Final Report

Application of CAMx and CMAQ Models to the August - September, 1997 SCOS Episode CRC Project A-40-2

Prepared for
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METEOROLOGICAL MODELING

The MM5 meteorological model was applied to the South Coast Air Basin (SoCAB) for the August-September 1997 period on a 45/15/5 km resolution grid. Numerous MM5 sensitivity simulations were carried out to try to improve the representation of meteorological conditions in the SoCAB during the modeling period. Based on the surface meteorological observations, a more optimal MM5 model configuration was identified that produced improved MM5 model performance over the previous sensitivity runs. CAMx and CMAQ meteorological inputs were then generated using the final MM5 outputs and the, respectively, MM5CAMx and MCIP meteorological processors.

EMISSIONS MODELING

Hourly gridded and point source speciated emissions for the CAMx model were generated for the August-September 1997 period using the California Air Resources Board (ARB) Gridded Emissions Model (GEM) setup for the August 3-6, 1997 episode and gridded biogenic emissions for August 3-7 and September 26-28, 1997. Emissions for other days from August-September, 1997 modeling period were generated by matching like days (e.g., day-of-week and similar temperatures) for days GEM emission inputs were available. Three-dimensional emissions for the CMAQ model were generated using a CAMx-to-CMAQ emissions processor that uses the CAMx two-dimensional gridded low-level and point source stack emissions files, the CAMx meteorological inputs and the CAMx plume rise algorithm.

PHOTOCHEMICAL GRID MODELING

The CAMx and CMAQ models were applied to the SoCAB 5 km resolution modeling domain for the August-September 1997 period and evaluated using available ozone, VOC, NOx, PM_{10} and speciated fine and coarse particulate matter (PM) data.

Ozone Model Performance

The ozone performance of the CAMx and CMAQ models for the August-September 1997 period is mostly poor with the two models exhibiting a large underestimation bias for the higher observed ozone days. The 187 ppb episode peak observed 1-hour ozone concentrations is underestimated by the CAMx and CMAQ models by approximately –20% and –30%, respectively, unpaired by location, and by approximately –40% by both models at the station location. EPA's 1-hour ozone $<\pm15\%$ normalized bias performance goal is rarely met by either model during the two-month modeling period with normalized bias levels for the two models typically between –20% and –50%. Similar underestimation bias was seen with 8-hour ozone model performance. On many high ozone days there was evidence of recirculation of pollutants out over the Ocean, as evident by observed elevated ozone levels on Santa Catalina and San Clemente Islands, that were not captured by either of the MM5/CAMx or MM5/CMAQ modeling systems. The CAMx and CMAQ models exhibited similar ozone model performance.

PM_{10} Model Performance

The two models underestimated the observed daily maximum PM_{10} peaks by approximately –50% for most days during the modeling period. During August 1997, the CAMx and CMAQ models exhibited some skill in estimating PM_{10} concentrations with most days exhibiting relatively low normalized bias (<±40%). In September 1997 the PM_{10} model performance was worse with several days exhibiting normalized bias greater than 100%. The PM_{10} performance for both CAMx and CMAQ models is very similar with both models exhibiting better and worse model performance on the same days.

Speciated PM Model Performance

Speciated PM observations were available at three sites for two 2-day intensive periods (August 21-22 and 27-28) during the August-September 1997 modeling period. The two models generally overstated the observed fine ($PM_{2.0}$) Elemental Carbon (EC) concentrations, with the overestimation being greater for PM_{10} EC because many PM_{10} EC measurements were less than their $PM_{2.0}$ EC counterparts due to measurement uncertainties. The two models exhibit an underestimation tendency for Organic Matter (OM) of –75% to –85% that is likely partly due to missing OC in the inventory, Secondary Organic Aerosol (SOA) formation processes not accounted for in the two models and meteorological uncertainties.

CMAQ exhibited near zero bias for fine ammonium, but a –50% to –60% under-prediction bias for fine+coarse ammonium. CAMx, on the other hand, exhibited bias for fine ammonium of from 0% to –86% and understated fine+coarse ammonium by –5% to –53%. The two models exhibited similar performance for ammonium with CMAQ performing slightly better for fine ammonium and CAMx performing slightly better for fine plus coarse (PM_{10}) ammonium.

Both models greatly (>100%) overestimate fine nitrate in the SoCAB for all four intensive days. CMAQ does a better job than CAMx in simulating fine+coarse nitrate with normalized bias values of –44% to 45%, whereas CAMx exhibits an overestimation bias of 20% to 118%. However, CAMx does a slightly better job in reproducing the observed sulfate concentrations with the CAMx bias for fine sulfate ranging from –31% to 21%, whereas CMAQ estimates an underestimation bias across all four days that range from –10% to –44%. Both models underestimate fine+coarse sulfate with the CAMx bias levels (-27% to –45%) being slightly better than seen for CMAQ (-45% to –55%).

(VOC) Volatile Organic Compound Emissions Sensitivity Tests

A VOC emission sensitivity test was performed using the CAMx model that increased VOC emissions by 40% (1.4 x VOC); the 1.4 factor was based on comparisons of VOC and NOx predictions and observations. Ozone model performance was greatly improved in the enhanced VOC emissions sensitivity test, both in terms of the performance statistics and in the spatial distribution of ozone predicted concentrations. The enhanced VOC emission sensitivity test had less effect on PM performance with EC and OM performance not affected, nitrate performance slightly degraded and sulfate performance slightly improved.

CONCLUSIONS

Similar poor ozone model performance is exhibited by the CAMx and CMAQ models for the August-September 1997 simulation of the SoCAB. The primary reason believed for this poor ozone performance is due to inadequate meteorological fields that, among other things, fail to reproduce the recirculation of pollutants in the SoCAB. Insufficient VOC or too much NOx emissions may also be contributing to the ozone under-prediction bias. The performance of the two models for PM in the SoCAB is more encouraging, although performance problems still exist. However, the models exhibited some skill in predicting sulfate and some other PM species components with PM performance for most species similar to other CAMx and CMAQ applications. With the possible exception of nitrate, where CAMx exhibited a larger overestimation tendency than CMAQ, the two models exhibited very similar ozone and PM model performance and tracked each others day-by-day performance tendencies, both good and bad, very well and neither model exhibited superior model performance to the other across all species and days in the modeling period.

RECOMMENDATIONS

Additional sensitivity analysis of the ozone and nitrate performance is warranted. Ozone sensitivity to meteorology and emissions, including use of MM5 fields of Boucouvala and Bornstein (2003) is recommended. Model ozone sensitivity to chlorine emissions (e.g., sea salt, swimming pools, etc.) and re-nitrification (i.e., the decomposition of nitric acid to NO_2 that is not treated in the Carbon Bond IV mechanism) is also needed. For nitrate, model sensitivity to deposition, ammonia emissions, and heterogeneous chemistry is needed to improve model formulation.

1.0 INTRODUCTION

BACKGROUND

The Coordinating Research Council (CRC) funded the implementation of full-science aerosol chemistry and sectional size modules developed by Carnegie Mellon University (CMU) and the California Institute of Technology (CIT) in the Comprehensive Air-quality model with extensions (CAMx) under CRC Project A-30 (ENVIRON, 2003; Morris et al., 2003a,b). The particulate matter (PM) version of CAMx was then applied to the South Coast (Los Angeles) Air Basin (SoCAB) region of Southern California for the October 1995 episode that occurred during the PM_{10} Technical Enhancement Program (PTEP). The emphasis in CRC Project A-30 was on the development and testing of the new PM version of the CAMx model. Thus, the October 1995 SoCAB modeling databases were based on readily available information with meteorological fields developed using the CALMET diagnostic meteorological model. The CALMET interpolated fields were less than optimal for photochemical grid modeling and not dynamically balanced. Thus, although the CAMx model was successfully applied for the October 1995 SoCAB episode and the modeling results generally appeared reasonable, there was a need to apply CAMx for PM in the SoCAB using more dynamically balanced meteorological fields.

Initial Modeling of September 26-28, 1997 SCOS Episode

CRC sponsored Project A-40-2 to apply the CAMx and the Models-3 Community Multi-scale Air Quality (CMAQ) models to the September 26-28, 1997 Southern California Ozone Study (SCOS) weekend episode during which elevated ozone and PM concentrations occurred in the SoCAB. MM5 meteorological modeling and emissions modeling using the California Air Resources Board (ARB) Gridded Emissions Model (GEM) were conducted to generate CAMx modeling inputs. Extensive MM5 sensitivity simulations were carried out to develop dynamically balanced meteorological fields for photochemical grid modeling of the SoCAB.

An initial application of the CAMx modeling using the September 26-28, 1997 MM5/GEM modeling databases exhibited poor ozone model performance; the model failed to reproduce the level of photochemical oxidants that were observed in the SoCAB. In particular, elevated (80-90 ppb) ozone concentrations observed at offshore islands (e.g., Catalina and San Clemente) were grossly underestimated suggesting that the modeling system failed to reproduce the recirculation of pollutants offshore. Note that the ARB and South Coast Air Quality Management District (SCAQMD) also attempted to model the September 26-28, 1997 weekend SCOS episode using UAM, CAMx, CALGRID and CMAQ for the 2003 Air Quality Management Plan (AQMP) and abandoned the episode due to poor ozone performance (SCAQMD, 2003) at about the same time.

Rather than proceeding with the CAMx and CMAQ PM modeling of the September 26-28, 1997 episode as originally planned, which would clearly produce inadequate secondary PM impacts due to incorrect depiction of photochemistry, the project was expanded to model the August-September 1997 two-month period using MM5, CAMx and CMAQ to investigate whether the ozone performance problems of the September 26-28, 1997 episode are related to the specific episode or are more endemic of air quality modeling of the SoCAB using the MM5/GEM/CAMx/CMAQ modeling systems.

OVERVIEW OF APPROACH

The application of CAMx and CMAQ to the August-September 1997 SCOS episode involved the following activities:

1. MM5 meteorological modeling of the August-September, 1997 period and evaluation of the MM5 meteorological variables estimates against observations.

2. Emissions modeling of the August-September 1997 period using the ARB Gridded Emissions Model (GEM) emissions databases for the August 3-7, 1997 and September 26-28, 1997 SCOS episodes and speciated into species used by CAMx4/PMCAMx and CMAQ.

3. Analysis and processing of the SCOS ambient air quality database to species and size-sections for use in the model evaluation.

4. CAMx modeling of the August-September 1997 period and evaluation of the model first against the SCOS ozone and then PM measurement database.

5. CMAQ modeling of the August-September 1997 period and evaluation against the SCOS measurement database.

6. Documentation of the study including Quarterly Progress Reports, Interim Reports, Draft Final and Final Reports.

REPORT ORGANIZATION

Section 2 discusses the development of the meteorological and emission inputs for the August-September 1997 two-month period and the CAMx and CMAQ models. The evaluation of the CAMx and CMAQ models for August-September 1997 episode and the SoCAB is presented in Section 3. Section 4 contains the summary and conclusions.

2.0 DEVELOPMENT OF METEOROLOGICAL AND EMISSION INPUTS FOR THE AUGUST-SEPTEMBER 1997 PERIOD

The development of the meteorological and emission inputs for the August-September 1997 SCOS modeling period and the CAMx and CMAQ models is summarized below.

INITIAL MM5 MODELING OF AUGUST – SEPTEMBER 1997

The MM5 meteorological model was exercised for the August-September 1997 period and the results subjected to a model performance evaluation. Numerous MM5 sensitivity simulations were performed for the SoCAB and the September 26-30, 1997 episode to test the MM5 model configuration and try to improve the MM5 and CAMx ozone model performance. Based on this preliminary analysis, the best performing MM5 configuration for the SoCAB and September 26-30, 1997 episode was as follows:

- 45/15/5-km two-way nested-grid modeling domain;
- Kain-Fritsch parameterization scheme for the 45 and 15 km resolution domains;
- Simple ice microphysics;
- Rapid Radiative Transfer Model (RRTM) radiation scheme;
- Medium Range Forecast (MRF) planetary boundary layer (PBL) parameterization scheme;
- NOAH OSU land-surface model (LSM); and
- Four Dimensional Data Assimilation (FDDA) of surface and 3D analysis nudging (AN) of wind, temperature, and moisture on the 45-km and 15-km grids to the Eta Data Assimilation System (EDAS) analysis fields.

This configuration was used for the initial MM5 simulation (Run1) of the August-September 1997 modeling period. The MM5 August-September 1997 Run1 simulation was subjected to a model performance evaluation that compared the MM5 estimated surface wind speed, wind direction, temperature and water vapor mixing ratio estimates to the observed value. Table 2-1 summarizes the MM5 Run1 model performance for wind speed and wind direction for the months of August and September 1997 and compares them against model performance benchmarks (Emery and Tai, 2001). For both the wind speed bias and RMSE, the MM5 model performance failed to achieve the model performance benchmarks. The model appears to underestimate the average wind speeds across the SoCAB for most days during the August-September 1997 period. Although the wind direction bias achieves the 10 degree performance benchmark, it exceeds the 30 degree gross error benchmark by a wide margin (43 and 49 degrees during August and September, respectively).

Table 2-1. Comparison of the MM5 Run1 meteorological model performance for surface wind speed and wind direction with model performance benchmarks for August and September 1997.

	Wind Speeds (m/s)				Wind Direction (Degrees)	
	Bias	Error	RMSE	IOA	Bias	Error
August	-1.27	1.97	2.41	0.64	2.19	44
September	-1.10	1.90	2.36	0.60	1.77	49
Benchmark	**≤ ±0.50**	**≤ 2.00**	**≤ 2.00**	**≥ 0.60**	**≤±10**	**≤ 30**

A summary of the MM5 model performance for temperature and mixing ratio and the August and September 1997 period is shown in Table 2-2. The MM5 exhibits an underprediction bias in temperature that exceeds the < ±0.5 degree performance benchmark. The temperature gross errors also exceeds the < 2.0 degree benchmark. The humidity is under-estimated by the simulation. Both the humidity bias and gross error for August and September fail to achieve the benchmark goals.

Table 2-2. Comparison of the MM5 Run1 meteorological model performance for temperature and water vapor mixing ratio (humidity) with model performance benchmarks for August and September 1997.

	Temperature (K)		Humidity (g/kg)	
	Bias	Error	Bias	Error
August	-0.96	2.84	-1.75	2.35
September	-1.07	2.90	-1.75	2.37
Benchmark	≤ ± 0.5	≤ 2.0	≤ ± 1.0	≤ 2.0

The model performance for the initial MM5 Run1 simulation of the August-September 1997 was sufficiently suspect that further analysis and testing of alternative MM5 configurations and inputs were performed.

MM5 SENSITIVITY TESTS AND FINAL CONFIGURATION

A series of MM5 sensitivity tests were performed to investigate alternative MM5 options and inputs to improve model performance that are summarized in the Table 2-3. These sensitivity tests differ in analysis input (EDAS/GDAS), Planetary Boundary Layer (PBL) schemes (ETA, MRF, and Blackadar), Land Surface Schemes (Noah Land Surface Model/Five-Layer Soil Model), and FDDA configurations (nudging coefficients, analysis/observation nudging, and 3D/Surface analysis nudging).

The experience gained by other researchers performing MM5 meteorological modeling of the SoCAB was instrumental in identifying enhancements and options for the final MM5 configuration (Bornstein et al., 2001; Boucouvala et al., 2003; Boucouvala and Bornstein, 2003).

Table 2-3. Design of MM5 sensitivity tests performed for the SoCAB.

Run	Analysis Input	PBL Scheme	LSM	FDDA	Nudging Coefficient (10E-4)			3-D and Surface Nudging	Obs Nudging
					45km	15km	5km		
1	EDAS	MRF	Noah	WD	2.5	1.0	--	Yes	
				T	2.5	1.0	--		
				RH	0.1	0.1	--		
2a	EDAS	ETA	Noah	WD	2.5	1.0	1.0	Yes	
				T	2.5	1.0	1.0		
				RH	0.1	0.1	0.1		
2b	EDAS	ETA	Noah	WD	2.5	1.0	1.0	Yes	
				T	2.5	1.0	1.0	No Sfc on Domain 3	
				RH	0.1	0.1	0.1		
2c	EDAS	ETA	Noah	WD	4.5	2.0	2.0	Yes	
				T	4.5	2.0	2.0		
				RH	0.2	0.2	0.2		
3	GDAS	Blackadar	SLAB	WD	2.5	1.0	1.0	Yes	
				T	2.5	1.0	1.0		
				RH	0.1	0.1	0.1		
3b	EDAS	Blackadar	SLAB	Same	As	Above			
4	GDAS	MRF	SLAB	WD	2.5	1.0	1.0	Yes	WD: 40.0
				T	2.5	1.0	1.0		
				RH	0.1	0.1	0.1		

Notes: WD = Wind direction RH = Relative Humidity
T = Temperature

One surprising finding was that for the episode period studied and the SoCAB domain, performing data assimilation using the lower resolution Global Data Assimilation Fields (GDAS) produced better MM5 performance than using the Eta Data Assimilation System (EDAS) fields that are typically used for US MM5 applications. The reasons for this are unclear but may be related to the fact that the August-September 1997 period was early in the implementation of EDAS and there may have been problems with some of these early fields due to start up problems.

