2.2 SIMULATIONS OF AN OZONE EPISODE DURING THE CENTRAL CALIFORNIA OZONE STUDY
PART II: CAMx AIR QUALITY MODEL SIMULATIONS

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1. INTRODUCTION

Ozone, the principal component of photochemical smog, frequently reaches concentrations that exceed the federal 1- and 8-hour standards (124 ppb and 84 ppb, respectively) in central California. The Central California Ozone Study (CCOS) was conducted in 2000 to investigate the causes of the region's high ozone. The study described in this paper uses CCOS data collected during a period of elevated ozone from July 31 to August 2, 2000, to numerically simulate the formation of ozone. In Part I of this paper (Wilczak et al., 2004), meteorological fields for this period were generated using several different options, including different representations of the land surface and with and without the use of four-dimensional data assimilation (FDDA; Stauffer and Seaman, 1994). In Part II of this paper we investigate the effects of using the different meteorological fields described in Part I on simulated ozone.

Previous photochemical modeling studies conducted for central California have shown mixed results in terms of the benefit of applying FDDA in generating meteorological fields for the purpose of improving simulations of ozone. Tanrikulu et al. (2000) applied FDDA in the MM5 meteorological model and produced improved statistical performance for wind and temperature fields, which in turn improved ozone modeling. Umeda and Martien (2002) applied FDDA in the CSU-RAMS meteorological model and also improved statistical performance of meteorological fields. However, they showed that the photochemical model performance did not improve when they used the meteorological fields generated with FDDA.

In this paper, we build on these earlier studies, by applying the Comprehensive Air quality Model with extensions (CAMx; ENVIRON, 2004) version 4.03 to the MM5 simulations detailed in Part I:

- Run 1 used the Noah Land-Surface Model (LSM; Chen and Dudhia, 2001) without FDDA,
- Run 2 used the Noah LSM with analysis nudging on the 36-km domain and observational nudging on the 4-km domain,
- Run 3 used the 5-layer soil model (Dudhia, 1996) without FDDA.

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The two objectives of this paper are, first, to present the ozone performance in central California for this modeling system with Run 3 meteorological fields, and second, to determine whether the meteorological fields with the best statistical performance necessarily generate the best ozone performance. To carry out the second objective, we investigate the importance of relatively subtle flow features, such as the location of a mesoscale convergence zone, to the photochemical modeling. Such features cover a small geographic area and may therefore be given little weight in a statistical evaluation of the meteorological model performance, but they could have a significant influence on the location and timing of peak ozone values, which are important in regulatory modeling applications.

2. MODELING DOMAIN

The modeling domain (Fig. 1) extends from north of Redding (in the upper Sacramento Valley) to south of Bakersfield, and from the Pacific Ocean in the west to east of the Sierra Nevada. Several major urban centers are located in the study domain: the San Francisco Bay Area (SFBA), the Sacramento metropolitan region, Fresno, and Bakersfield. During a typical ozone episode in this domain, the Eastern Pacific high-pressure system

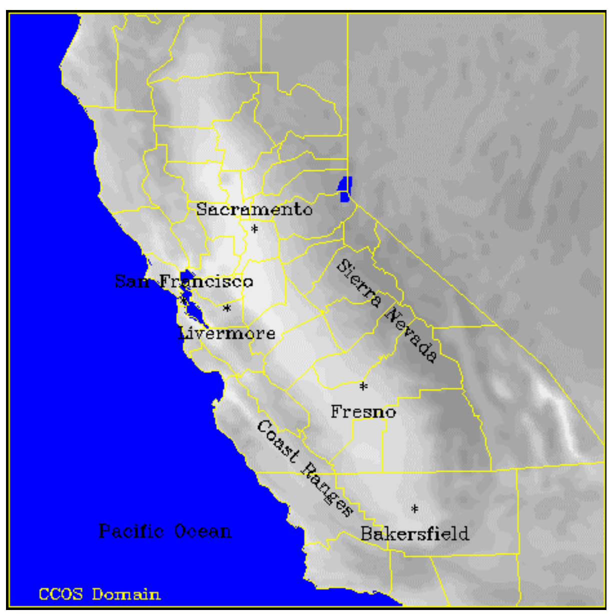

Fig. 1. The horizontal domain of the modeling study. Yellow lines denote county boundaries. Terrain is shaded gray.

exerts a major influence on meteorological conditions. The high-pressure system fosters subsidence, low-level divergence, and a shallow mixing depth. Such conditions, coupled with the emission characteristics of the region, can cause ozone in central California to exceed the federal ozone standards.

