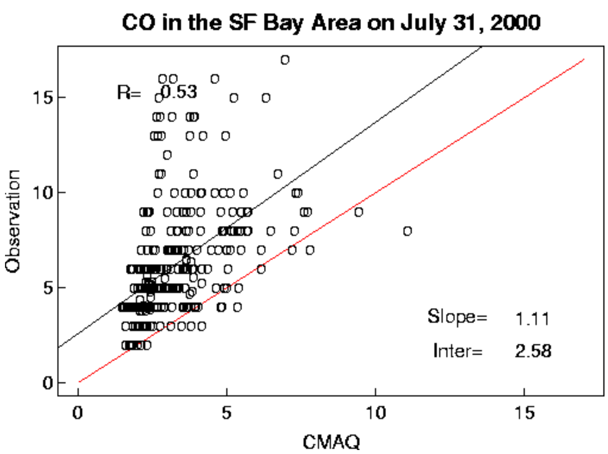

Figure 16. Scatter plot of hourly averaged CO (pptm) in CMAQ versus observations at 14 stations over the Bay Area on July 31, 2000. Notations are the same as in Figure 13.

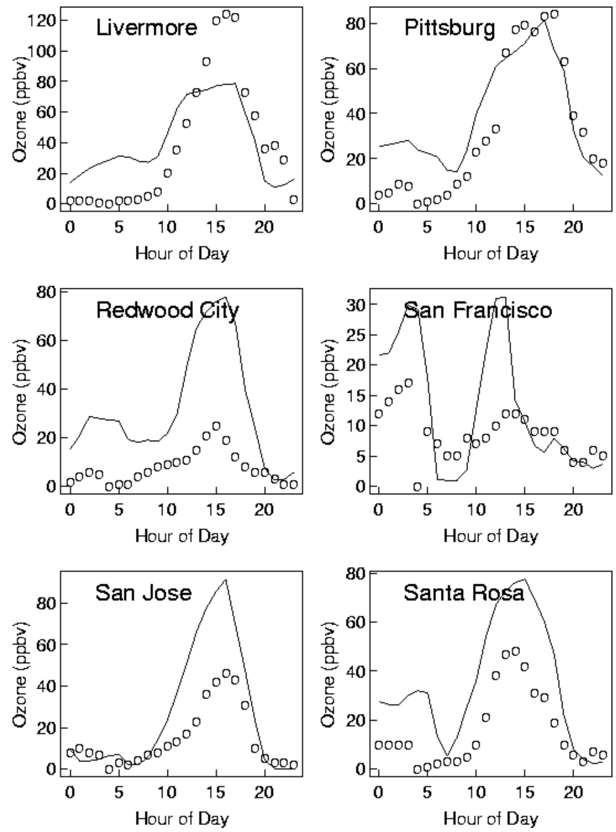

Figure 17. Time series of ozone at 6 stations over the Bay Area on July 31, 2000. The lines denote CMAQ model values, and ‘o’ denotes hourly averaged observations.

4.2 *Time Series of Ozone and its Precursors*

Figures 17-20 show time series plots of ozone and its precursors at selected stations over the Bay Area. Note that ozone precursors were not available at all stations. Observed diurnal variations were captured in CMAQ for ozone and NO_X at most stations (Figures 17-18). Since HCHO was observed on 3-hour averaged basis, the diurnal variation is less clear in observations. CMAQ predicted clear diurnal patterns with a maximum in the late afternoon at most stations. CO in CMAQ was significantly lower than observations, but the diurnal trend in CMAQ appeared to be similar to that in observations.