The final MM5 Run4 configuration is as follows:

- GDAS analysis as the “first guess”
- KF cumulus parameterization scheme for the 45 and 15 km resolution domains
- Simple ice microphysics
- RRTM radiation scheme
- Modified MRF PBL parameterization scheme
- SLAB soil model
- Surface and 3D analysis nudging of wind, temperature, and moisture for all three domains
- Observation nudging of wind for the 15km and 5km-resolution domains

Comparisons of daily statistics from MM5 Run1 and the final run (Run4) with the statistical performance benchmarks are summarized in Table 2-4. This statistical summary shows that there are significant improvements for surface wind speed and direction, temperature and humidity in the final run compared to Run1, especially for wind direction and humidity. Whereas in Run1 only 4 of the 11 (36%) MM5 statistical measures achieved the performance benchmarks, in the final Run4, 9 of 11 (82%) of the MM5 performance measures achieved the benchmarks.

Table 2-4. Comparison of the MM5 model performance statistics from two runs in the SCOS 5-km domain for August-September, 1997 with statistical performance benchmark values (shaded mean values exceed the benchmark).

		Run1			RunFin (Run4)		
Parameter	**Benchmark**	**Range**		**Mean**	**Range**		**Mean**
Wind Speed Bias	<± 0.5	-1.66	0.2	-1.18	-1.82	-0.84	-1.20
Wind Speed RMSE	< 2.0	2.05	2.68	2.39	1.33	2.39	1.75
Wind Speed IOA	<0.60	0.48	0.75	0.62	0.64	0.87	0.78
Wind Direction Bias	<± 10	-11.99	12.12	1.98	-1.37	9.26	3.75
Wind Direction Gross Error	< 30	35.96	70.79	46.47	17.53	30	22.59
Temperature Bias	<± 0.5	-2.55	3	-1.02	-2	1.93	-0.94
Temperature Gross Error	< 2.0	1.98	3.85	2.87	1.58	3.19	2.36
Temperature IOA	< 0.80	0.56	0.95	0.91	0.69	0.95	0.92
Humidity Bias	<± 1.0	-3.22	-0.09	-1.75	-1.62	1.75	-0.08
Humidity Gross Error	< 2.0	1.42	3.63	2.36	1.1	2.81	1.97
Humidity IOA	< 0.60	0.41	0.82	0.63	0.36	0.77	0.55

DEVELOPMENT OF EMISSION INPUTS

Gridded speciated anthropogenic emissions for the SoCAB were available for the CAMx model and the August 3-7, 1997 episode. In addition, gridded speciated biogenic emissions were available for the August 3-7, 1997 and September 26-28, 1997 episodes. Biogenic emissions for each day of the August-September 1997 episode were generated from the available biogenic emissions for the August and September episodes by matching up days with similar temperatures. For the anthropogenic emissions, an additional criterion of matching days, by day-of-week (weekday, Saturday and Sunday) was also added.

VERSIONS OF MODELS USED

CAMx Version 4.02 (July 9, 2003 release) was used in the August-September 1997 modeling of the SoCAB. CAMx v4.02 supports a Coarse/Fine (C/F) PM site representation mode where all secondary PM is assumed to be fine, and a full multi-section PM site representation where PM can grow and shrink across size sections. Originally the intent was to run CAMx using both the C/F and multi-section mode. However, when questionable performance was obtained using the C/F mode, more resources were devoted to developing improved meteorological fields.

CMAQ Version 4.4 (October 2004 release) was used for the simulation of the two-month episode period. The CMAQ represents PM size distribution using a modal approach with 3 modes, where secondary PM is assumed to reside in the first two modes. Although the size of the PM can grow above the fine mode, we assumed that the first two modes are fine PM.

3.0 CAMx AND CMAQ MODEL EVALUATION

In this section we evaluate the CAMx and CMAQ model performance for the August-September 1997 period in the South Coast Air Basin (SoCAB). We first discuss the ozone model performance, and then examine performance for particulate matter (PM).

OZONE MODEL PERFORMANCE

The ozone model performance was assessed for ozone monitors within the SoCAB portion of the modeling domain. Monitors close to the boundaries and within the San Diego and other portions of the modeling domain away from the SoCAB were excluded in the evaluation so that we could focus on model performance within the central SoCAB portion of the domain and minimize boundary effects. Figure 3-1 displays the locations of the ozone monitoring sites used in the ozone model performance evaluation for CAMx and CMAQ.

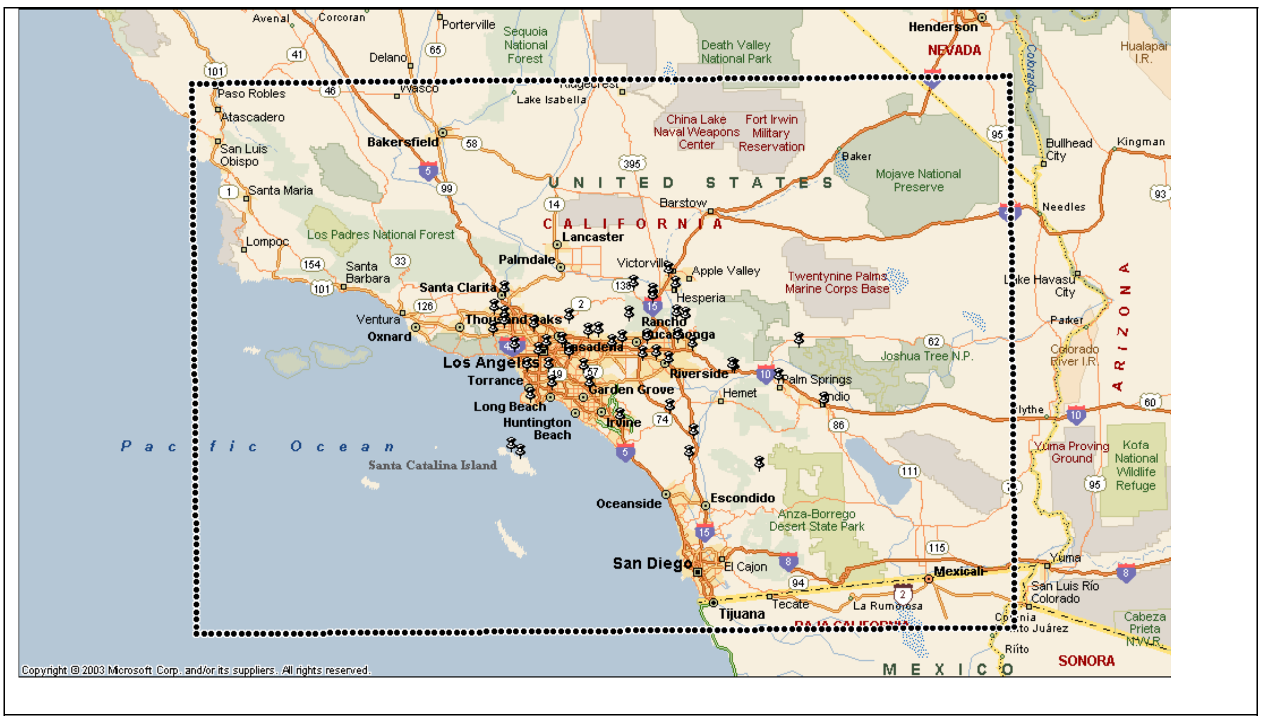


Figure 3-1. Modeling domain and locations of ozone monitors used in the ozone model performance evaluation of CAMx and CMAQ for the August-September 1997 period.

Summary 1-Hour Performance Statistics

EPA has developed 1-hour ozone performance goals for three statistical performance metrics (EPA, 1991):

- Unpaired Peak Prediction Accuracy <±20%;
- Normalized Bias <±15%; and
- Normalized Gross Error <35%.

Figure 3-2 summarizes the 1-hour ozone model performance for the CAMx and CMAQ base case simulation of the August through September 1997 period and the SoCAB. The observed 1-hour ozone peak in the SoCAB during August-September 1997 was 187 ppb and occurred on August 5, 1997. The peak CAMx and CMAQ estimated 1-hour ozone concentrations on this day were 144 and 128 ppb, respectively, so neither CAMx (-23%) or CMAQ (-31%) met the within ±20% performance goal for the unpaired peak on this day. The next highest observed 1-hour ozone concentration during the modeling period was 171 ppb on September 28, 1997 that is underestimated by the CAMx (73 ppb) and CMAQ (79 ppb) by over a factor of two. Two days had observed 1-hour ozone peaks of 170 ppb (August 6 and September 1). On August 6, 1997 the CAMx-estimated 1-hour peak was 147 thereby achieving the <±20% performance goal (-13%), whereas the CMAQ peak of 135 ppb falls right on the performance goal (-20%). On September 1, 1997, the CAMx (97 ppb) and CMAQ (79 ppb) 1-hour ozone peaks were, respectively, -43% and –54% below the observed value. The two models estimated 1-hour ozone peaks almost always are below the observed values with the <±20% performance goal only being achieved by the CAMx and CMAQ models on 33% and 47%, respectively, of the days during August-September 1997 modeling period (Figure 3-2a).

The Normalized Bias <±15% performance goal is rarely met by either CAMx (1 day) or CMAQ (9 days) during the two month modeling period. Both models exhibit an under-prediction bias on almost every day of the modeling period. The Normalized Error < 35% performance goal is met by the two models for approximately half (28 days) of the days during the modeling period.

Summary 8-Hour Ozone Performance Statistics

Although the Unpaired Peak, Normalized Bias and Error performance goals were developed for 1-hour ozone performance, they are applied to 8-hour ozone performance metrics to assist in the interpretation of the 8-hour ozone model performance. Both models tend to underestimate the observed peak 8-hour ozone concentrations in the SoCAB during the modeling period (Figure 3-3a). The within ±20% unpaired peak performance goal is met on only 47% and 33% of the days for, respectively, the CMAQ and CAMx models and 8-hour ozone peaks. The 8-hour ozone normalized bias indicates an underestimation bias throughout the August-September 1997 modeling period, with the <±15% performance goal being met only 7% (CMAQ) and 2% (CAMx) of the days. The less stringent <35% normalized bias performance goal is also met less than half the time by the CMAQ (47% of the days) and CAMx (42% of the days) models.

In 1999 EPA published draft 8-hour ozone modeling guidance that included new approaches for projecting future-year 8-hour ozone attainment that uses the model in a relative fashion through relative reduction factors (RRFs). RRFs are used to project future year Design Values and are defined as the ratio of the highest daily maximum 8-hour ozone concentration near the monitor for the future-year scenario to the current year scenario. The RRFs are applied to the current year observed 8-hour ozone Design Value to obtain the future-year projected 8-hour ozone Design Value. Thus, the 8-hour ozone model performance for the maximum 8-hour ozone concentrations near the monitor is an important performance metric. Thus, EPA included a performance goal of this value being within ±20% of the observed value on most days in their draft 8-hour modeling guidance (EPA, 1999). For near the monitor we use the same 7 x 7 array of 5 km grid cells as required in the attainment test. Three different approaches have been used to select the predicted daily maximum 8-hour ozone concentrations near the monitor for comparison with the observed value:

- The maximum estimated daily maximum 8-hour ozone concentrations near the monitor, as used in the attainment test;
- The nearest estimated daily maximum 8-hour ozone concentrations to the observed value; and
- The estimated daily maximum 8-hour ozone concentrations at the monitor (spatially paired).

Figure 3-4 displays scatter plots of the predicted and observed daily maximum 1-hour (Figure 3-4a) and 8-hour (Figure 3-4b) ozone concentrations near the monitor using the maximum, nearest and spatially paired definitions of near the monitor given above. Also shown in these figures are the Quantile-Quantile plots (i.e., cumulative distribution of predictions and observations). The performance of CAMx and CMAQ is comparable for this performance metric with a majority of the predicted daily maximum 1-hour and 8-hour ozone concentrations being within ±20% of the observed value. CMAQ appears to produce slightly higher 8-hour ozone than CAMx that results in slightly improved performance. However, both models exhibit worse model performance than typically seen for ozone, especially under higher observed ozone conditions.

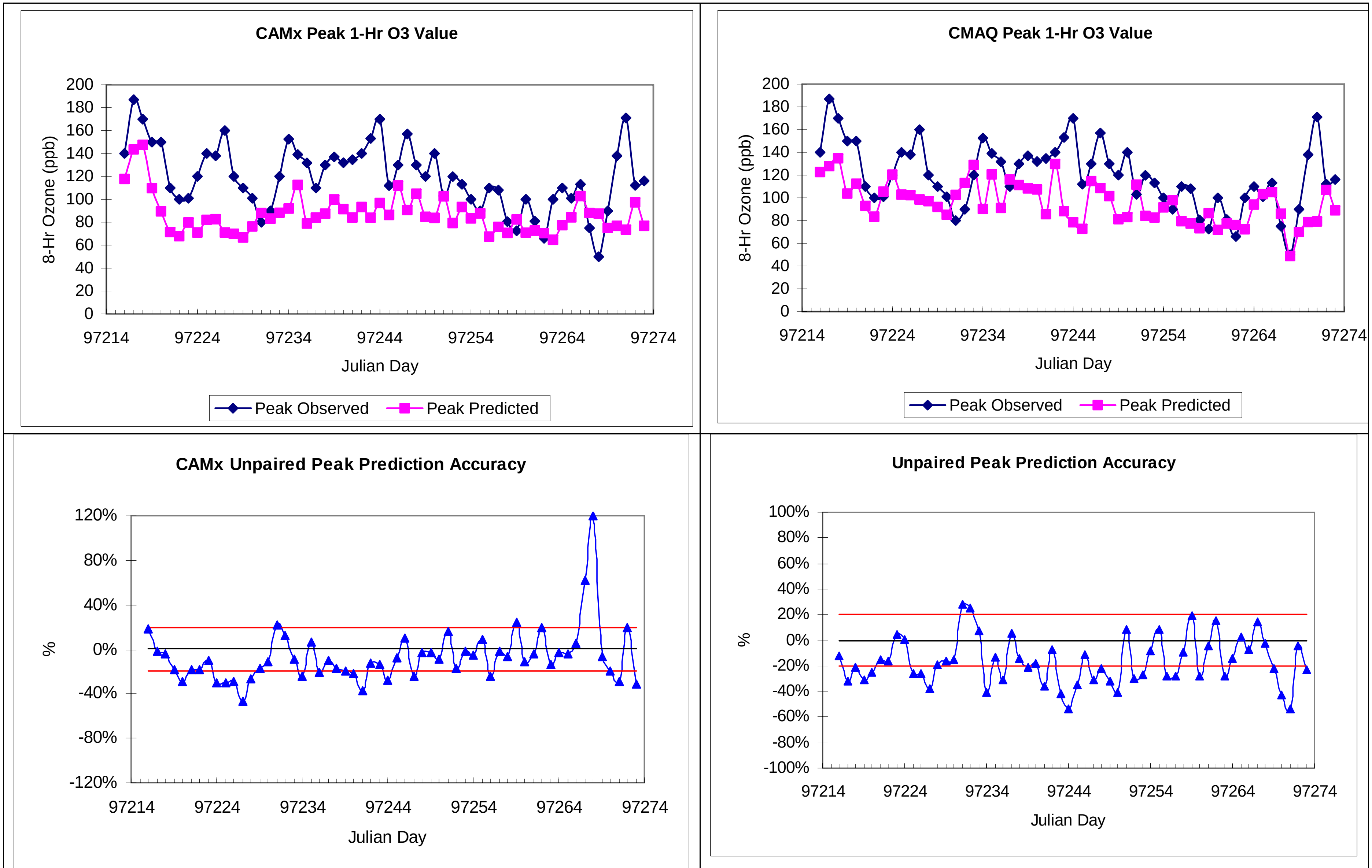


Figure 3-2a. Peak 1-hour ozone performance in the SoCAB for August-September 1997 and the CAMx (left) and CMAQ (right) models.