3. OBSERVATIONAL DATA

Continuous meteorological and air quality measurements were made during CCOS from June 26 to October 2, 2000 (Fujita et al., 2001). Additional meteorological and air quality data were collected during intensive operation periods (IOPs) when ozone was predicted to be high. These additional data included aircraft measurements, hydrocarbon and carbonyl measurements, as well as rawinsonde and ozonesonde measurements. For this study, the period from July 31 to August 2, part of a CCOS IOP, was selected for simulating ozone because during this period ozone exceeded the federal 1-hour standard in all major metropolitan areas of the study region. In addition, July 31 was shown to be representative of high ozone days in the SFBA (Fairley et al., 2004).

Table 1 shows the observed ozone for the July 31 to August 2, 2000, period at selected stations in the SFBA, the Sacramento Valley, and the San Joaquin Valley. During this period, ozone exceeded the federal 1-hour ozone standard in the SFBA on July 31, in the Sacramento Valley on August 1, and in the San Joaquin Valley on August 2. The ozone exceedance in the SFBA on July 31 occurred at Livermore (126 ppb) in the eastern SFBA (Fig. 1) at 1600 PST.

The observed ozone distribution for the entire CCOS domain at the time of the SFBA peak ozone is shown in Fig. 2. Ozone in the Sacramento Valley is generally low at this time. There are some elevated observed ozone values in the San Joaquin Valley at this time (above 100 ppb), but none exceeded the federal 1-hour standard.

Note that the observed high ozone at Livermore occurred in an isolated region, surrounded by stations with maximum observed ozone less than 85 ppb. This isolated high value makes it challenging to accurately simulate the observed ozone peak. However, isolated high ozone at Livermore is not uncommon. Fairley et al. (2004) showed that between 1995 and 2002, there were 36 days that exceeded the 1-hour ozone standard in the SFBA. Out of these 36 days, the highest ozone in the entire SFBA was observed at Livermore on 20 days. Livermore was the only station that exceeded the federal 1-hour ozone standard on 15 of the 36 days.

4. MODEL DESCRIPTION AND INPUTS

The CAMx version 4.03 model (ENVIRON, 2004) was run for a 5-day period for each of the three MM5 meteorological inputs described above. All simulations started on 0400 PST on July 29, 2000, and continued to 0000 PST on August 3, 2000. In each case, an 185x185 grid was used with 4 km grid resolution. This grid matched the inner MM5 grid after removing 2 cells from each edge of the grid. The telescoping vertical grid structure has 20 layers. Each MM5 layer matches a CAMx layer for the lowest 2 layers. Each 2 MM5 layers are collapsed into one CAMx layer for CAMx layers 3-5 and 18-20. Each 3 MM5 layers are collapsed into one CAMx layer for CAMx layers 6-17.

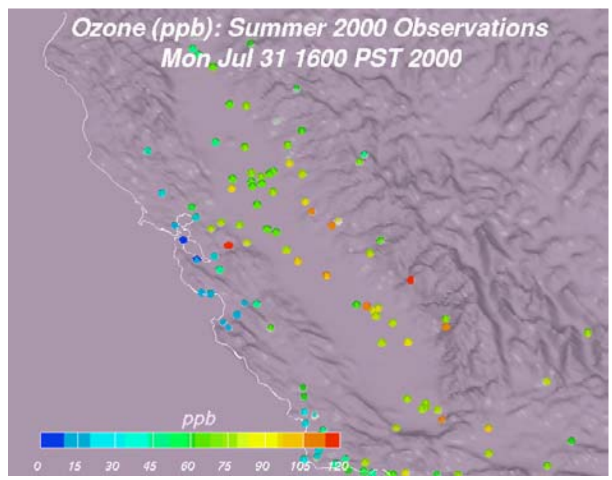

Fig. 2. The distribution of the observed ozone at 1600 PST, July 31, 2000 over the CCOS domain.