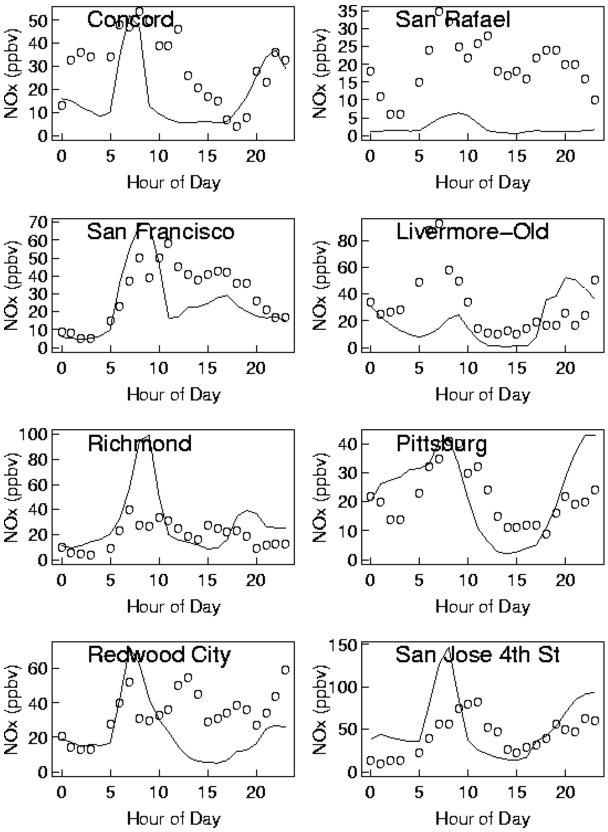

Figure 18. Time series of NO_X at 8 stations over the Bay Area on July 31, 2000. Notations are the same as in Figure 17.

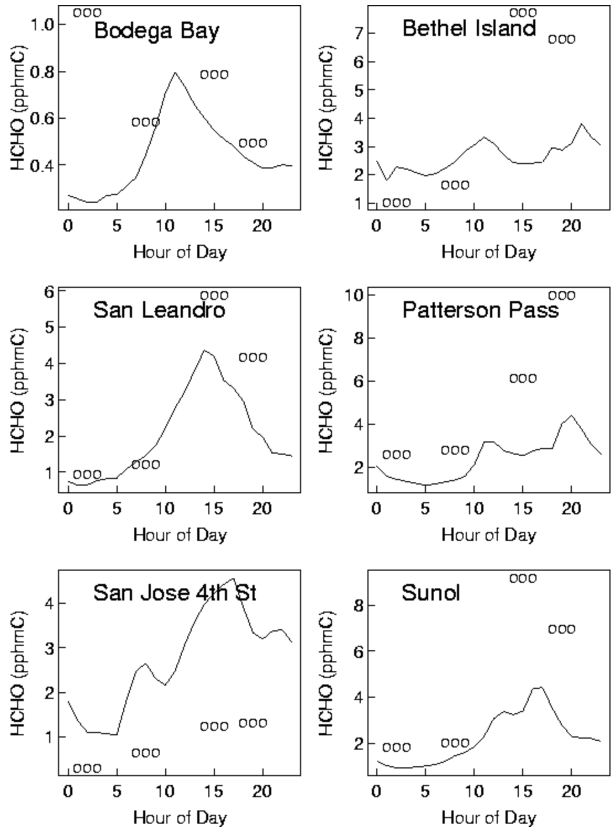

Figure 19. Time series of HCHO at 6 stations over the Bay Area on July 31, 2000. Notations are the same as in Figure 17.

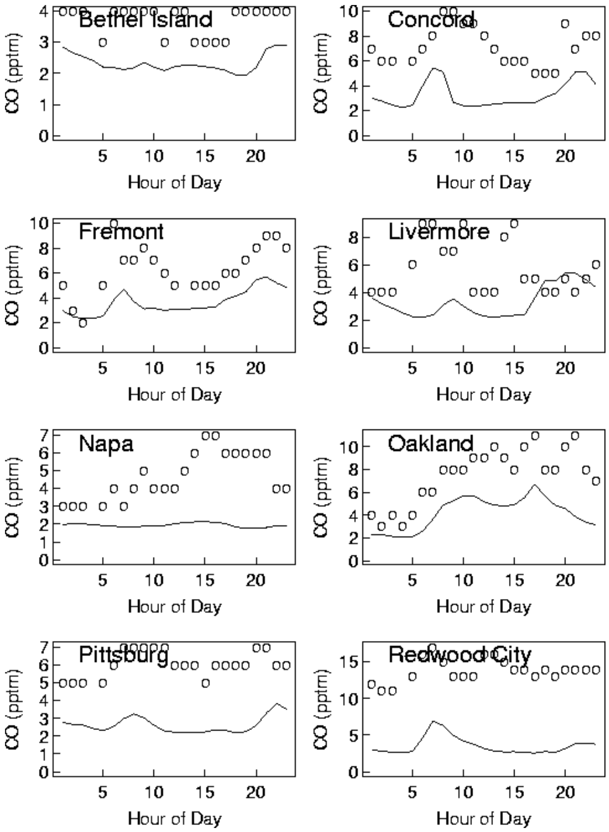

Figure 20. Time series of CO at 8 stations over the Bay Area on July 31, 2000. Notations are the same as in Figure 17.