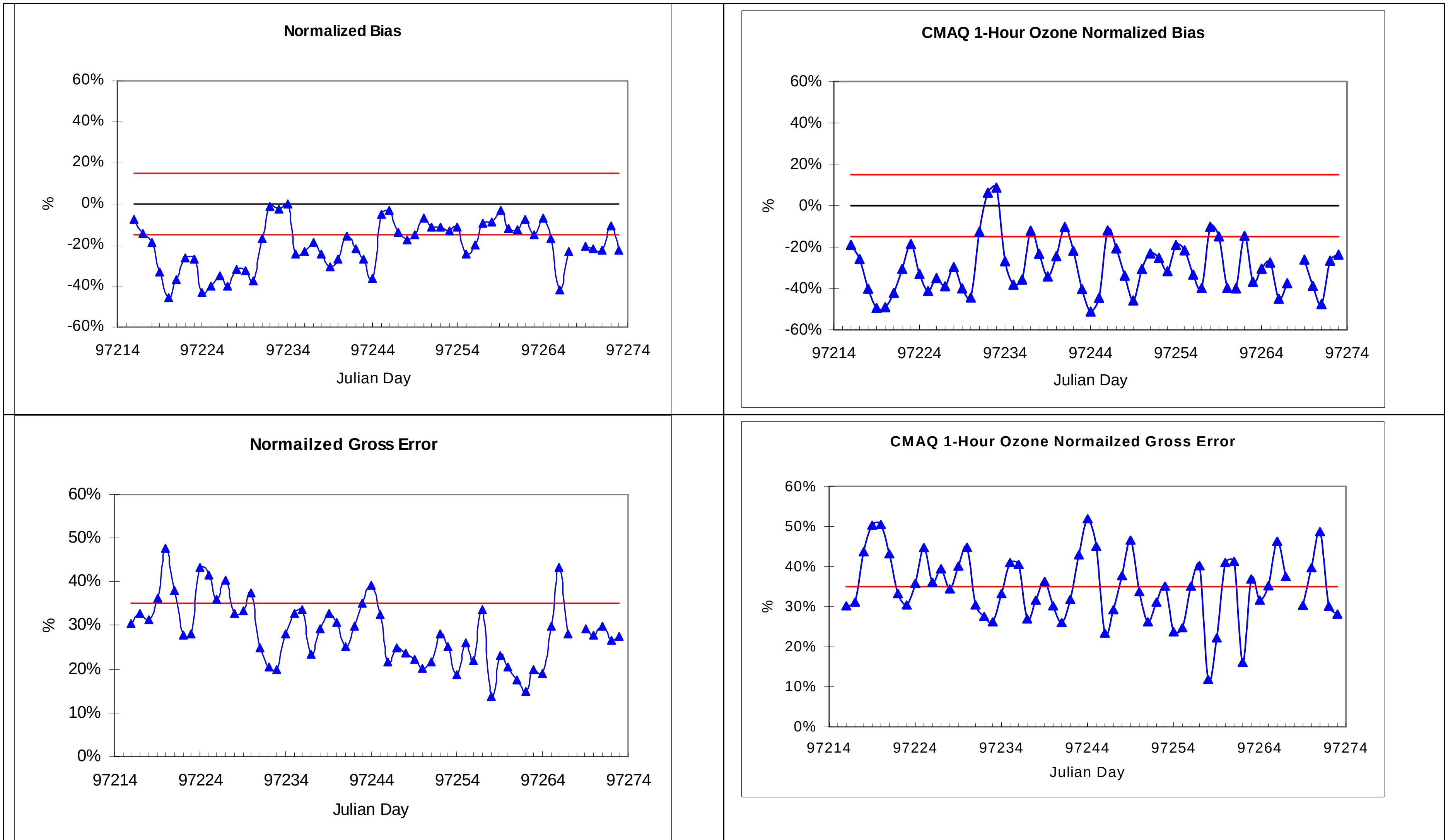


Figure 3-2b. Normalized bias (top) and normalized gross error (bottom) for 1-hour ozone concentrations and the CAMx (left) and CMAQ (right) simulations of the SoCAB and the August-September 1997 period.

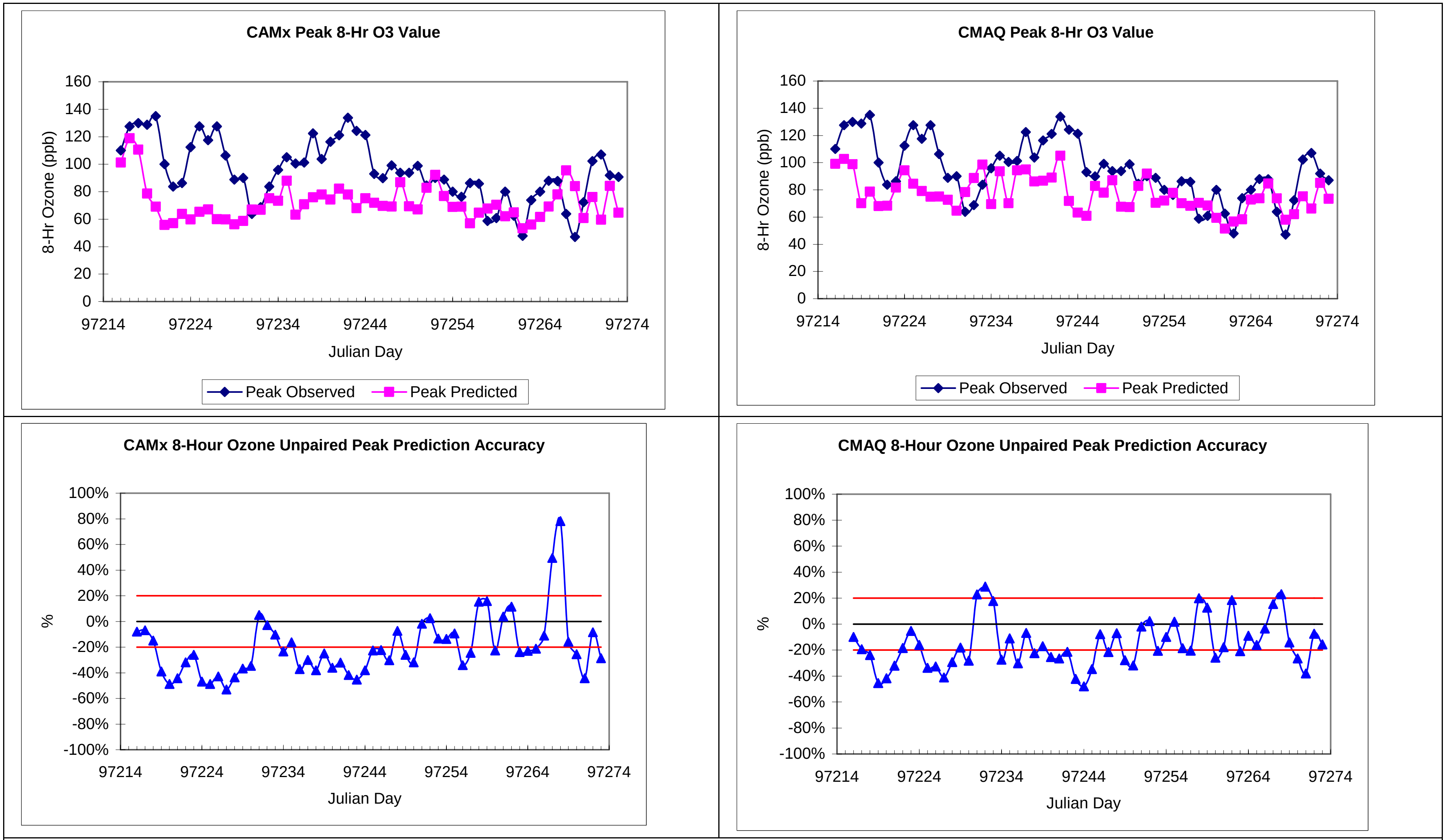


Figure 3-3a. Peak 8-hour ozone performance in the SoCAB for August-September 1997 and the CAMx (left) and CMAQ (right) models.

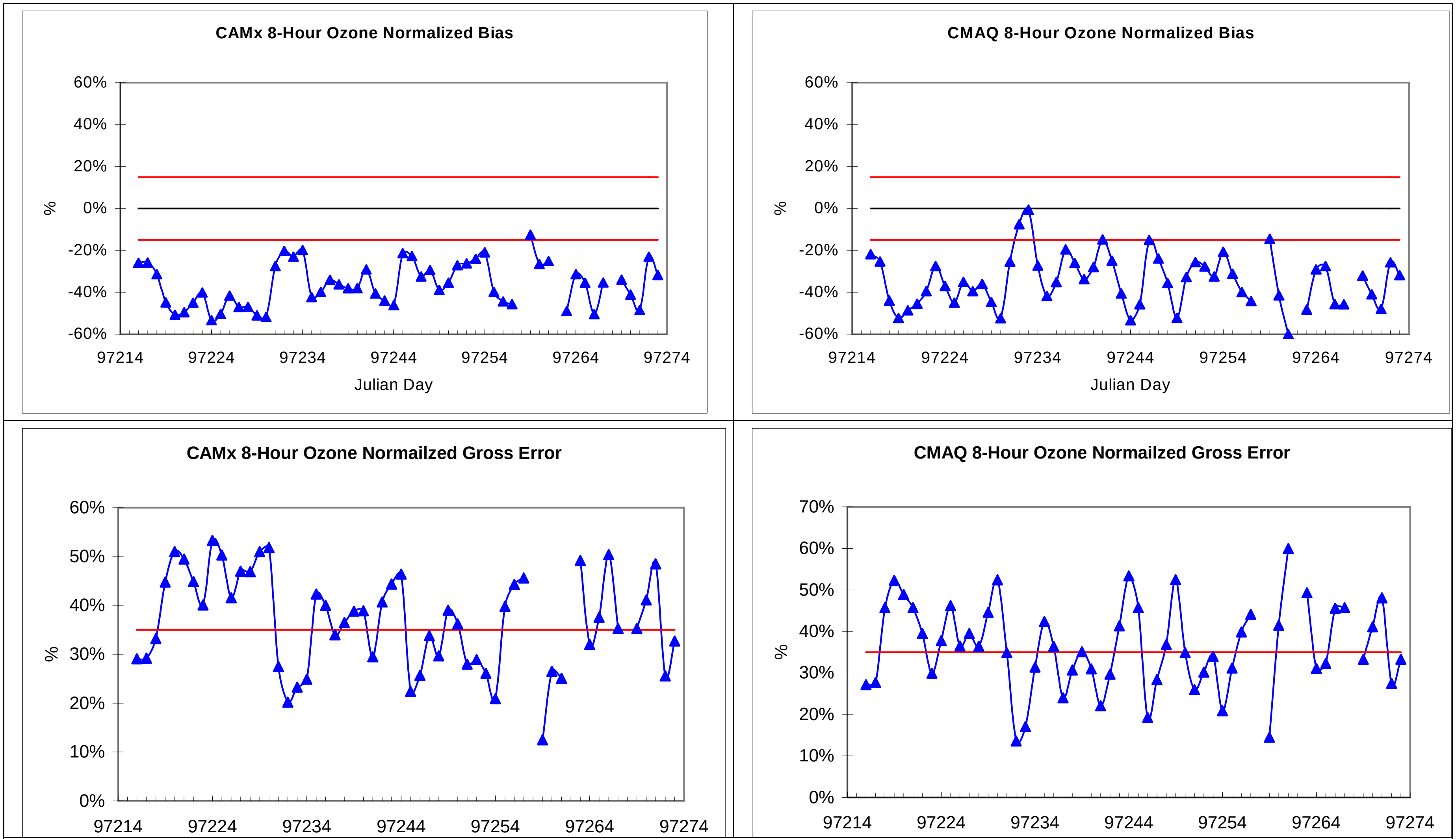


Figure 3-3b. Normalized bias (top) and normalized gross error (bottom) for 8-hour ozone concentrations and the CAMx (left) and CMAQ (right) simulations of the SoCAB and the August-September 1997 period.

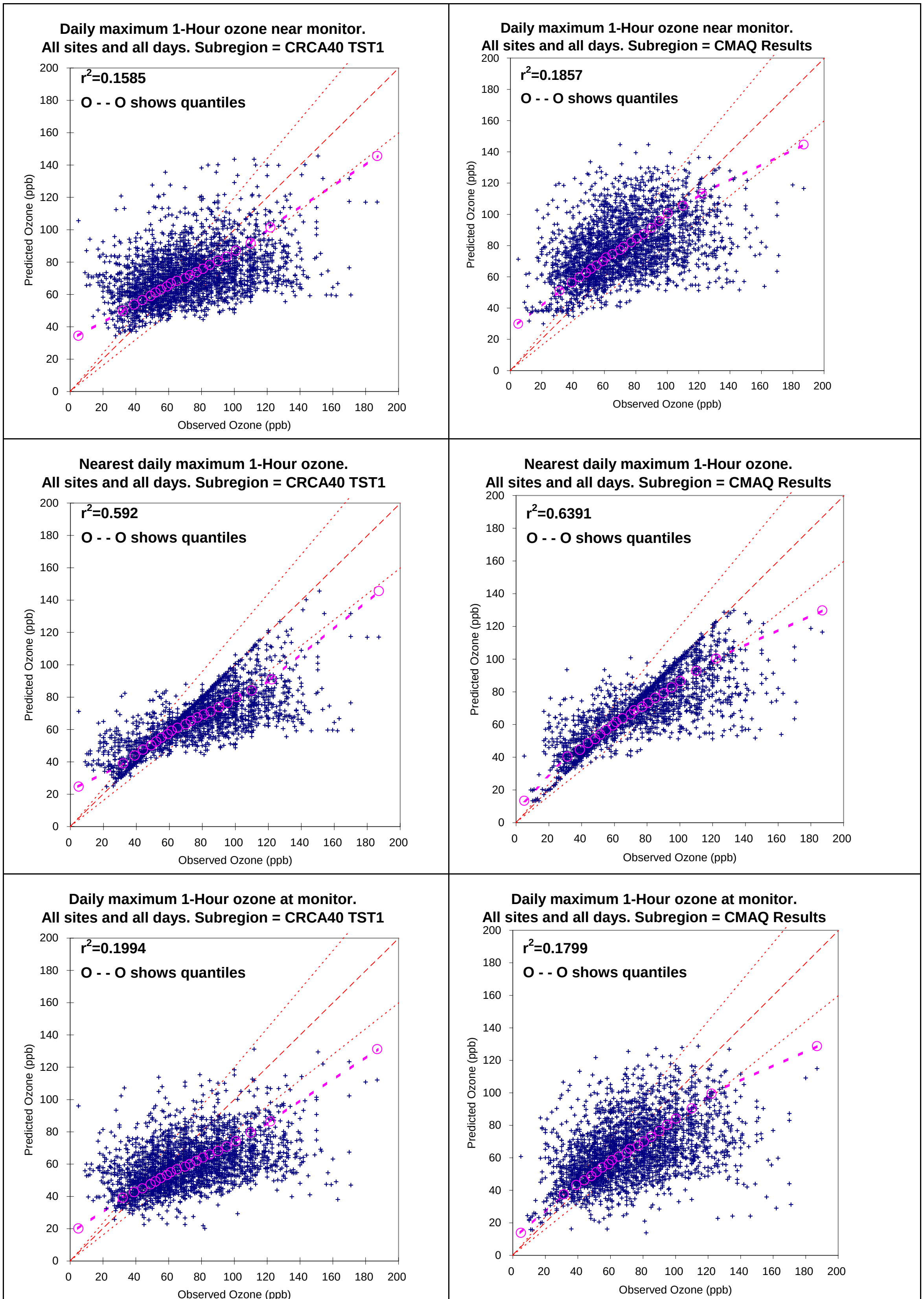


Figure 3-4a. Predicted and observed daily maximum 1-hour ozone concentrations near the monitor for CAMx (left) and CMAQ (right) using maximum (top), closest (middle) and spatially paired ozone estimate near the monitor.

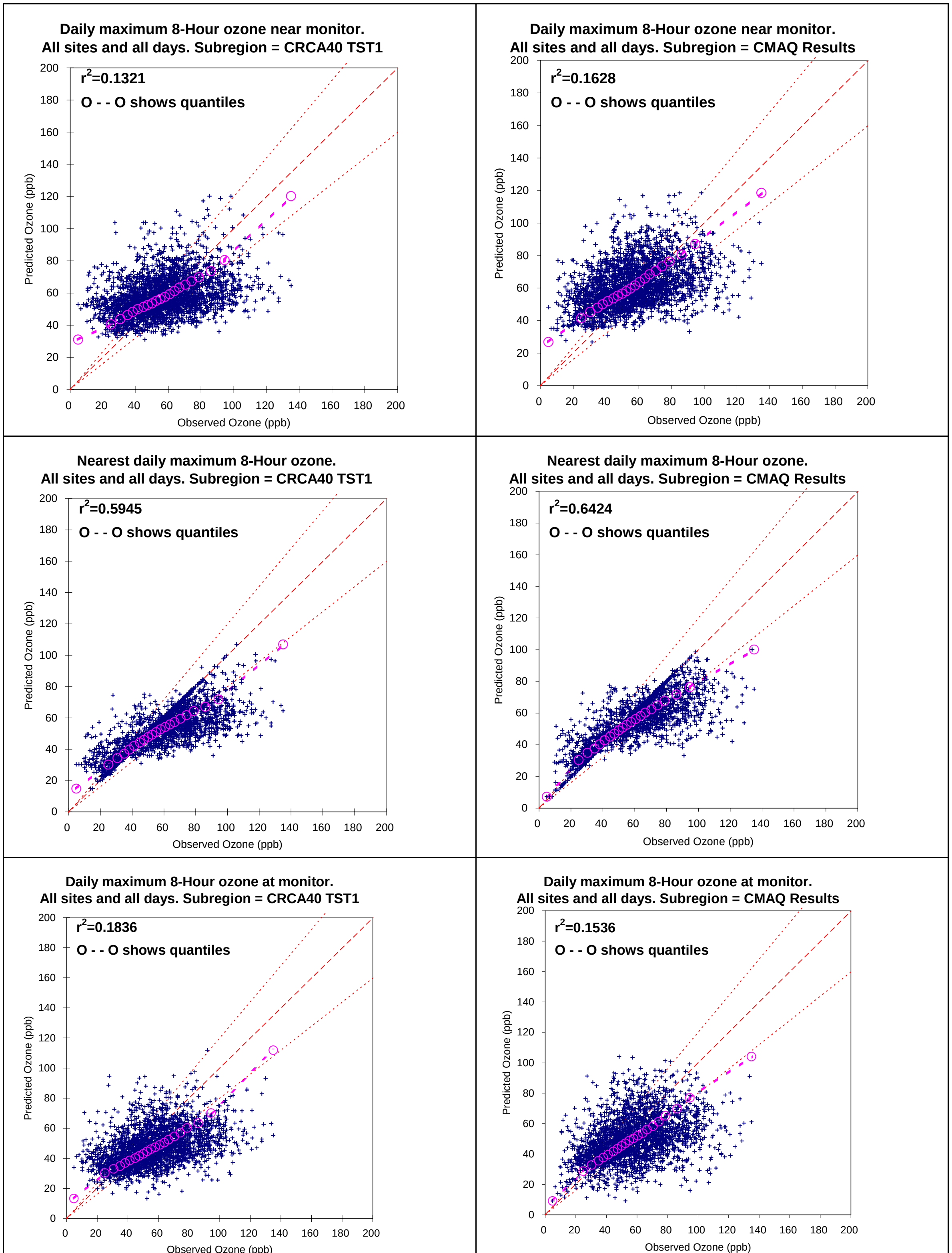


Figure 3-4b. Predicted and observed daily maximum 8-hour ozone concentrations near the monitor for CAMx (left) and CMAQ (right) using maximum (top), closest (middle) and spatially paired ozone estimate near the monitor.