Table 1. The observed ozone at selected stations

Day	7/31/2000							8/1/2000							8/2/2000						
Hr (PST)	12	13	14	15	16	17	18	12	13	14	15	16	17	18	12	13	14	15	16	17	18
SFBA																					
Livermore - Old 1st	68	88	116	123	126	73	53	73	86	92	81	68	65	52	88	93	98	84	69	57	49
Sacramento Area																					
Sloughhouse		100	92	87	78	74	66	88	112	133	126	119	112	95	98	102	101	103	98	66	77
San Joaquin Valley																					
Edison	115	110	106	94	81	74	38	113	109	93	102	102	96	83	129	151	139	121	76	51	45
Turlock	75	91	104	105	96	88	64	100	101	97	104	86	85	73	98	95	114	117	116	131	106
Modesto - 14th	74	87	94	90	84	81	60	80	84	99	87	94	91	70	90	94	95	113	131	128	85

The shaded cells are those exceeding the federal 1-hour ozone standard.

All simulations described in this study applied the SAPRC-99 chemical mechanism (Carter, 2000). Day-specific emissions for point, area, biogenic, and on-road mobile sources for this modeling period were prepared by the California Air Resources Board. Initial and boundary conditions were adapted from those used in the SARMAP air quality modeling (DaMassa et al., 1996). These boundary conditions were modified slightly based on an average of four CCOS aircraft flights collected over the Pacific Ocean at about 250 km offshore. Average mixing ratios for ozone on lateral boundaries were set to 40 ppb. For oxides of nitrogen (NOx), mixing ratio boundary conditions were set to 1 ppb. For hydrocarbons and aldehydes, boundary conditions were set to 25 ppb and 7 ppb, respectively.

5. RESULTS

Three CAMx simulations were made using the results from the 3 MM5 runs as inputs. For easy reference, the CAMx runs are referred to as Run 1, Run 2 and Run 3, corresponding to the names of the three MM5 runs given in Section 1.

5.1 *Simulated Ozone Distribution in Central California*

Fig. 3 shows the peak simulated ozone distribution in Run 3 over the entire CCOS domain at 1600 PST, July 31, 2000, the date and time of the peak simulated ozone in the SFBA. There is a clear relationship between the areas of predicted high ozone and the distribution of the region's metropolitan areas and a large forest fire that occurred during this period. Fig. 3 shows five areas of high ozone mixing ratios in the Central Valley. Starting from the north, there is an area of high ozone just east of Sacramento, followed to the south by regions of high ozone close to the two Central Valley cities of Stockton and Modesto. Continuing further southward, there is an ozone high just south of Fresno and another near Bakersfield. The high ozone northeast of Bakersfield in the southern Sierra Nevada is due to the Manter forest fire, which had burned more than 60,000 acres by July 31, 2000.

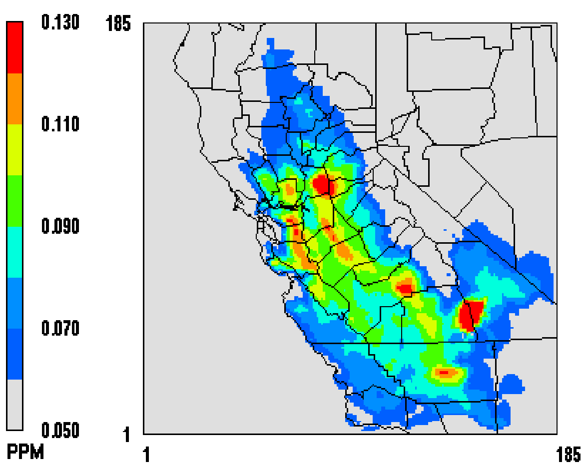

Fig. 3. The simulated ozone distribution in Run 3 over the CCOS domain at 1600 PST, July 31, 2000.