4.3 *Statistical Metrics*

To evaluate model performance for ozone, the U.S. EPA recommends three model performance statistics for air quality modeling (U.S. EPA, 1991), namely the unpaired predicted-to-observed peak ozone ratio, the normalized gross error, and the normalized bias. The normalized gross error parameter provides an overall assessment of model performance and can be interpreted as precision, and the normalized bias parameter measures a model's ability to reproduce observed spatial and temporal patterns and can be interpreted as accuracy. The U.S. EPA criteria require an unpaired predicted-to-observed peak ozone ratio of < ±20%, a mean normalized bias (MNB) of < ±15%, and a normalized gross error (NGE) of < 35% above a threshold of 40-60 ppb. We show in Figure 21 each of these three parameters calculated for the Bay Area, Sacramento, and the San Joaquin Valley. CMAQ met the U.S. EPA guidelines in the Bay Area on July 31, 2000. The other areas also met the U.S. EPA performance criteria, but there was no ozone exceedance in those regions on this day.

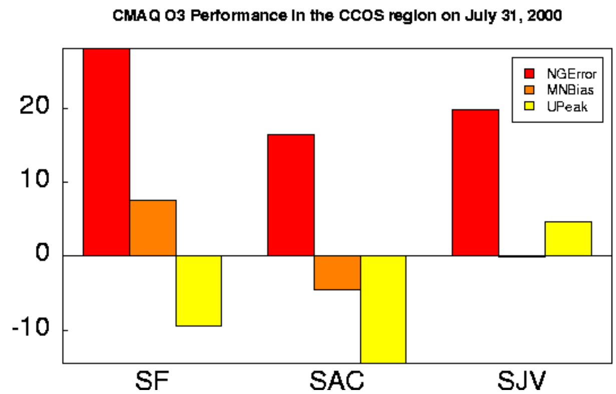

Figure 21. The normalized gross error (NGError, red), the normalized bias (MNBias, orange), and the deviation from 1 of the unpaired predicted-to-observed peak ozone ratio (Upeak, yellow) of ozone (as a percentage) in CMAQ over the Bay Area (SF), Sacramento (SAC), and the San Joaquin Valley (SJV) on July 31, 2000. The cutoff value is 40 ppb.

Figure 22 shows the normalized gross error and normalized bias of NO_X, NMHCs, HCHO, and CO as well as O_3 in CMAQ for the Bay Area on July 31, 2000. The cutoff value is 0 ppb for ozone precursors. With both measures, ozone was better predicted than its precursors. HCHO has the largest error (80%), and CO has the largest bias in magnitude (-40%).

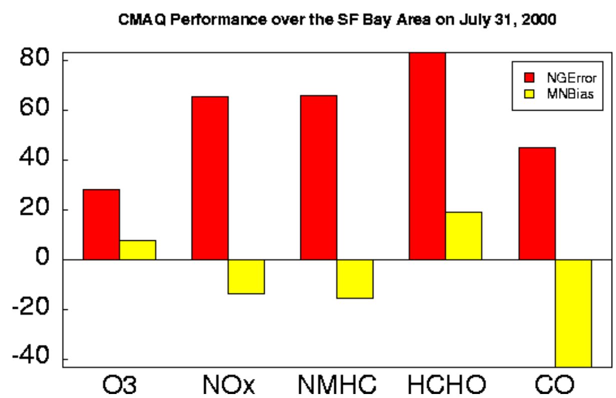

Figure 22. The normalized gross error (red) and mean normalized bias (yellow) of O_3, NO_X, NMHCs, HCHO, and CO (in percentage) in CMAQ for the Bay Area on July 31, 2000.

5. SUMMARY

We employed CMAQ to simulate an ozone episode captured during a comprehensive field monitoring campaign conducted in central California during the summer of 2000. Our companion paper evaluated CAMx model performance. This paper focused on comparing CAMx and CMAQ predictions, and on evaluating CMAQ model performance for ozone and its precursors.

We designed the model setup for CAMx and CMAQ to be as similar to each other as possible, and compared the temporal and spatial distributions of ozone and its precursors in the two models in the study domain. We found that CAMx predicted larger areas with elevated surface ozone - exceeding the federal 1-hour ozone standard - than CMAQ, but the model maximum in CAMx was lower than CMAQ in areas affected by forest fire. The stronger vertical transport in CMAQ, compared to CAMx, could be responsible for this difference, based on comparisons of CO distributions in the two models. We evaluated ozone and its precursors in CMAQ with observations especially over the Bay Area. We showed that CMAQ met the U.S. EPA model performance criteria for ozone in the Bay Area. As in previous studies, this study found that model performance for ozone precursors was less successful than for ozone.

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