Spatial Maps of Predicted and Observed Ozone Concentrations

Appendices A and B display daily maximum 1-hour and 8-hour ozone concentrations estimated by the CAMx and CMAQ models with superimposed daily maximum 1-hour and 8-hour observations for the five days from August-September 1997 in which the peak 1-hour observed ozone concentrations were 160 ppb or higher. The spatial maps comparing daily 1-hour predicted and observed ozone for the two highest ozone days, August 5, 1997 and September 28, 1997, are also shown in Figures 3-5 and 3-6.

August 5, 1997: On August 5, 1997 the episode maximum 1-hour observed value of 187 ppb occurred at the Rubidoux monitor where CAMx and CMAQ daily maximum 1-hour estimated ozone peaks were 112 ppb (-41%) and 115 ppb (-39%) (Figures 3-5 and A-1). South of the Rubidoux monitor CAMx estimates a cloud of elevated 1-hour ozone > 130 ppb with a peak of 144 ppb, whereas CMAQ also estimates elevated 1-hour ozone in the 120-130 ppb at the same location. Both models estimate elevated 1-hour ozone in the San Diego and Tijuana areas with the CAMx ozone levels (120-130 ppb) being slightly lower than those seen for CMAQ (140-152 ppb). There are similarities and differences in the spatial distribution of the CAMx and CMAQ 1-hour ozone clouds on August 5th. Probably the biggest difference is the elevated (120-130 ppb) 1-hour ozone cloud estimated by CMAQ north of Los Angeles in the San Bernardino Mountains surrounded by observed 1-hour ozone peaks of 86-142 ppb where CAMx estimates slightly lower ozone levels of 100-110 ppb). The similarity in the CMAQ and CAMx model performance on this day suggests the under-prediction bias is driven by deficiencies in the meteorological and/or emission inputs common to the two models, rather than a deficiency in model formulation. Similar results and spatial patterns are seen for 8-hour ozone on this day (Appendix B-1).

August 6, 1997: The peak observed 1-hour ozone on August 6, 1997 was 170 ppb and occurred at Lake Arrowhead just north of San Bernardino where the CAMx (124 ppb) and CMAQ (87 ppb) models reproduce the observed ozone peak to within –27% and –49%, respectively (Figure A-2). CAMx estimates high 1-hour ozone in Riverside (> 140 ppb) that stretches northward into San Bernardino-Lake Arrowhead region, whereas the CMAQ estimated peak in Riverside (145 ppb) is very localized and does not stretch northward resulting in the poorer model performance at the location of the observed 1-hour ozone peak. Despite this difference, the spatial distribution of the CAMx and CMAQ estimated daily maximum 1-hour ozone concentrations are quite similar with elevated ozone concentrations in Riverside, the San Bernardino Mountains, Palm Springs, San Diego and Mexicali. Similar results are seen for the daily maximum 8-hour ozone comparisons on this day (Figure B-2) where the observed 8-hour ozone peak of 130 ppb is reproduced by the CAMx (93 ppb) and CMAQ (60 ppb) models to within –29% and –54%, respectively.

August 15, 1997: The observed 160 ppb peak 1-hour ozone at Lake Arrowhead on August 15^{th} is underestimated by the CAMx (63 ppb) and CMAQ (77 ppb) models by –61% and –52%, respectively (Figure A-3). Both CAMx and CMAQ estimate fairly clean conditions in and downwind of the SoCAB despite observed values of > 130 ppb occurring north of San Bernardino at several sites in the San Bernardino Mountains (e.g., Mount Baldy, Phelan and Lake Arrowhead). CMAQ estimates slightly higher ozone than CAMx, which is likely due to the higher vertical mixing rate in the CMAQ than CAMx inputs. 1-hour and 8-hour (Figure B-3) ozone model performance for both models is very poor on this day.

September 1, 1997: The 170 ppb observed 1-hour ozone peak on September 1st again occurs at Lake Arrowhead, but elevated observed ozone also occurs at the San Bernardino (149 ppb), Crestline (144 ppb) and Fontana (142 ppb) monitoring sites. Both CAMx and CMAQ severely underestimate the observed ozone concentrations on this day with the CAMx estimated ozone at the four sites listed above where the observed 1-hour peak exceeded 140 ppb ranging from 62-67 ppb, similar values for CMAQ are 42-44 ppb. Clearly neither CAMx nor CMAQ are capturing the meteorological and chemical processes that led to high observed 1-hour (Figure A-4) and 8-hour (Figure B-4) ozone on this day.

September 28, 1997: The two models exhibit extremely poor ozone model performance on Sunday September 28, 1997 (Figure 3-6 and A-5). Both models estimate an ozone hole < 40 ppb centered on Los Angeles where observed values are > 100 ppb. At Upland, where the observed ozone peak of 171 ppb occurs, CAMx and CMAQ estimate 1-hour ozone peaks of 47 ppb and 31 ppb, respectively. Similar poor 8-hour ozone model performance is exhibited by the two models with a severe ozone underestimation bias (Figure B-5).

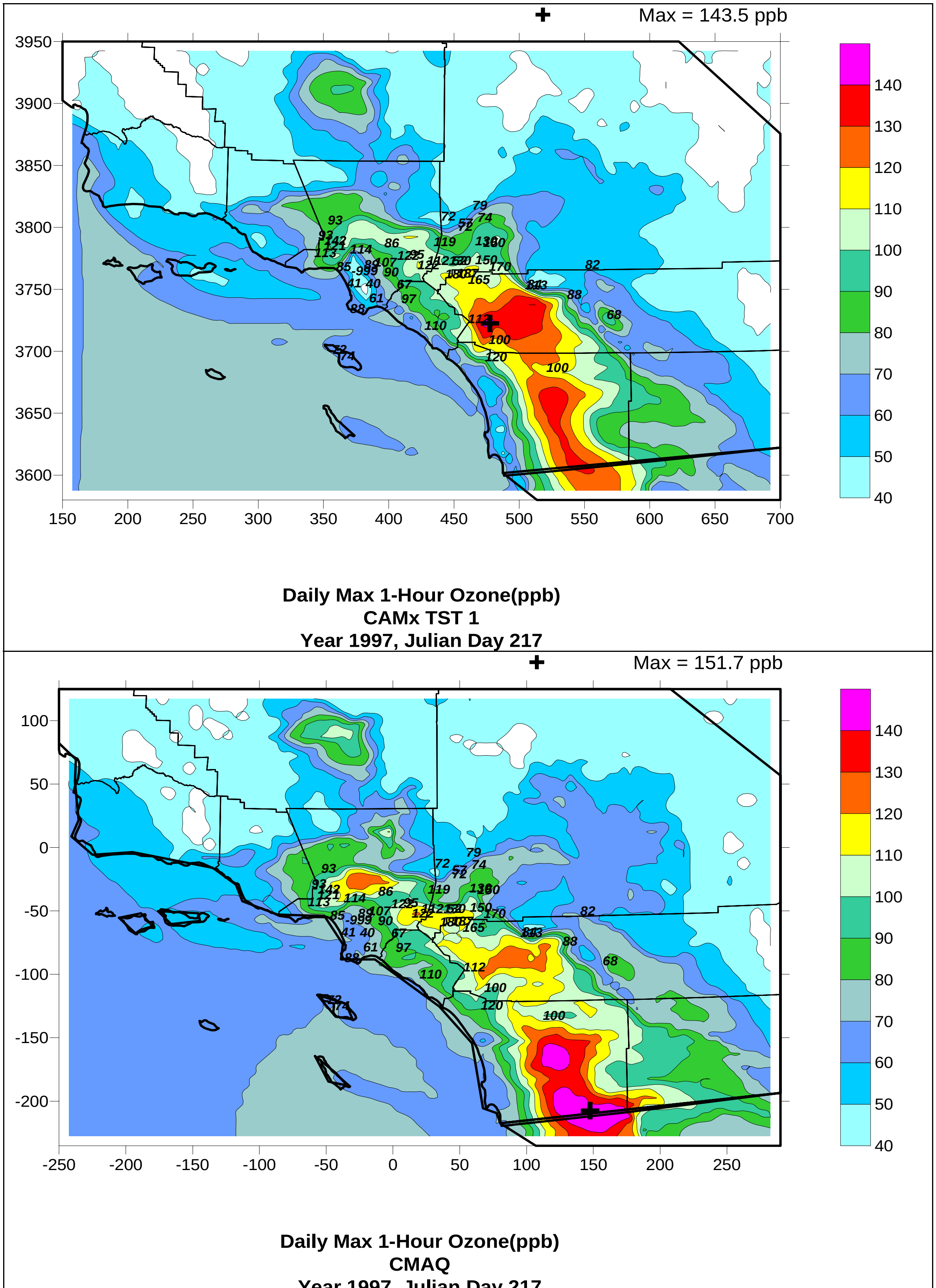


Figure 3-5. Daily maximum observed and CAMx (top) and CMAQ (bottom) estimated 1-hour ozone concentrations in the SoCAB on August 5, 1997.

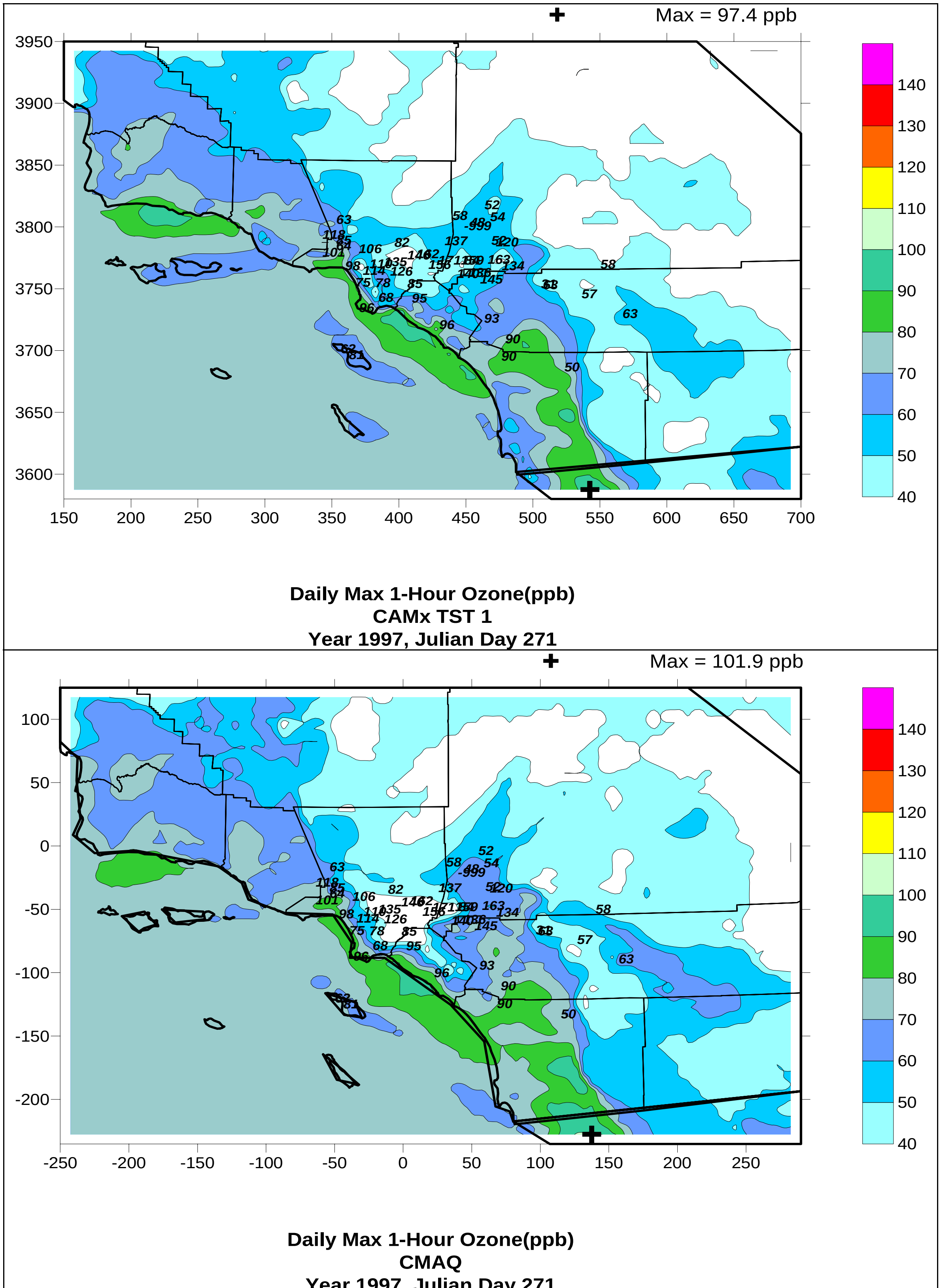


Figure 3-6. Daily maximum observed and CAMx (top) and CMAQ (bottom) estimated 1-hour ozone concentrations in the SoCAB on September 28, 1997.

VOC Emissions Sensitivity Test

VOC measurements were collected at four sites in Southern California during the August-September 1997 episode (El Rio, Simi Valley, Bakersfield and San Diego) and NOx measurements were collected at several additional sites. Figure 3-7 compares the predicted and observed VOC concentrations at two of the sites where VOC was observed and shows that the model tends to underestimate early morning observed VOC concentrations by factors of 2 to 5. The VOC-to-NOx ratio is also underestimated by on average 30-50%. Thus a sensitivity test was conducted that increased the total VOC emissions in the SoCAB by 40% (1.4 factor) to see whether understated VOC emissions may be part of the CAMx and CMAQ ozone underestimation bias. The 1.4 x VOC (tst3) sensitivity test was performed using the CAMx model, results for CMAQ would be expected to be similar since they use the same chemical mechanism (CB4). Results for August 5 and September 28, 1997, the two highest observed ozone days, are shown in Figure 3-8 that can be compared with the CAMx results using the base case VOC emissions in Figures 3-5 and 3-6.

Increasing the VOC emissions by 40% results in substantial improvement in the CAMx ozone model performance on August 5, 1997. The observed ozone 1-hour ozone peak of 187 ppb, that was underestimated by –41% (112 ppb) using the base emissions, is underestimated by only -13% (163 ppb) using the enhanced VOC emissions (Figure 3-5 top versus Figure 3-8 top). The ozone performance on September 28, 1997 is also improved with the enhanced VOC emissions. Whereas using the base emissions CAMx estimated an ozone hole (< 40 ppb) over and east of downtown Los Angeles where elevated (> 100 ppb) ozone was observed, with the enhanced VOC emissions the model estimates an ozone enhancement of similar magnitude to the observed values. At Upland, where the observed 171 ppb 1-hour peak occurred on September 28th, the estimated peak is increased from 31 ppb to 105 ppb when the VOC emissions are increased by 40%.

The increased VOC emissions sensitivity test suggests that some of the CAMx and CMAQ ozone underestimation bias may be due to a deficient VOC emissions inventory. Note that over estimated NOx emissions would have a similar effect as not enough VOC, so errors in the NOx emissions also could be an issue. However, meteorological characterization of the SoCAB also is believed to be a major cause of the model ozone underestimation bias.