A scatter plot of simulated versus observed surface-level ozone (Fig. 4) shows a reasonable degree of correlation for each of the three days. The correlation coefficient of the linear regression for the three days combined is 0.78. The slope of the regression equation is 0.92 and the intercept is 0.2 ppb. However, there are some disagreements between predicted and observed peak values. There is an overprediction of the daily maximum ozone in the Sacramento Valley on July 31 (crosses in Fig. 4). The simulated maximum ozone for July 31 in the Sacramento area was 145 ppb, whereas, the observed maximum was 103 ppb. In the San Joaquin Valley, the simulated maximum ozone for July 31 was 132 ppb (outside the area obviously influenced by the Manter forest fire) versus the observed 115 ppb. However, this overprediction problem is not systematic. The model underpredicted the daily maximum ozone in the Sacramento area by 9 ppb on August 1 (circles) and in the San Joaquin Valley by 38 ppb on August 2 (triangles), respectively, the days when each area exceeded the federal 1-hour ozone standard. Table 2 shows performance statistics for three regions: the SFBA, the Sacramento area and the San Joaquin Valley. The statistics are defined as follows:

Unpaired peak prediction accuracy:
$UPP = 100 \times (peak_{pred} / peak_{obs} - 1)$

Normalized Bias: $NB = 100 \times (\frac{1}{N} \sum_{i=1,N} (\frac{pred_i - obs_i}{obs_i}))$

Normalized Error: $NE = 100 \times (\frac{1}{N} \sum_{i=1,N} |\frac{pred_i - obs_i}{obs_i}|)$.

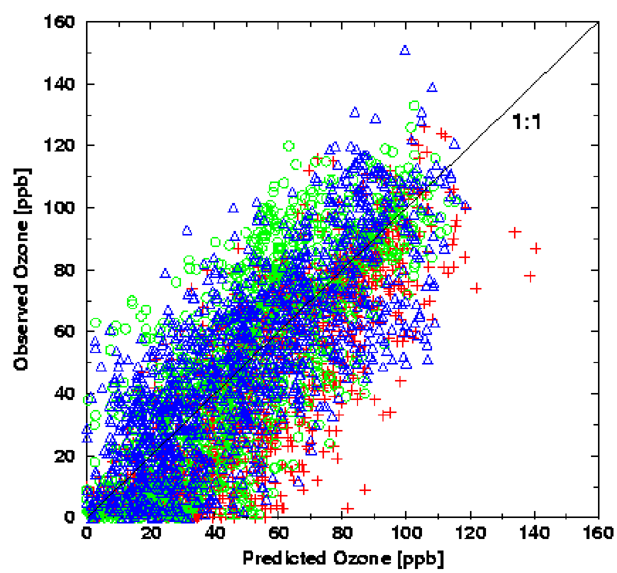

Fig. 4. Scatter plot of observed and simulated ozone with Run 3 meteorological inputs for July 31 (crosses), August 1 (circles), and August 2 (triangles).

In computing UPP, $peak_{pred}$ is the predicted value on the same day and within a 25 km radius of the location of the observed peak for a given region. In computing the normalized bias and error, the predicted ozone is paired (in time and space) to the observed value. Observations below 40 ppb were not included in the statistics. Table 2 shows that most of the statistics are within the U.S. EPA's suggested performance criteria.

The features of the predicted ozone described here for Run 3 also appear in Run 1 and Run 2. There are slight differences in the locations and the values of the maximum ozone among these runs. Yet, these slight differences can have important implications for regulatory applications. A detailed discussion on the differences among the runs for the SFBA on July 31 will be presented in the next subsection.

5.2 *Simulated Ozone Distribution in the SFBA on July 31, 2000*

In this paper, the SFBA coincides with the area under the jurisdiction of the Bay Area Air Quality Management District, the boundaries of which are indicated with a solid black line in Figs. 5 and 6. The SFBA topography and ozone observation stations are also shown in Fig. 5. As mentioned in section 2, the ozone exceedances at Livermore account for nearly half of the total ozone exceedance in the SFBA. Livermore is situated in the south end of the Tri-Valley, an L shaped valley area that roughly connects Concord to Livermore. A major highway (I-680) runs north-south in the western part of the valley and another highway (I-580) runs east-west in the southern part of the valley. The traffic is often congested on both highways and the mountains around the valley channel the local winds and reduce their speed.