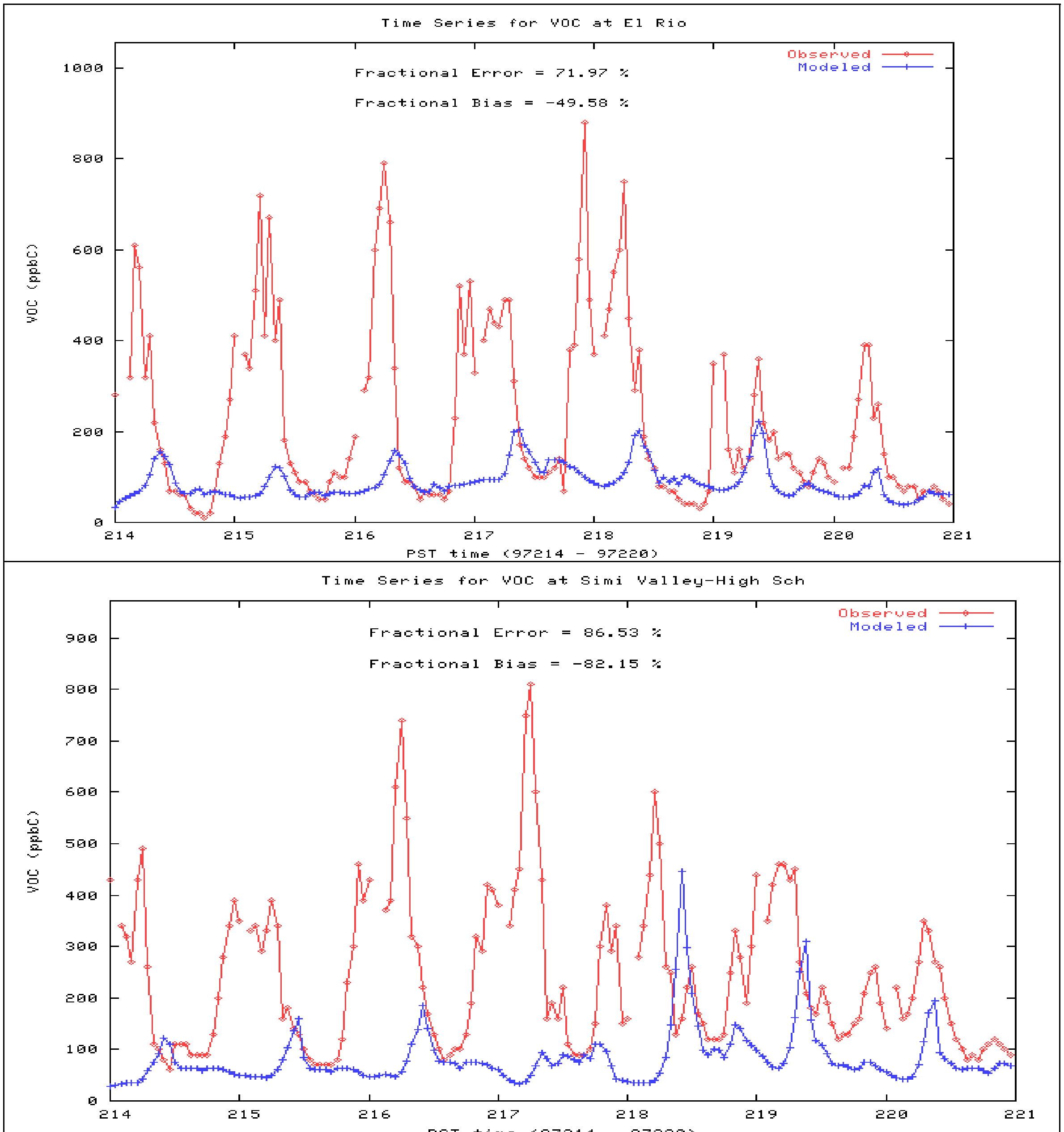
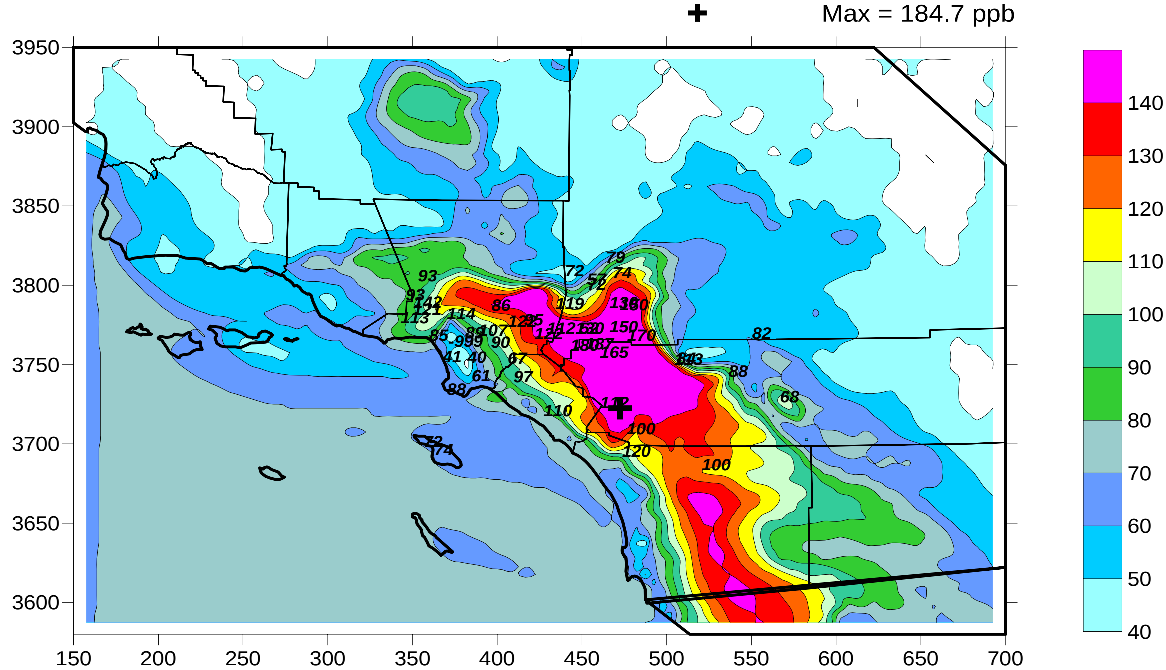
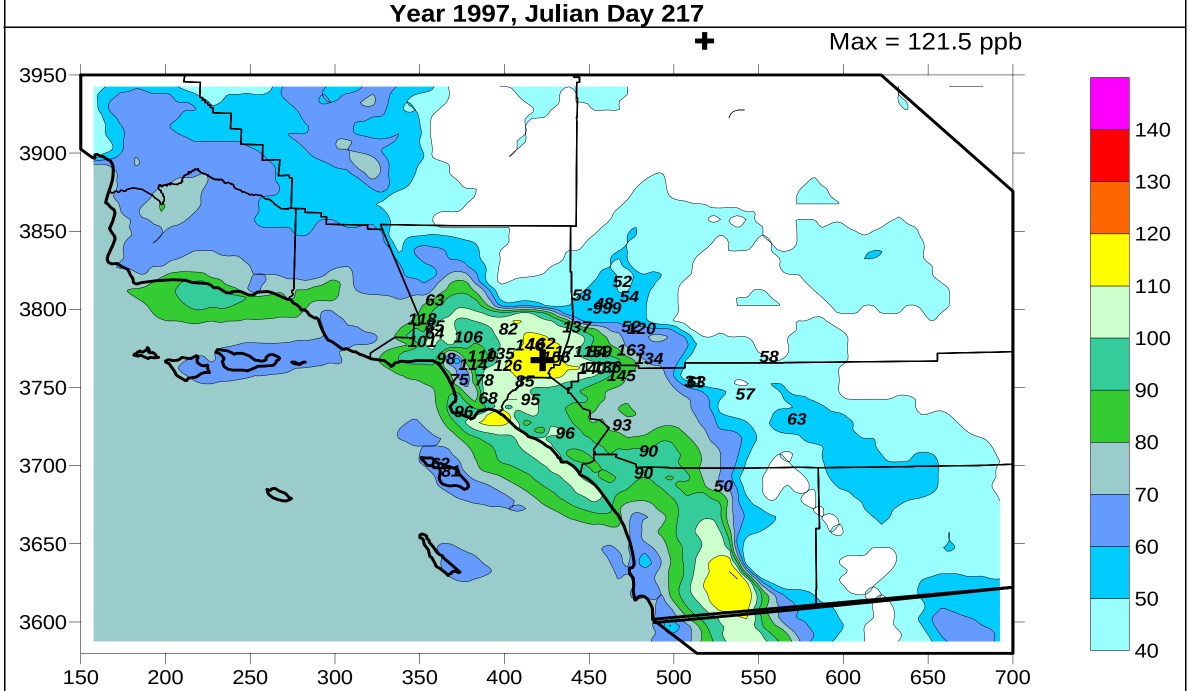


Figure 3-7. Time series of CAMx estimates (blue) and observed (red) VOC concentrations (ppbC) at the El Rio (top) and Simi Valley (bottom) monitoring sites for August 2-8, 1997.



Daily Max 1-Hour Ozone(ppb)
CAMx TST 3
Year 1997, Julian Day 217



Daily Max 1-Hour Ozone(ppb)
CAMx TST 3
Year 1997, Julian Day 271

Figure 3-8. Daily maximum observed and CAMx estimated 1-hour ozone concentrations in the SoCAB on August 5, 1997 and September 28, 1997 for the 1.4 x VOC emissions sensitivity test.

PM MODEL PERFORMANCE EVALUATION

24-hour average PM_{10} observations were available for 17 sites in Southern California during the August-September 1997 modeling period. In addition, hourly observations of speciated PM_2 and PM_{10} concentrations were available for the two August 21-22 and 27-28, 1997 2-day intensive periods at three sites: (1) Los Angeles – North Main; (2) Azusa; and (3) Riverside. The intensive sampling measured PM_2 (< 2μm) rather than the more common $PM_{2.5}$ (< 2.5μm) but this is not expected to have much impact on the model performance evaluation.

PM_{10} Evaluation

Figure 3-9 displays the PM_{10} performance statistics for CAMx and CMAQ and the August-September 1997 simulation using the 24-hour PM_{10} measurements from the 17 sites in Southern California. Both CAMx and CMAQ underestimate the peak 24-hour observed PM_{10} concentration on almost every day of the modeling period (Figure 3-9a). Of the 60 modeling days, the peak observed PM_{10} concentrations exceeded the 24-hour PM_{10} standard of 150 $\mu g/m^3$ on 44 (73%) of the days, whereas the CAMx and CMAQ models estimate the standard would only be exceeded on 19 (32%) and 6 (10%) of the days. The CAMx model predicts the peak observed 24-hour PM_{10} concentrations a little better than CMAQ as evident by an average Unpaired Peak Prediction Accuracy across the two-month period of –27% for CAMx compared to –41% for CMAQ. CAMx and CMAQ exhibit similar PM_{10} performance attributes for normalized bias and error (Figure 3-9b). During the first part of the modeling period (August 1-9) both models exhibit relatively low bias (0% to –40%) and error (<~80%), albeit with an underestimation tendency, followed by a large overestimation on August 10th. Low bias (< ±40%) is also seen for August 21-30 followed by an overprediction bias of >80% in August 31. Performance for PM_{10} in September is not as good as seen for August with several days with a large (>100%) PM_{10} over-prediction bias for both models.

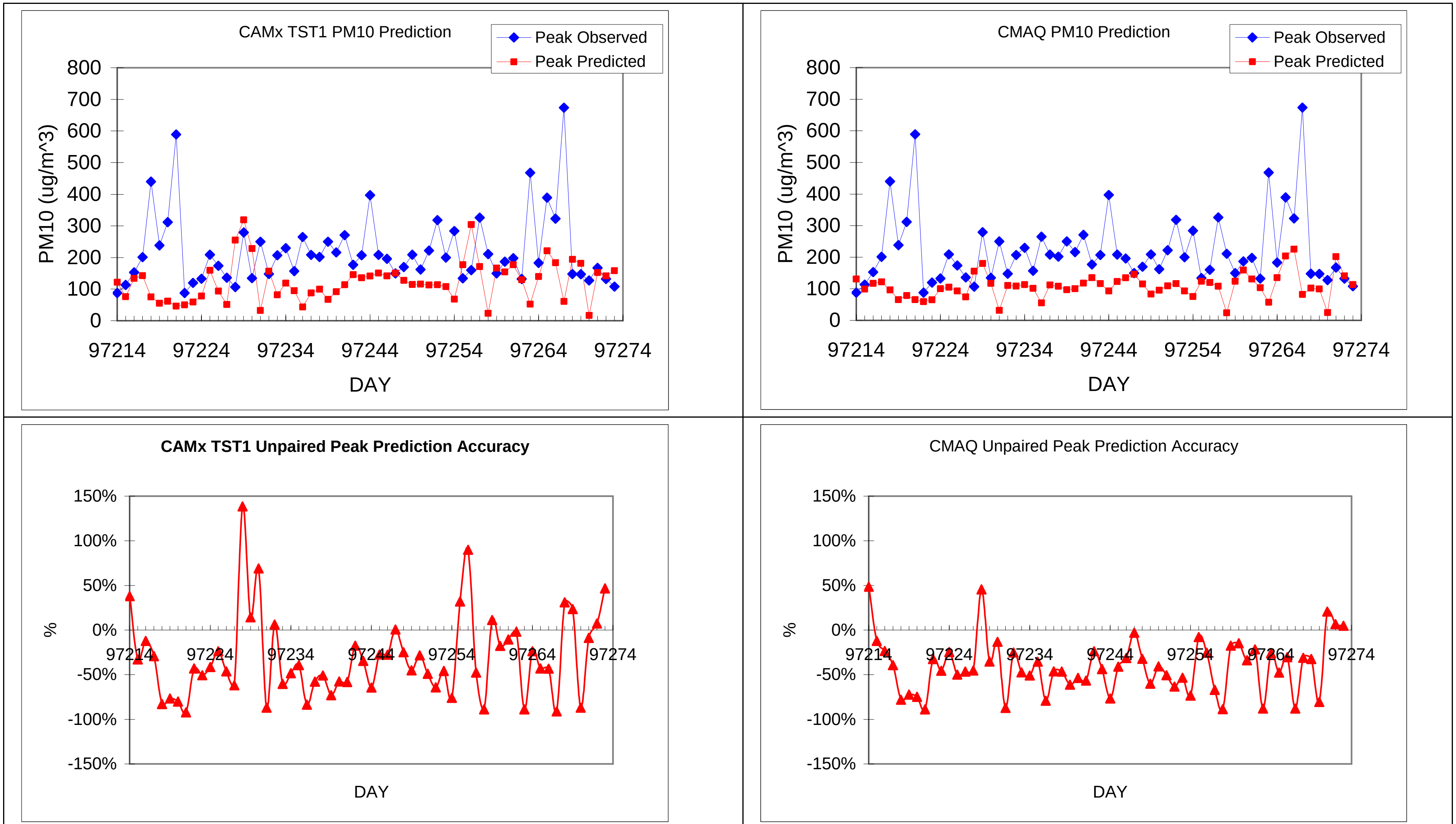


Figure 3-9a. Peak 24-hour PM_{10} performance in the SoCAB for August-September 1997 and the CAMx (left) and CMAQ (right) models.

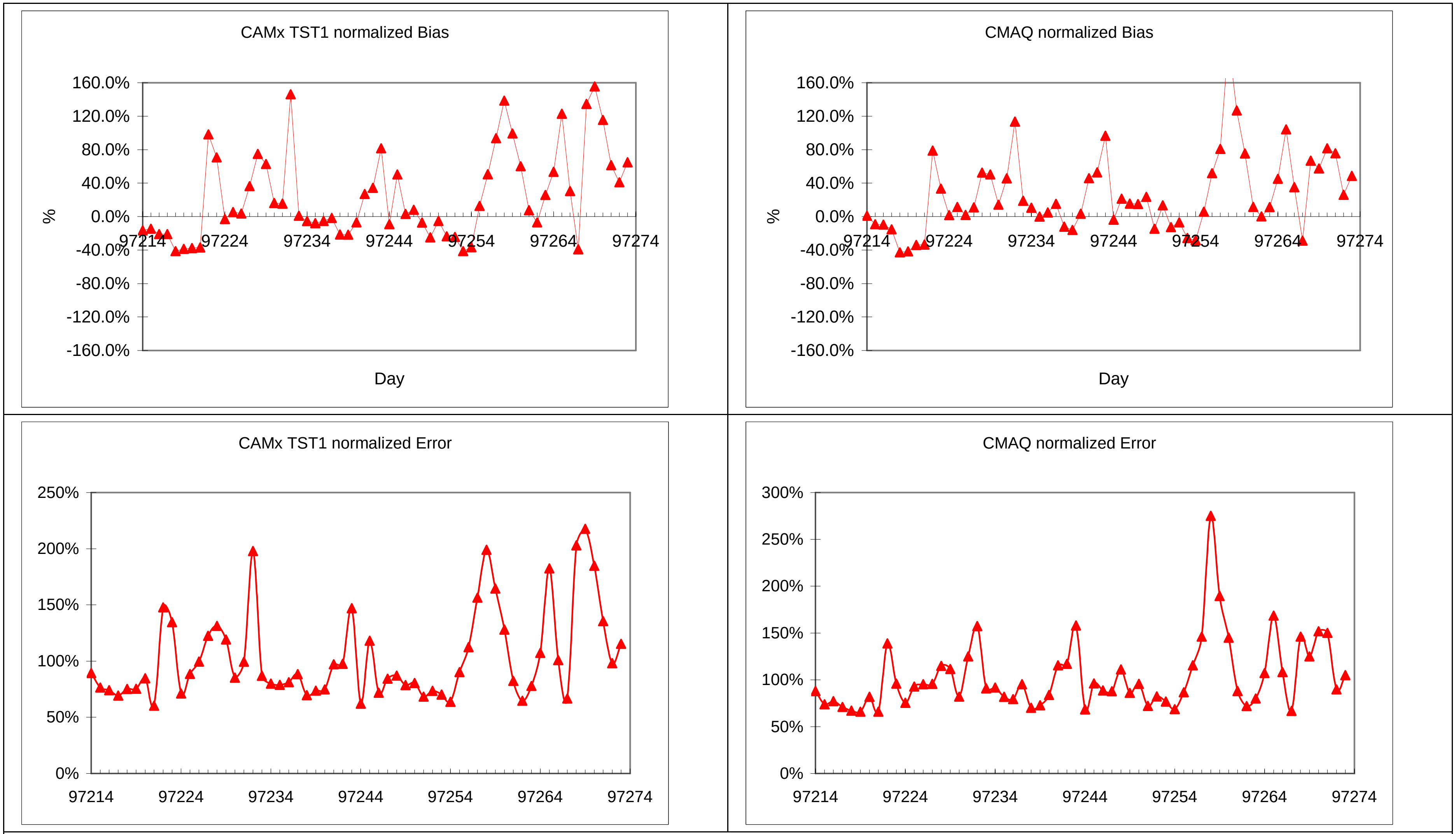


Figure 3-9b. Normalized bias (top) and normalized gross error (bottom) for 24-hour PM_{10} concentrations and the CAMx (left) and CMAQ (right) simulations of the SoCAB and the August-September 1997 period.