Fig. 6 shows the wind pattern at 1400 PST, July 31, 2000, 2 hours before the observed ozone maximum at Livermore. The wind coming from the Pacific Ocean splits into two branches after entering the San Francisco Bay: one tends southward toward the Santa Clara Valley (which contains San Martin, Fig. 5) and the other tends northward through the Carquinez Strait (south of Vallejo between San Pablo and Pittsburg). The northwesterly wind at the north end of the Tri-Valley is correlated with high ozone in Livermore. Several large refineries and power plants are located along the

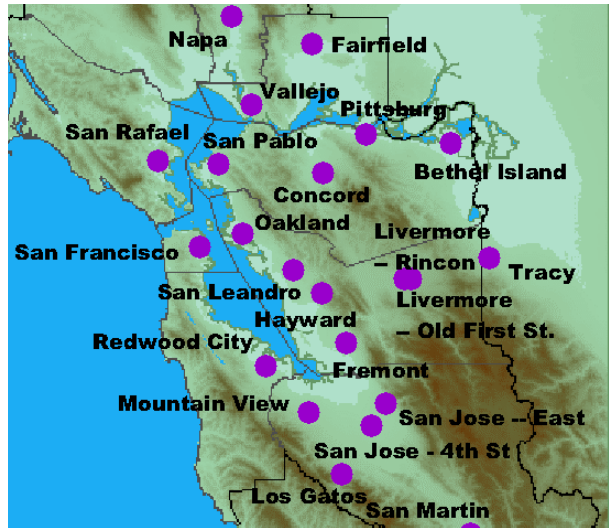

Fig. 5. The SFBA topography and ozone observation stations.

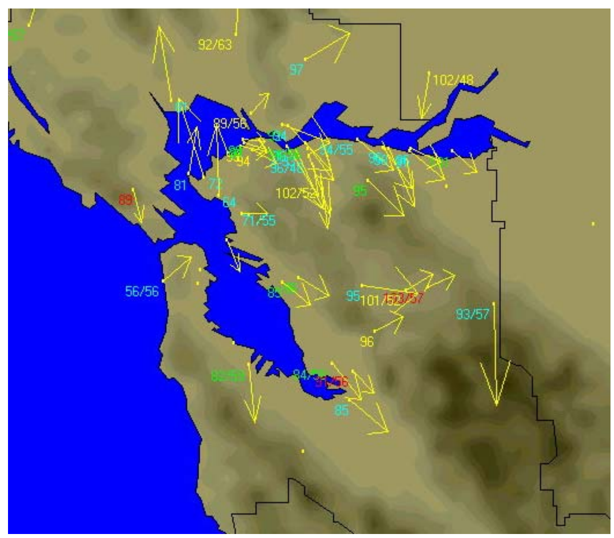

Fig. 6. The wind distribution in the SFBA at 1400 PST, July 31, 2000.

Table 2. Model Performance statistics for Run 3.

Day	7/31/2000			8/1/2000			8/2/2000		
Statistic	UPP (%)	NB (%)	NE (%)	UPP (%)	NB (%)	NE (%)	UPP (%)	NB (%)	NE (%)
SFBA	-2	15	22	-16	-16	26	10	-12	27
Sacramento Area	11	9	20	-6	-21	25	12	-2	26
San Joaquin Valley	12	3	19	9	-3	22	-23	-10	26

EPA guidance suggests that the unpaired peak prediction accuracy (UPP) should be within ± 20%; the normalized bias should be within ± 15%; and the normalized error should be < 35%.

Carquinez Strait. We suspect that this northwesterly wind transports additional emissions to Livermore. It may be the combination of the abundant emission sources and the enclosed valley that make the Livermore area particularly conducive to the formation of high ozone.