Evaluation of PM Components

Table 3-1 displays CAMx and CMAQ summary statistics based on three sites that measured PM species components using a 1.9 µm (PM_2) and 10 µm (PM_{10}) size cut-point:

- Elemental Carbon (PECpm02 and PECpm10);
- Ammonium (PNH4pm02 and PNH4pm10);
- Nitrate (PNO3pm02 and PNO3pm10);
- Organic Carbon Compounds (PORGPApm02 and PORGPApm10); and
- Sulfate (PSO4pm02 and PSO4pm10).

The normalized bias and error performance statistics in Table 3-1 are based on multi-hour observations measured on four days during the two-month modeling period, August 21-22 and August 27-28, 1997 (Allen et. al., 2000). Also shown in Table 3-1 are the unpaired peak predicted and observed fine and fine+coarse PM components. However, because of the limited spatial extent of the three monitors where speciated coarse and fine PM were collected, the unpaired peak comparisons are fairly meaningless unless the predicted peak is less than the observed peak in which case an under-prediction bias is indicated. Note that CAMx as run in its Coarse/Fine (i.e., without multi-sections) and CMAQ's modal representation of PM size distribution does not allow secondary and primary Carbon PM compounds to be in the coarse mode. Consequently, the same model species mappings are used to match up the modeled species to the fine (PM_2) and fine+coarse (PM_{10}) modes of the PM components.

Elemental Carbon: CAMx and CMAQ exhibit similar model performance attributes for fine EC (PECpm02) with normalized bias levels that indicate an overestimation bias that ranges from slight (20%-25% on August 22, 1997) to medium (64%-69% for August 27, 1997) to moderately large (147%-183% on August 21 and 28, 1997). Surprisingly, when comparing the modeled EC with the observed PM_{10} EC (PECpm10) the over-prediction bias seen with the PM_2 EC is increased. As PM_2 is contained in PM_{10} the fact that the observed PECpm10 is less than the observed PECpm02 is physically impossible. We reviewed the final report for the 1997 PM species collection (Allen et al., 2000) and found that there were numerous cases of measured EC PM_{10} being less than EC PM_2 with the differences being due to uncertainties in the sampling technology. The uncertainty bounds in the EC PM_{10} measurements were quite large more than encompassing the EC $PM_{2.}$ measurement. Thus, these results are attributed to measurement artifacts.

Ammonium: CMAQ exhibits near zero bias for fine ammonium (PNH4pm02) with normalized bias value ranging from -5% to +1%, whereas CAMx bias values range from 13% to 86%. Both models underestimate PM_{10} ammonium with the CAMx underestimation bias (-5% to –53%) not being as large as CMAQ (-48% to –61%).

Nitrate: Both models severely overestimate fine nitrate with CAMx producing normalized bias values of 397% to 1036%, corresponding values for CMAQ are 142% to 585%. The over-prediction bias for PM_{10} nitrate is not as bad, with CMAQ exhibiting normalized bias levels of –45%, -14%, -44% and –21% for the four days and CAMx still overestimating with bias values ranging from 20% to 118%.

Organic Matter: The two models produce essentially identical bias and error performance statistics for fine (PORGPApm02) and fine+coarse (PORGPApm10) organic matter with normalized bias values of –75% to –85% and normalized error of 78% to 85%. The models appear to understate organic matter, which is likely due to understated organic carbon emissions and the fact the two models do not completely account for all secondary organic carbon from biogenic sources.

Sulfate: Both models exhibit better model performance for sulfate in the SoCAB. The CAMx/CMAQ normalized bias values for August 21-22 and 27-28 using fine sulfate measurements (PSO4pm02) are –31%/-44%, 21%/-10%, -1%/-25% and –4%/-29%. Similar CAMx/CMAQ bias values for fine+coarse sulfate (PSO4pm10) are –45%/-55%, -29%/-48%, -27%/45% and –30%/-48%. The normalized error values for fine and fine+coarse coarse sulfate and the two models are also fairly reasonable ranging from 32% to 70%.

Neither model is performing sufficiently better than the other for PM that model performance of one model can be considered superior to the other. CAMx produces slightly better sulfate predictions, whereas CMAQ produces slightly better nitrate predictions and organic aerosol performance is nearly identical. However, neither model produces performance for PM species that would be considered good.

Enhanced VOC Emissions Sensitivity Test: Increasing the VOC emissions by 40% has very little effect on the PM species performance. Elemental Carbon is not affected at all, ammonium performance is improved slightly, but nitrate performance is degraded (i.e., overestimation bias increased). Sulfate performance improves slightly, but surprisingly organic matter performance is unchanged, suggesting that secondary organic aerosols are not a major component of the modeled organic matter. PM_{10} model performance is also not affected very much when the VOC emissions are enhanced by 40%. The episode average normalized bias for PM_{10} degrades slightly from 25% to 29% with the enhanced VOC emissions.

Table 3-1a. Summary PM_2 and PM_{10} component performance statistics for the CAMx base case simulation on days with enhanced PM monitoring in August/September 1997.

Case	CAMx Statistics	Aug. 21	Aug. 22	Aug. 27	Aug. 28
PECpm02	Peak Observed	5.9	6.2	4.8	4.4
	Peak Predicted	7.8	9.2	9.7	11.1
	Unpaired Peak Prediction Accuracy	32%	47%	103%	154%
	Bias (normalized)	154%	25%	67%	167%
	Error (normalized)	168%	56%	84%	177%
PECpm10	Peak Observed	5.6	5.6	5.9	3.3
	Peak Predicted	7.8	9.2	9.7	11.1
	Unpaired Peak Prediction Accuracy	39%	64%	64%	240%
	Bias (normalized)	167%	88%	597%	824%
	Error (normalized)	190%	112%	617%	833%
PNH4pm02	Peak Observed	4.4	2.7	3.3	3.9
	Peak Predicted	7.7	12.2	10.8	12
	Unpaired Peak Prediction Accuracy	75%	357%	226%	206%
	Bias (normalized)	13%	86%	71%	0%
	Error (normalized)	79%	116%	98%	0%
PNH4pm10	Peak Observed	6.9	5.4	7.5	7.3
	Peak Predicted	7.7	12.2	10.8	12
	Unpaired Peak Prediction Accuracy	12%	128%	44%	63%
	Bias (normalized)	-53%	-29%	-30%	-5%
	Error (normalized)	55%	46%	45%	45%
PNO3pm02	Peak Observed	7.6	3.1	5.9	7.4
	Peak Predicted	23.7	36.8	34.2	38.1
	Unpaired Peak Prediction Accuracy	213%	1093%	481%	415%
	Bias (normalized)	749%	1036%	397%	640%
	Error (normalized)	794%	1077%	433%	661%
PNO3pm10	Peak Observed	9.9	8.7	17.4	17
	Peak Predicted	23.7	36.8	34.2	38.1
	Unpaired Peak Prediction Accuracy	140%	324%	97%	124%
	Bias (normalized)	107%	118%	20%	78%
	Error (normalized)	186%	179%	84%	119%
POApm02	Peak Observed	27.1	35.9	33.8	28.7
	Peak Predicted	8.6	13.4	12.4	14.3
	Unpaired Peak Prediction Accuracy	-68%	-63%	-64%	-50%
	Bias (normalized)	-79%	-76%	-81%	-75%
	Error (normalized)	79%	76%	81%	75%
POApm10	Peak Observed	31.8	42.3	40.2	43.8
	Peak Predicted	9.6	13.4	13.9	12.1
	Unpaired Peak Prediction Accuracy	-70%	-68%	-66%	-72%
	Bias (normalized)	-83%	-78%	-85%	-81%
	Error (normalized)	83%	78%	85%	81%
PSO4pm02	Peak Observed	6.3	4.4	3	5.3
	Peak Predicted	4.5	5.6	4.9	3.9
	Unpaired Peak Prediction Accuracy	-29%	27%	64%	-28%
	Bias (normalized)	-31%	21%	-1%	-4%
	Error (normalized)	40%	70%	32%	49%
PSO4pm10	Peak Observed	8.4	5.9	3.8	7.4
	Peak Predicted	4.5	5.8	4.9	7.2
	Unpaired Peak Prediction Accuracy	-47%	-2%	30%	-3%
	Bias (normalized)	-45%	-29%	-27%	-30%
	Error (normalized)	48%	38%	35%	42%

Table 3-1b. Summary PM_2 and PM_{10} component performance statistics for the CMAQ base case simulation on days with enhanced PM monitoring in August/September 1997.

Species	CMAQ Statistics	Aug. 21	Aug. 22	Aug. 27	Aug. 28
PECpm02	Peak Observed	5.9	6.2	4.8	4.4
	Peak Predicted	5.4	8.1	9.1	9.4
	Unpaired Peak Prediction Accuracy	-8%	30%	90%	116%
	Bias (normalized)	147%	20%	69%	173%
	Error (normalized)	169%	54%	90%	183%
PECpm10	Peak Observed	5.6	5.6	5.9	3.3
	Peak Predicted	5.4	8.1	9.1	9.4
	Unpaired Peak Prediction Accuracy	-3%	45%	53%	190%
	Bias (normalized)	165%	84%	586%	810%
	Error (normalized)	189%	112%	610%	818%
PNH4pm02	Peak Observed	4.4	2.7	3.3	3.9
	Peak Predicted	15.1	23.7	22.3	17.9
	Unpaired Peak Prediction Accuracy	241%	784%	576%	358%
	Bias (normalized)	-5%	0%	1%	0%
	Error (normalized)	76%	51%	55%	0%
PNH4pm10	Peak Observed	6.9	5.4	7.5	7.3
	Peak Predicted	21.4	22.3	22.3	17.9
	Unpaired Peak Prediction Accuracy	210%	314%	198%	143%
	Bias (normalized)	-61%	-60%	-58%	-48%
	Error (normalized)	70%	60%	65%	55%
PNO3pm02	Peak Observed	7.6	3.1	5.9	7.4
	Peak Predicted	17.1	48.6	45.6	42.5
	Unpaired Peak Prediction Accuracy	126%	1478%	674%	475%
	Bias (normalized)	585%	340%	142%	261%
	Error (normalized)	628%	359%	185%	273%
PNO3pm10	Peak Observed	9.9	8.7	17.4	17
	Peak Predicted	28.6	48.6	45.6	42.5
	Unpaired Peak Prediction Accuracy	189%	460%	162%	150%
	Bias (normalized)	45%	-14%	-44%	-21%
	Error (normalized)	143%	75%	73%	61%
PORGPApm02	Peak Observed	27.1	35.9	33.8	28.7
	Peak Predicted	6.1	9.2	8.9	10.7
	Unpaired Peak Prediction Accuracy	-78%	-74%	-74%	-63%
	Bias (normalized)	-80%	-78%	-81%	-74%
	Error (normalized)	80%	78%	81%	74%
PORGPApm10	Peak Observed	31.8	42.3	40.2	43.8
	Peak Predicted	11.6	9.2	10.4	13.9
	Unpaired Peak Prediction Accuracy	-63%	-78%	-74%	-68%
	Bias (normalized)	-84%	-79%	-85%	-80%
	Error (normalized)	84%	79%	85%	80%
PSO4pm02	Peak Observed	6.3	4.4	3	5.3
	Peak Predicted	3.1	3.5	2.7	3.5
	Unpaired Peak Prediction Accuracy	-51%	-22%	-9%	-36%
	Bias (normalized)	-44%	-10%	-25%	-29%
	Error (normalized)	47%	60%	34%	46%
PSO4pm10	Peak Observed	8.4	5.9	3.8	7.4
	Peak Predicted	3.1	3.4	2.7	4.1
	Unpaired Peak Prediction Accuracy	-63%	-43%	-28%	-44%
	Bias (normalized)	-55%	-48%	-45%	-48%
	Error (normalized)	57%	48%	45%	50%

4.0 SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

METEOROLOGICAL MODELING

The MM5 meteorological model was applied to the South Coast Air Basin (SoCAB) for the August-September 1997 period on a 45/15/5 km resolution grid that included special measurements by the Southern California Ozone Study (SCOS) field study. Numerous MM5 sensitivity simulations were carried out to try to improve the representation of meteorological conditions in the SoCAB during the modeling period. These MM5 sensitivity tests included the introduction of new MM5 modeling techniques for the SoCAB as discussed by Boucouvala and co-workers (2003). Some improvements in the MM5 model performance were seen in the sensitivity tests. CAMx and CMAQ meteorological inputs were then generated using the final MM5 outputs and formatted for air quality modeling using, respectively, the MM5CAMx and MCIP meteorological processors.

EMISSIONS MODELING

Hourly speciated gridded low-level and point source emissions for the CAMx model were generated for the August-September 1997 period using the California Air Resources Board (ARB) Gridded Emissions Model (GEM) setup for the August 3-6, 1997 episode and gridded biogenic emissions for August 3-7 and September 26-28, 1997. Emissions for other days from August-September 1997 were generated by matching like days (e.g., day-of-week and similar temperatures) for days in which GEM emission inputs were available. Three-dimensional emissions for the CMAQ model were generated using a CAMx-to-CMAQ emissions processor that uses the CAMx two-dimensional gridded and point source stack emissions files, the CAMx meteorological inputs and the CAM_X plume rise algorithm.

PHOTOCHEMICAL GRID MODELING

The CAMx and CMAQ models were applied to the SoCAB 5 km resolution modeling domain for the August-September 1997 period and evaluated using available ozone, VOC, NOx, PM_{10} and speciated fine and coarse PM data. One major deficiency in the SCOS97 field study was the lack of a comprehensive data archival system. Consequently, not all data collected during the field study are available on the SCOS97 data archive CD (http://www.arb.ca.gov/research/scos/scos.htm). Although additional data were obtained from some researchers (e.g., Allen et al., 2000) not all data collected during the field study were available for use in the evaluation. However, sufficient gaseous and PM species data were available to provide some conclusions regarding the CAMx and CMAQ model performance for the SoCAB and the August-September 1997 period.

Ozone Model Performance

The ozone performance of the CAMx and CMAQ models for the August-September 1997 period is mostly poor with the two models exhibiting a large underestimation bias for the higher ozone days. The performance for the August 3-6, 1997 period, that was the focus Boucouvala et al.,

(2003) model improvements and modeled for the 2003 Air Quality Management Plan, (AQMP) is better than for the rest of the episode suggesting that specific MM5 meteorological improvements for this episode may not be universally applicable to the other days of the two-month period. The 187 ppb episode peak observed 1-hour ozone concentration is underestimated by the CAMx and CMAQ models by approximately –20% and –30%, respectively, unpaired by location, and by approximately –40% by both models at the station location. EPA's 1-hour ozone <±15% normalized bias performance goal is rarely met by either model during the two-month modeling period with normalized bias levels for the two models typically between –20% and –50%. Similar underestimation bias was seen with 8-hour ozone model performance. The CAMx and CMAQ models exhibited similar poor ozone model performance for the two-month modeling period, with CMAQ's ozone levels being slightly higher than CAMx resulting in marginally better performance when analyzed across the two-month period, although CAMx exhibits better ozone performance than CMAQ on the August 5th peak observed ozone day.

PM_{10} Model Performance

PM_{10} model performance was evaluated for the two models using 24-hour PM_{10} observations collected at 17 sites in Southern California. The observed daily maximum PM_{10} peaks were underestimated by the two models for most days during the modeling period. Whereas the observations indicated that an exceedance of the Federal 24-hour PM_{10} standard of 150 $\mu g/m^3$ occurred on 73% of the days during the two-month modeling period, the CAMx and CMAQ models only estimated that 32% and 10%, respectively, of the days were PM_{10} exceedance days in Southern California. Although the highest observed PM_{10} concentrations were understated by both models, across the monitoring network there were several days with high model overestimation with normalized bias values exceeding 80% for both models. During August 1997, the CAMx and CMAQ models exhibited some skill in estimating PM_{10} concentrations with most days exhibiting relatively low normalized bias (<±40%). In September 1997 the PM_{10} model performance was worse with several days exhibiting normalized bias greater than 100%. The PM_{10} performance for both CAMx and CMAQ models is similar with both models exhibiting better and worse model performance on the same days.

Speciated PM Model Performance

Multi-hour speciated fine ($PM_{2.0}$) and fine+coarse (PM_{10}) PM component measurements were collected at three sites during two 2-day intensive periods (August 21-22 and 27-28) during the modeling period. For comparison with the fine and fine+coarse PM components, consistent model species mappings were used (i.e., the modeled PM species are assumed to all be within the fine mode for the PM components analyzed). The two models generally overestimated fine ($PM_{2.0}$) Elemental Carbon (EC), with the overestimation bias ranging from slight (~20%) to moderate (~60%) to large (>100%). When the modeled EC is compared to the observed PM_{10} EC, surprisingly the overestimated bias seen for the fine EC is increased, which is counter intuitive since $PM_{2.0}$ is contained within PM_{10}. An examination of the EC fine and fine+coarse measurements revealed that the PM_{10} EC is frequently less than the $PM_{2.0}$ EC which is attributable to the different measurement techniques used (Allen et al., 2000). The two models exhibit an underestimation tendency for Organic Matter (OM) of –75% to –85% that is likely due to missing OC in the inventory, Secondary Organic Aerosol (SOA) formation processes not accounted for in the two models (Morris et al., 2005) and meteorological uncertainties.