The simulated ozone distribution in the SFBA for Run 3 at 1600 PST, July 31, 2000 is shown in Fig. 7. The ozone mixing ratios are less than 60 ppb by the coast and in the central urban region rimming the San Francisco Bay. The predicted high ozone in the northeastern corner of Fig. 7 is located downwind of Sacramento. In the SFBA, there is an arc-shaped line of high ozone surrounding Livermore. The maximum simulated ozone in the SFBA was 123 ppb 16 km north of Livermore. The maximum observed ozone at Livermore, as shown in Table 1, was 126 ppb

Fig. 8 shows the MM5-generated surface-level wind vectors superimposed on the ozone distribution. One of the most prominent features of this wind field is the strong sea breeze, which transports the relatively clean offshore air to the onshore coastal areas. Over the land, this simulation captured most of the main wind features presented in Fig. 6: The northward and southward branching of the wind over the San Francisco Bay, the northwesterly flow at the north part of Tri-Valley, and the wind convergence near Livermore. Just east of Livermore, the direction of the wind is from north, matching the observed wind direction. Fig. 8 also indicates that, in this particular case, the wind and emissions did not pass over the Altamont Pass (between Livermore and Tracy) to the Central Valley. There is a close association between the location of maximum wind convergence and the location of the peak ozone. This association between convergence zones and peak ozone also exists in Run 1 and Run 2 simulations.

The overall simulated ozone distribution and wind pattern at 1600 PST, July 31, 2000 for Run 1 (Fig. 9) and Run 2 (Fig. 10) are quite similar to those for Run 3. There are some subtle differences in the Tri-Valley area. The wind in Run 1 has a more westerly component south of the Carquinez Strait. This may prevent the stationary-source emissions along the Strait from entering the Tri-Valley. Near Livermore, the westerly is also stronger. These stronger westerly components of the wind can be attributed to the stronger temperature contrast between the ocean and the Central Valley in the runs with the Noah LSM. The effect of this stronger westerly is to move the southern part of the high ozone area further to the east, from near Livermore to Tracy (Fig. 5), a station 20 km east of Livermore. The northern part of the high ozone area also moved eastward slightly. The simulated maximum ozone is located 23 km northeast of Livermore with a magnitude of 120 ppb.

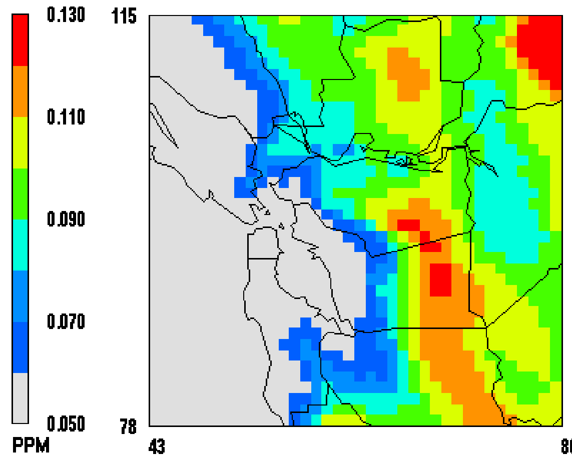

Fig. 7. The simulated ozone distribution over the SFBA for Run 3 at 1600 PST, July 31, 2000.

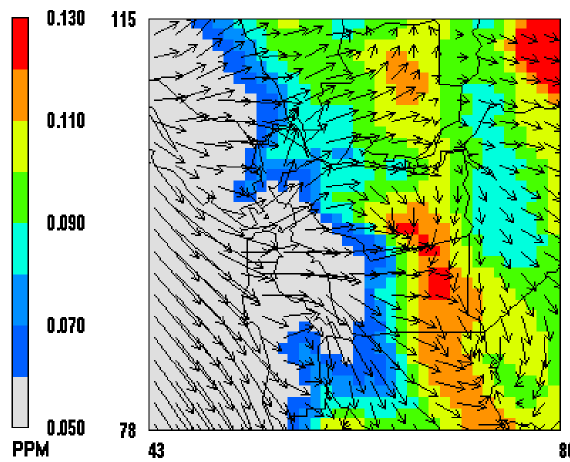

Fig. 8. Same as Fig. 5, but with simulated wind vectors.

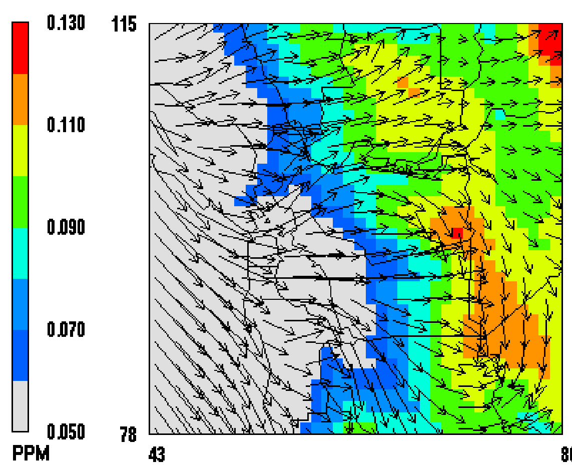

Fig. 9. Same as Fig. 8, but for Run 1.

The application of FDDA in Run 2 improved the wind near the Carquinez Strait, but it further increased the westerly wind speed near Livermore and moved the southern part of the convergence line further toward the east. As a result, the southern part of the high ozone line moved past Tracy into the Central Valley. (The maximum observed ozone at Tracy was 91 ppb on this day, significantly less than that at Livermore.) The northern part of the high ozone line also moved further eastward but it stayed in the boundary of the SFBA. The location of maximum ozone did not change from that in Run 1. The magnitude of the simulated peak was 126 ppb, which is identical to the observed maximum ozone at Livermore.

5.3 *Statistical Performance Evaluation of Ozone on July 31, 2000 in the SFBA*

The errors of the simulations can also be defined and compared via statistical methods. A scatter plot of the simulated versus observed ozone for the three runs for all hours of July 31, 2000, in the SFBA is shown in Fig. 11. This is a paired comparison wherein all simulated values were interpolated to the location of the observation stations. The plotted pairs in Fig. 11 can be classified into 3 distinct regimes: (1) a few observations with ozone around 120 ppb; (2) a large cluster of ozone observations below 20 ppb; and (3) the rest of the observations with ozone between 20 and 100 ppb. There is a general overprediction of ozone in regimes 2 and 3. This overprediction may be caused in part by the lateral boundary conditions, where the ozone is set to a constant 40 ppb.

Most of the plotted pairs in regime 2 are nighttime values, when the observed ozone mixing ratios were very small, but when the simulated ozone tends to be in the range of 10-30 ppb. Fig. 11 suggests that Run 3 is performing best for the observed high ozone in regime 1. Run 2 appears to be the second best simulation, followed by Run 1. Since the difference between the simulated and the observed values in regime 1 is a combination of errors in the prediction of the maximum ozone and the prediction of the location of the maximum ozone, the better performance of Run 3 is actually a reflection of the fact that Run 3 gives the most accurate prediction of the location of the peak ozone. As mentioned previously, the maximum ozone simulated in Run 2 exactly matches the observed maximum value; however, that value is not located at an observation station and therefore does not appear in Fig. 11.

Fig. 12 shows the normalized bias and error and the unpaired peak prediction accuracy for the 3 runs. The normalized bias and errors are derived from the paired values shown in Fig. 11. Using the unpaired peak prediction accuracy as the measure, Run 2 performed the best with no error and Run 1 performed the worst with an underprediction of 5%. However, the normalized bias for Run 1 is the smallest, less than 10%. This smaller bias occurred because while Run 1 under-

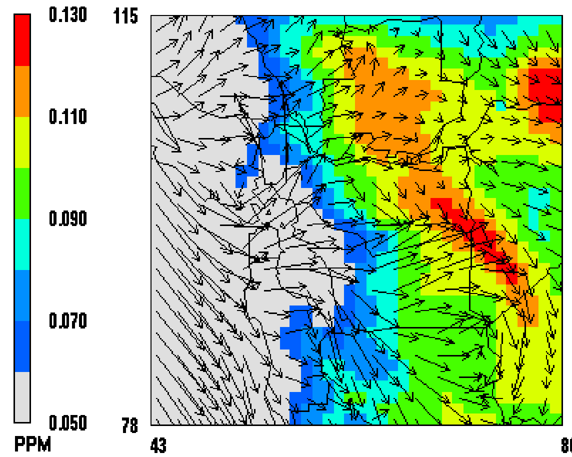

Fig. 10. Same as Fig. 8, but for Run 2.