CMAQ exhibited near zero bias for fine ammonium, but a –50% to –60% under-prediction bias for fine+coarse ammonium. CAMx, on the other hand, exhibited bias for fine ammonium that ranged from 0% to –86% and understated fine+coarse ammonium by –5% to –53%. The two models exhibited similar performance for ammonium with CMAQ performing slightly better for fine ammonium and CAMx performing slightly better for fine + coarse ammonium.

Both models greatly (>100%) overestimated fine nitrate concentrations in the SoCAB for all four intensive days. CMAQ does a better job than CAMx in simulating fine+coarse nitrate with normalized bias values of –44% to 45%, whereas CAMx exhibits an overestimation bias of 20% to 118%. However, CAMx does a slightly better job in reproducing the observed sulfate concentrations with the CAMx bias for fine sulfate ranging from –31% to 21%, whereas CMAQ exhibits an underestimation bias for fine sulfate across all four days that range from –10% to –44%. Both models underestimate fine+coarse sulfate with the CAMx bias levels (-27% to –45%) being slightly better than seen for CMAQ (-45% to –55%).

VOC Emissions Sensitivity Tests

A comparison of predicted and observed VOC concentrations at four sites in Southern California indicated that early morning VOC concentrations were underestimated by the model by a factor of 2 to 5 and that the VOC-to-NOx ratios were underestimated by, on average, 30%-50%. Thus a VOC emission sensitivity test was performed using the CAMx model that increased VOC emissions by 40% (1.4 x VOC). Ozone model performance was greatly improved in the enhanced VOC emissions sensitivity test both in terms of the performance statistics and in the spatial distribution of ozone concentrations. The enhanced VOC emission sensitivity test had less effect on PM performance with EC and OM performance not affected, nitrate performance slightly degraded and sulfate performance slightly improved.

Discussion of Results

Despite performing extensive MM5 meteorological sensitivity tests to improve the meteorological model performance in the SoCAB, when used in the photochemical grid models the improved MM5 meteorological model performance did not result in substantial improvements in ozone model performance. The MM5 meteorological fields still fail to account for the recirculation of pollutants in the SoCAB on some days. Perhaps implementation of more processed based evaluation using tracers to examine potential pollutant flows would provide more insight into the MM5 model performance than use of traditional surface based meteorological observations that fail to evaluate the model aloft or the model’s ability to simulate return flows. On many days, CMAQ estimates slightly higher ozone levels than CAMx which is believed to be due to the higher vertical turbulent exchange coefficients (Kv) and minimum Kv (1.0 m^2/s) in CMAQ than CAMx (the CMAQ Kv profile typically results in mixing heights one layer deeper than the CAMx default Kv and the CAMx minimum K_V values range from 0.1 to 1.0 m^2/s).

As part of the development of the 2003 Air Quality Management Plan (AQMP), the South Coast Air Quality Management District (SCAQMP) and the California Air Resources Board (ARB) exercised several models (CAMx, CALGRID and UAM) using the CB4 and SAPRC chemical mechanism and reported ozone model performance results, some of which are summarized in Table 4-1, along with the CAMx and CMAQ performance results from this study.

Table 4-1. Summary ozone performance from 2003 AQMP process and this study for 1-hour ozone peak on August 5, 1997.

Model	Peak Observed (ppb)	Peak Predicted (ppb)	Unpaired Peak Accuracy (%)
2003 AQMP Development			
CAMx/CB4	187	166	-11%
CALGRID/CB4	187	161	-14%
CAMx/SAPRC99	187	168	-10%
CALGRID/SAPR99	187	172	-8%
UAM/CM4	187	200	+20%
CRC Project A-40			
CAMx	187	144	-23%
CMAQ	187	128	-31%

The SCAQMD/ARB achieved superior ozone model performance than obtained in this study. The UAM/CB4 model was ultimately selected as the final model for use in the 2003 AQMP. However, in the SCAQMD/ARB modeling the recirculation of pollutants was not simulated any better. Furthermore, some model inputs were selected based on better ozone model performance, rather than better science. For example, the MM5 meteorological modeling was conducted with the terrain heights cut in half because it produced improved model performance in the ozone models. In addition, the UAM model is based on old science and contains some parameterizations (e.g., overstated photolysis rates) that are known to be incorrect. Thus, although the 2003 AQMP reports better ozone model performance for the early August 1997 episode than we were able to achieve in this study, such improved performance may be due in part to compensatory errors.

PM performance for the two models is more encouraging with model performance levels not that different from what is seen in recent regional PM modeling (e.g., Morris et al., 2004a,b). Nitrate performance is more disappointing, but the summer nitrate overestimation tendency is a fairly common result using the CAMx and CMAQ models. The performance for the other species is generally within the range that other studies have seen.

The improved ozone performance in the enhanced (1.4 x) VOC emissions sensitivity test suggests that a deficient VOC emissions inventory, or alternatively too much NOx, may be partially responsible for the ozone underestimation bias. However, inadequate meteorology is believed to be the major cause of the poor ozone model performance.

CONCLUSIONS

Similar poor ozone model performance is exhibited by CAMx and CMAQ for the August-September 1997 simulation of the SoCAB. The primary reason for this poor ozone performance appears to be to inadequate meteorological fields that, among other things, fail to reproduce the recirculation of pollutants in the SoCAB. Insufficient VOC and/or too much NOx emissions may also be contributing to the ozone under-prediction bias. The performance of the two models for PM in the SoCAB is more encouraging, although performance problems still exist. The models exhibited some skill in predicting sulfate and some other PM species components with PM performance for most species similar to other CAMx and CMAQ applications. With the possible exception of nitrate, where CAMx exhibited a larger overestimation tendency, the two models exhibited very similar ozone and PM performance and closely tracked each other's day-by-day performance tendencies, both good and bad.

RECOMMENDATIONS

Two areas of model performance deserve additional analysis to understand and improve performance in the SoCAB. These are the ozone and nitrate performance for CAMx and CMAQ.

Ozone Recommendations

As noted above, much of the questionable ozone performance is likely due to deficient meteorological fields. The group out of San Jose State University has reported improved MM5 meteorological representation of the August 3-6, 1997 episode (Boucouvala et al., 2003; Boucouvala and Bornstein, 2003).

These SJSU MM5 fields should be used in the CAMx and CMAQ models. Further emission sensitivity tests should also be conducted that examine increased VOC and/or reduced NOx and other sensitivity. The sensitivity of the model estimated ozone concentrations to chlorine emissions (through sea salt or direct emissions) should be examined along with re-nitrification chemistry (i.e., the decomposition of nitric acid to NO_2 that is not treated in the Carbon Bond IV chemical mechanism).

Nitrate Performance

The CAMx and CMAQ nitrate performance should be analyzed in more detail. This is an issue that has also come up in the regional visibility modeling using the two models. The sensitivity of the 2 models nitrate performance to the following factors needs to be examined.

- Dry deposition
- Ammonia emissions
- Heterogeneous chemistry
- N_2O_5 chemistry

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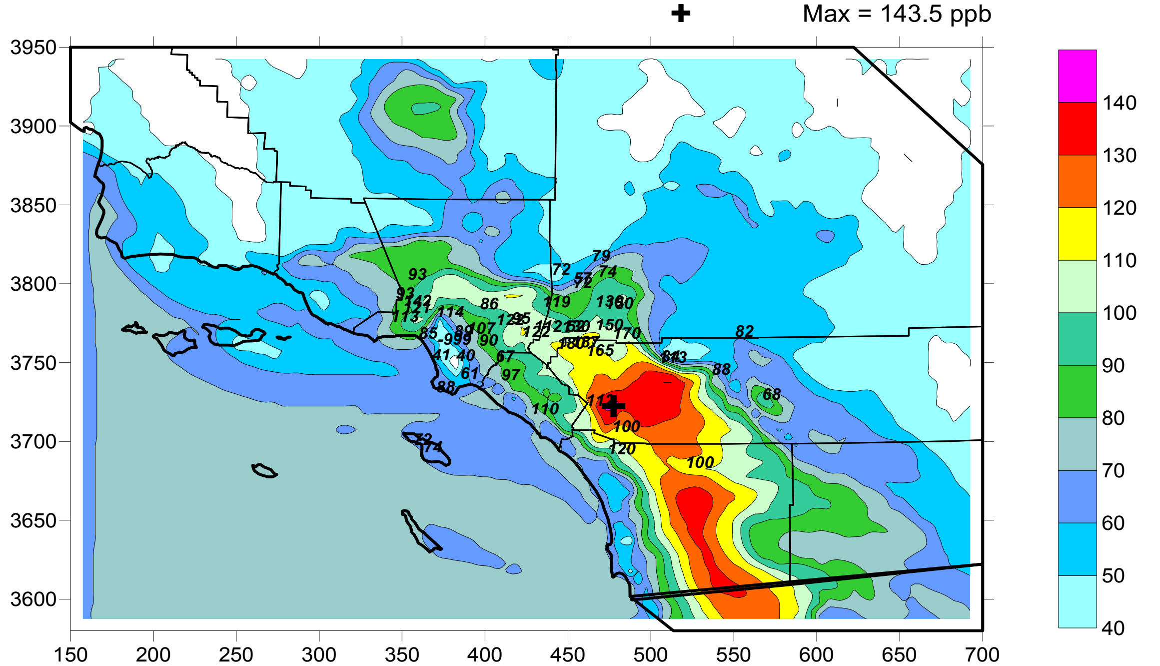
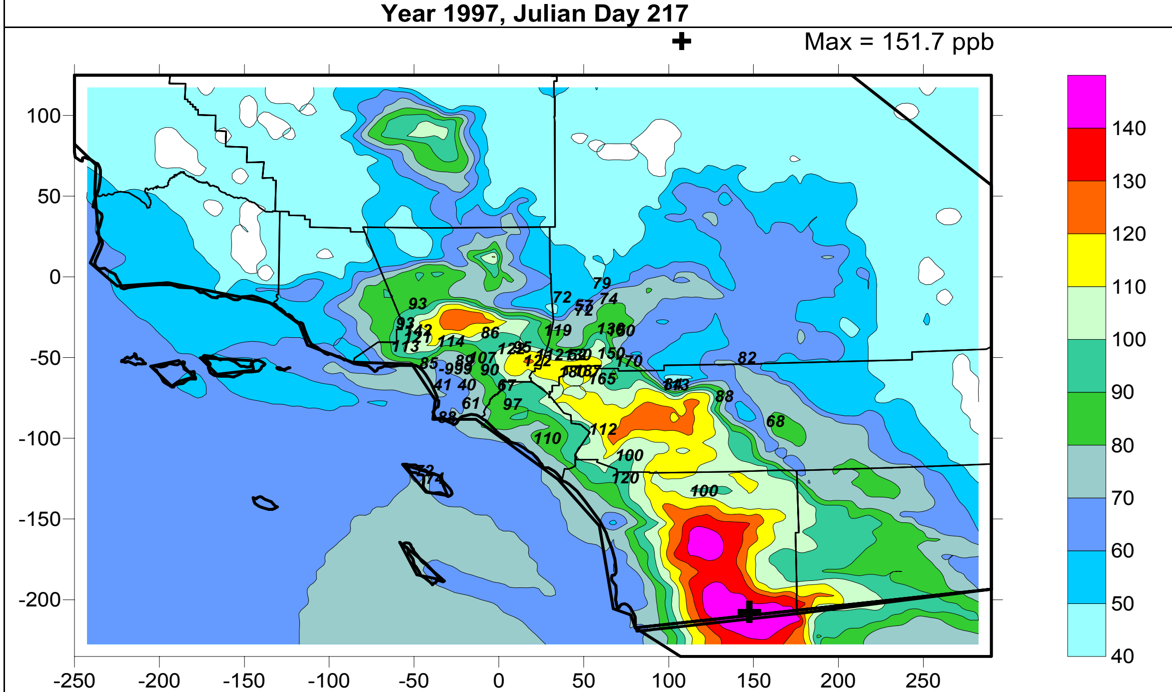
Appendix A

Spatial Maps of Predicted and Observed Daily Maximum 1-Hour Ozone Concentrations (ppb) for the CAMx and CMAQ Base Case Simulations

Day 217; August 5, 1997
Day 218; August 6, 1997
Day 227; August 15, 1997
Day 244; September 1, 1997
Day 271; September 28, 1997



Daily Max 1-Hour Ozone(ppb)
CAMx TST 1
Year 1997, Julian Day 217



Daily Max 1-Hour Ozone(ppb)
CMAQ
Year 1997, Julian Day 217

Figure A-1. Peak observed and CAMx (top) and CMAQ (bottom) estimated 1-hour ozone concentrations in the SoCAB on August 5, 1997.