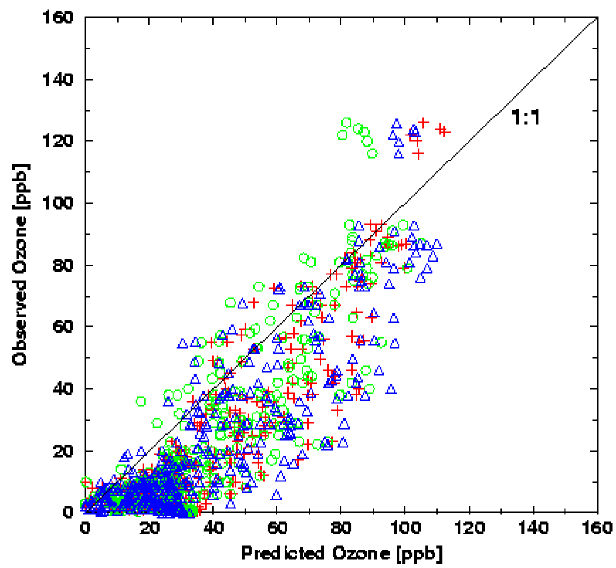

Fig. 11. The scatter plots of the observed and the simulated ozone in the SFBA for Run 1 (circles), Run 2 (triangles) and Run 3 (crosses).

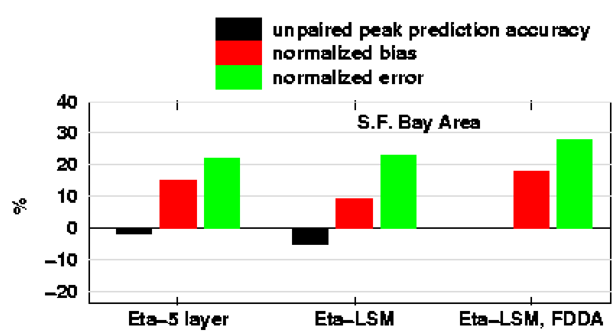

Fig. 12. The normalized bias, error and the unpaired peak prediction accuracy of ozone for Run 3 (Eta-5 layer), Run 1 (Eta-LSM) and Run 2 (Eta-LSM, FDDA).

predicted the high ozone values in regime 1, it has less of a tendency to overpredict the lower values in regimes 2 and 3. The normalized errors in Run 3 and Run 1 are comparable while the normalized error in Run 2 is the largest. The cause for this larger normalized error in Run 2 is the larger overprediction of ozone in regime 3, the mid-range ozone values.

6. SUMMARY AND CONCLUSIONS

This paper has shown that the MM5-CAMx couple produced reasonable predictions of ozone in central California during the July 31-August 2, 2000, period. It also produced reasonable predictions of the locations and timing of peak ozone in the SFBA on July 31, 2000. The prediction skill varied from region to region and from time to time.

Locations of the wind convergence zone and the locations of simulated high ozone were found to be closely related. The overall surface-wind patterns in the SFBA are similar in the 3 MM5 runs, but there are subtle differences in the wind patterns among the runs in and near the Livermore Valley. The runs with the 5-layer soil model, as reported in Part I of the paper, underpredicted Central Valley temperatures and therefore produced a weaker sea breeze. This weaker sea breeze created a convergence line close to Livermore and produced an ozone pattern that, among the three simulations, compared best with observations.

The MM5 runs using the Noah LSM, while producing a reasonable Central Valley temperature, created a much stronger sea breeze. This stronger sea breeze moved the convergence zone about 20 km east of Livermore. This trade-off between accurate inland temperature and accurate sea-breeze predictions may indicate a deficiency in the current MM5 model.

There are several possible explanations for this problem. One explanation is that the second-order advection scheme used in MM5 requires such large diffusion values that the mountain-blocking effect is reduced and the sea breeze front is propagated too far inland. Another possible explanation is the lack of a mountain drag parameterization that would tend to reduce the speed of the sea breeze in the Tri-Valley and more accurately channel the flow. A third possible explanation is the lack of vertical resolution in the original data input to MM5 to define the inversion layer during this high ozone period. A comparison between the MM5 output and the observed vertical profiles of temperature did show that the strength of the inversion is underpredicted.

An important conclusion, then, is that some relatively subtle flow features, which may not be fully appreciated in meteorological model performance evaluations, can have a significant influence on the performance of a photochemical model.

Acknowledgements

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