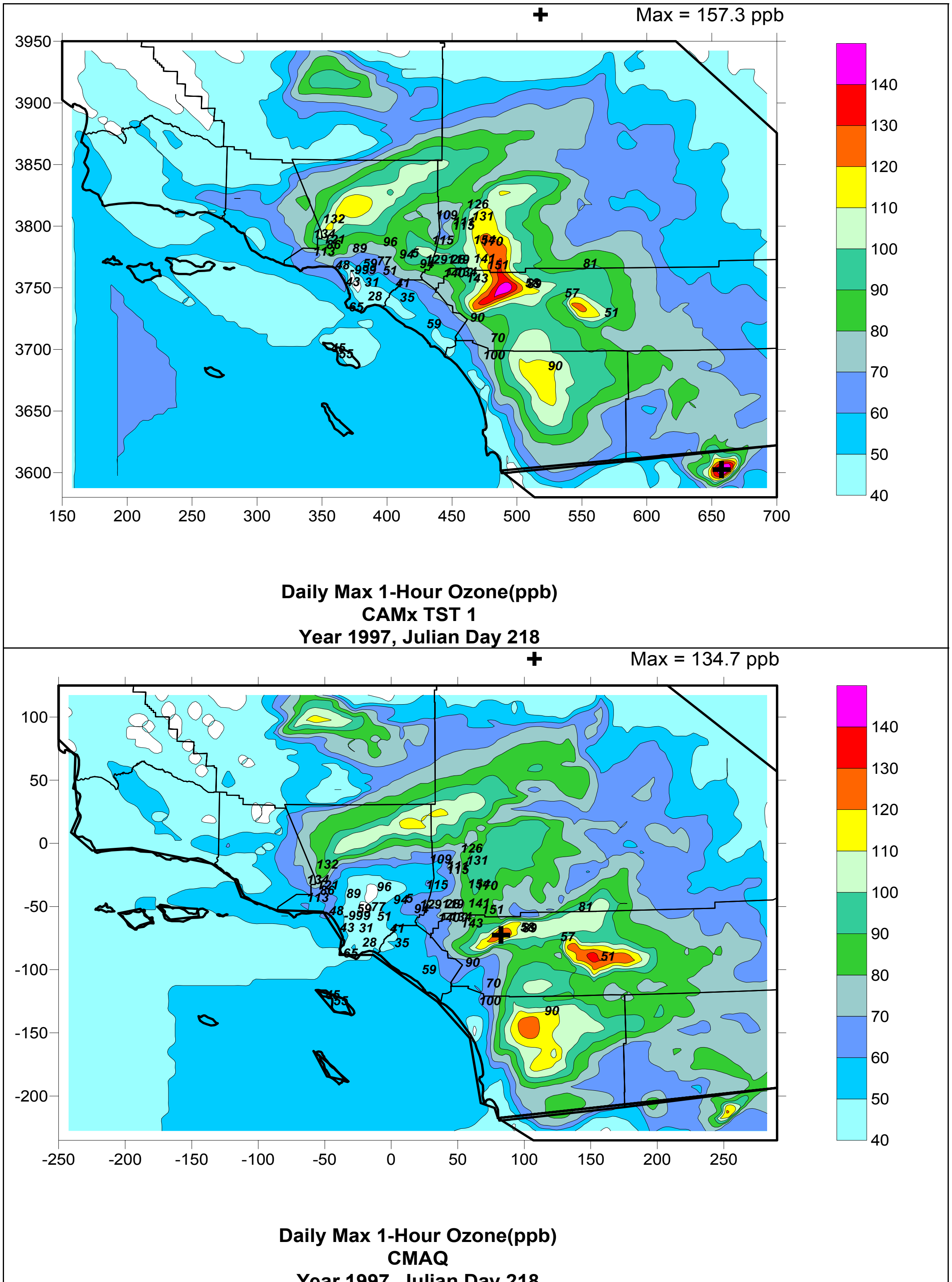
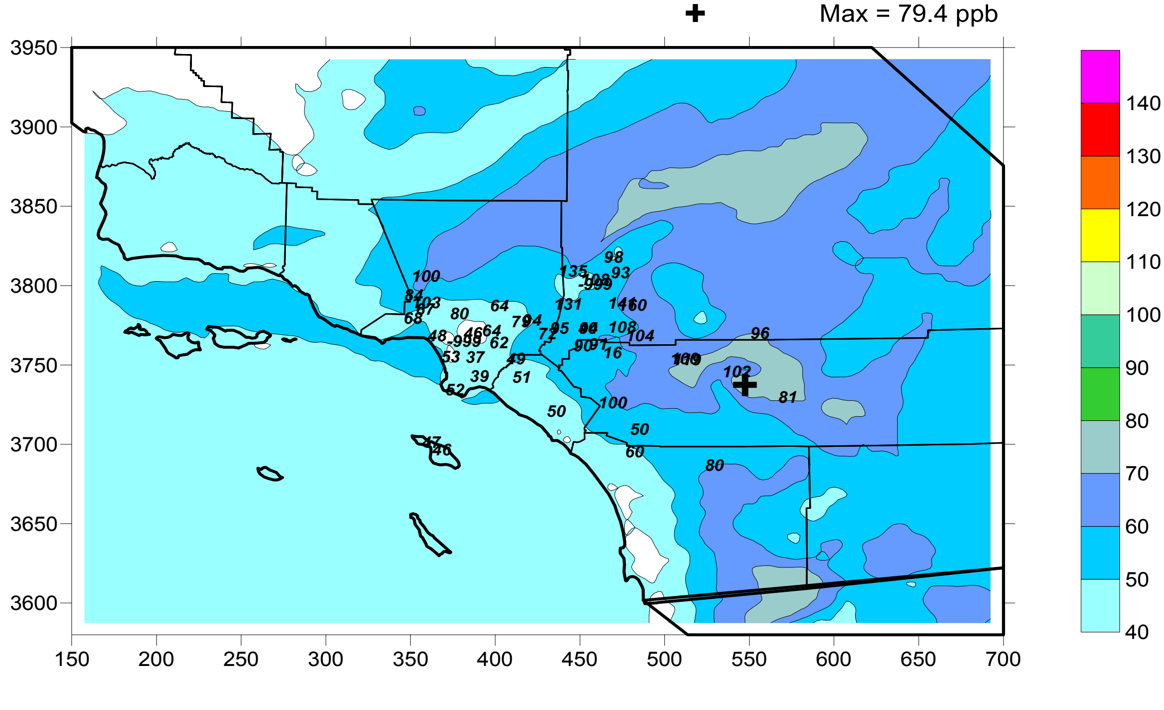
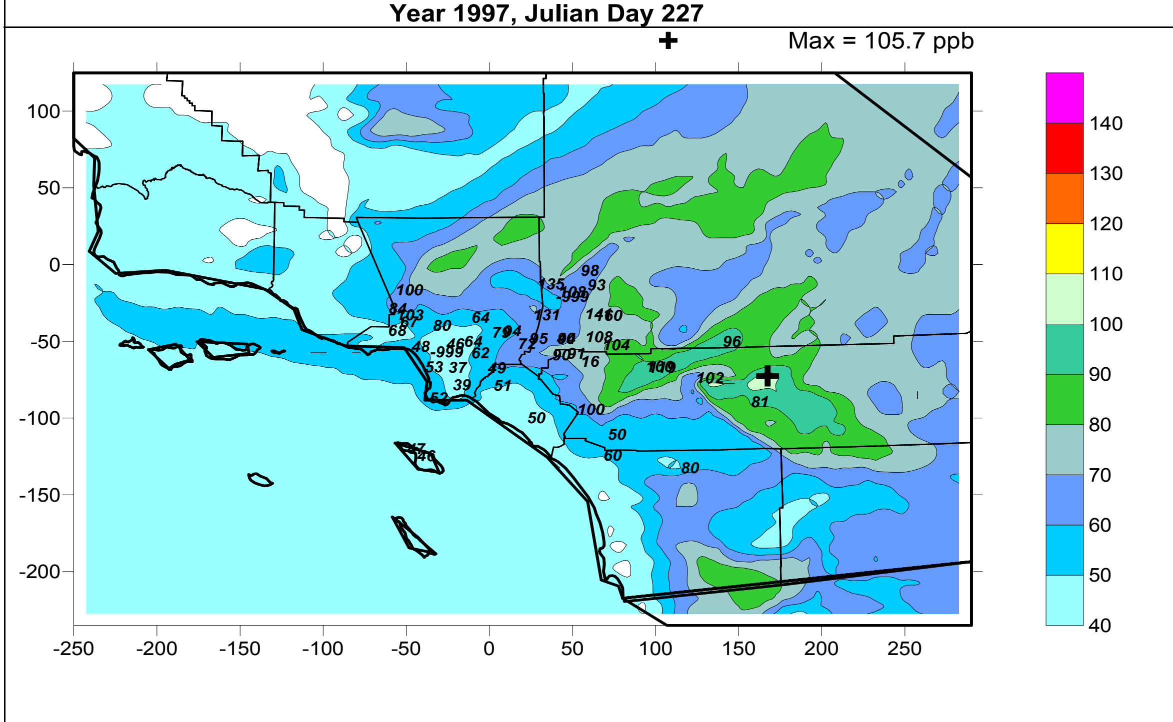


Figure A-2. Peak observed and CAMx (top) and CMAQ (bottom) estimated 1-hour ozone concentrations in the SoCAB on August 6, 1997.



Daily Max 1-Hour Ozone(ppb)
CAMx TST 1
Year 1997, Julian Day 227



Daily Max 1-Hour Ozone(ppb)
CMAQ
Year 1997, Julian Day 227

Figure A-3. Peak observed and CAMx (top) and CMAQ (bottom) estimated 1-hour ozone concentrations in the SoCAB on August 15, 1997.

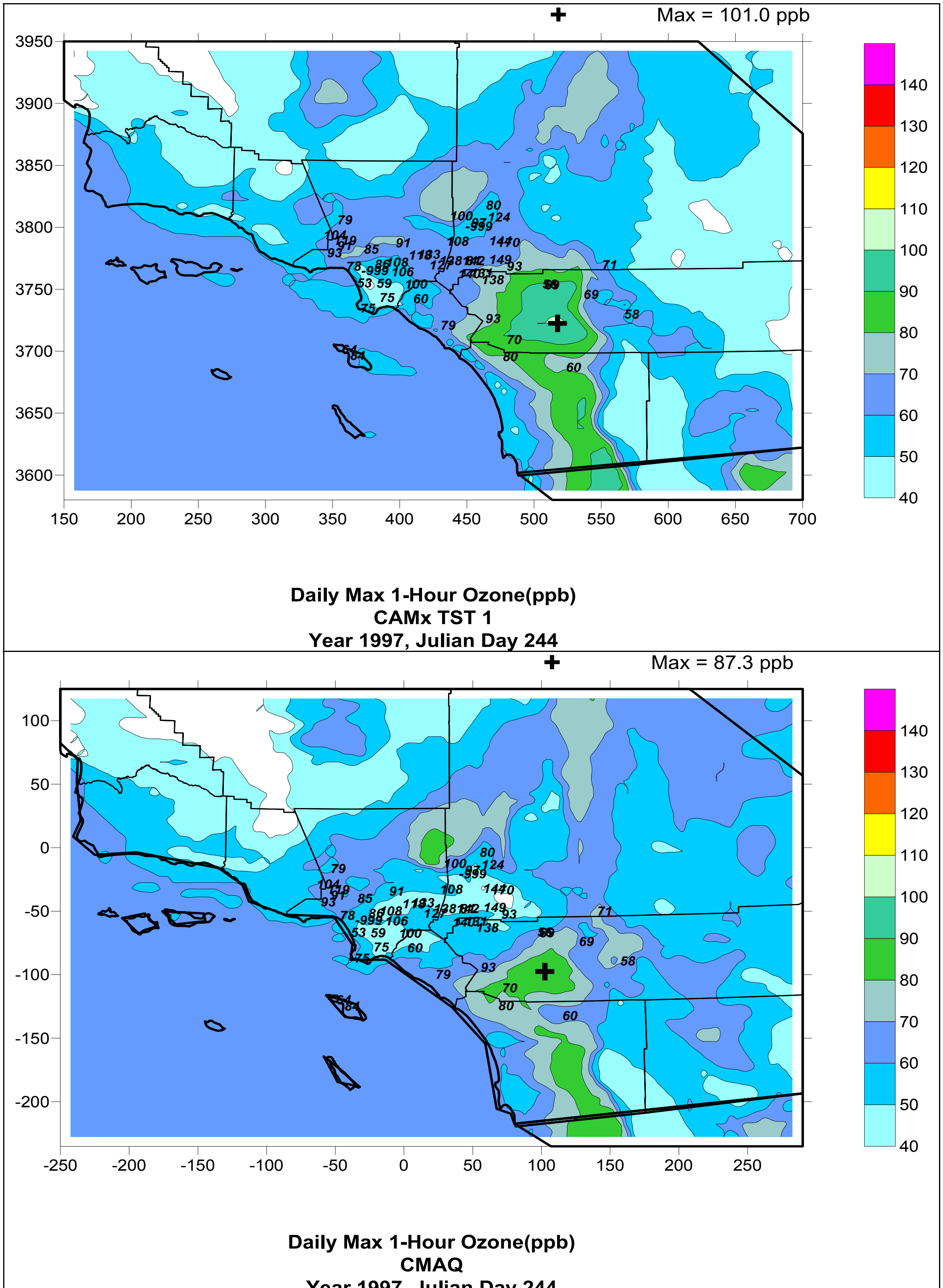


Figure A-4. Peak observed and CAMx (top) and CMAQ (bottom) estimated 1-hour ozone concentrations in the SoCAB on September 1, 1997.

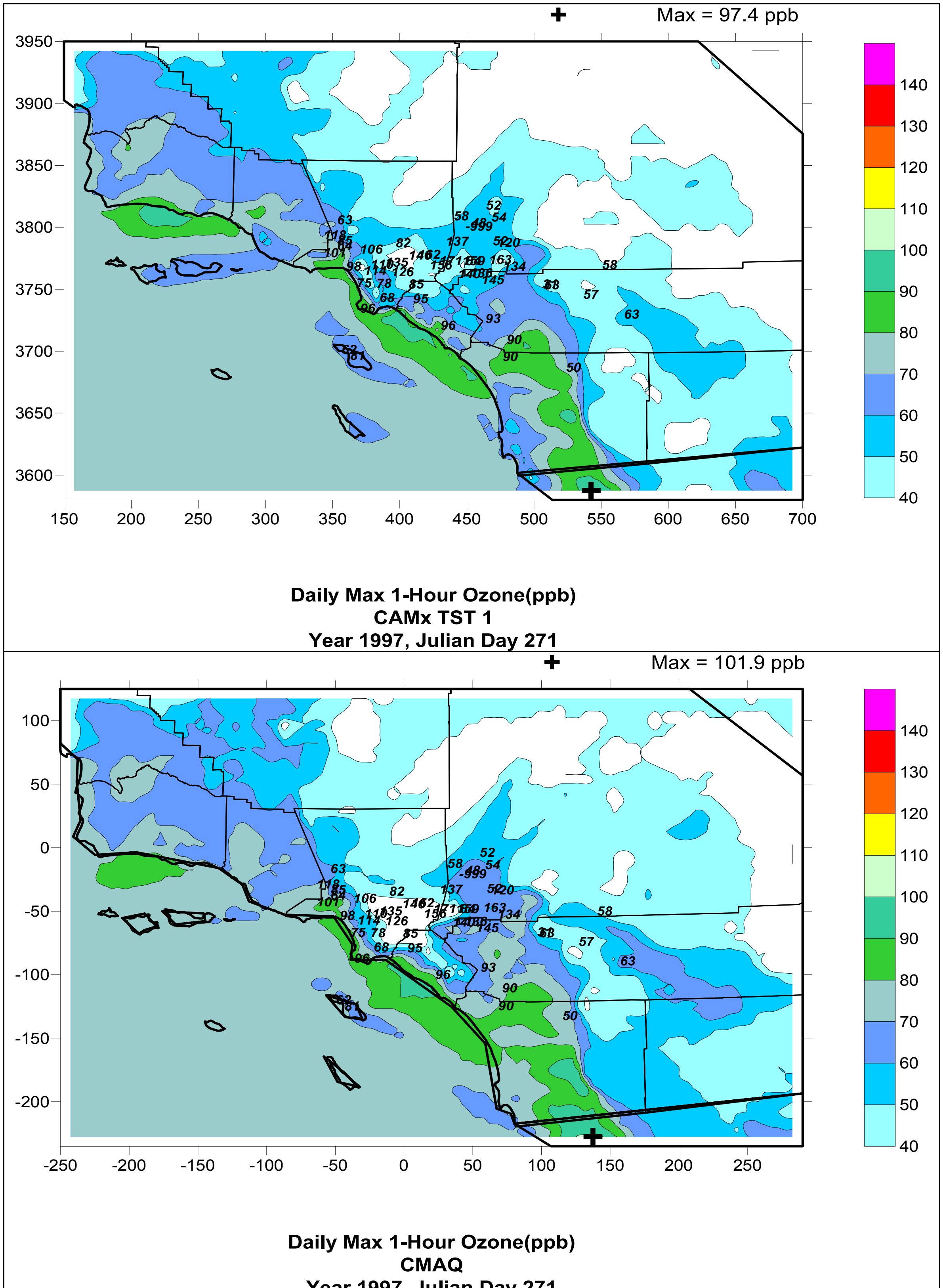


Figure A-5. Peak observed and CAMx (top) and CMAQ (bottom) estimated 1-hour ozone concentrations in the SoCAB on September 28, 1997.

Appendix B

Spatial Maps of Predicted and Observed Daily Maximum 8-Hour Ozone Concentrations (ppb) for the CAMx and CMAQ Base Case Simulations

Day 217; August 5, 1997
Day 218; August 6, 1997
Day 227; August 15, 1997
Day 244; September 1, 1997
Day 271; September 28, 1997

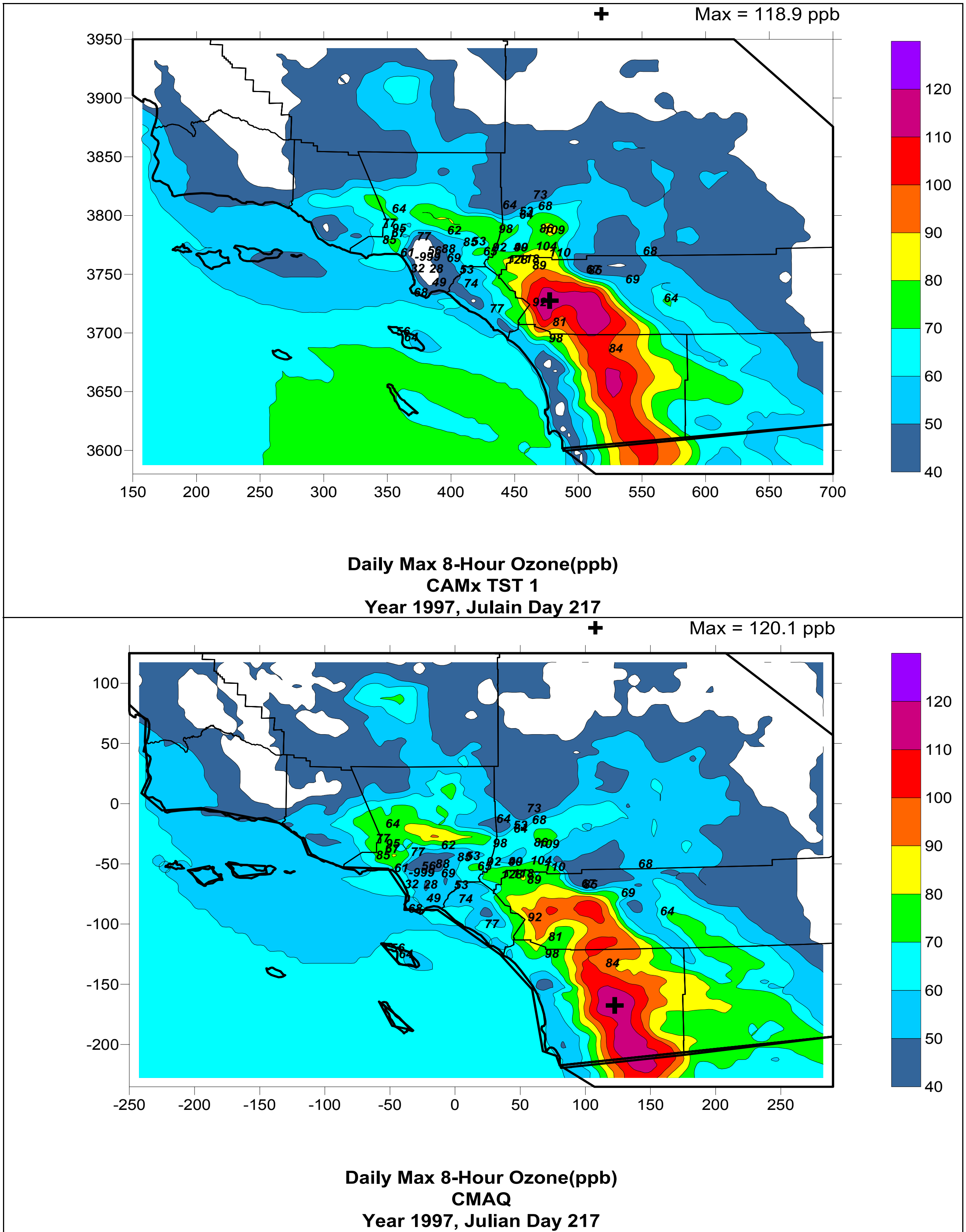


Figure B-1. Peak observed and CAMx (top) and CMAQ (bottom) estimated 8-hour ozone concentrations in the SoCAB on August 5, 1997.

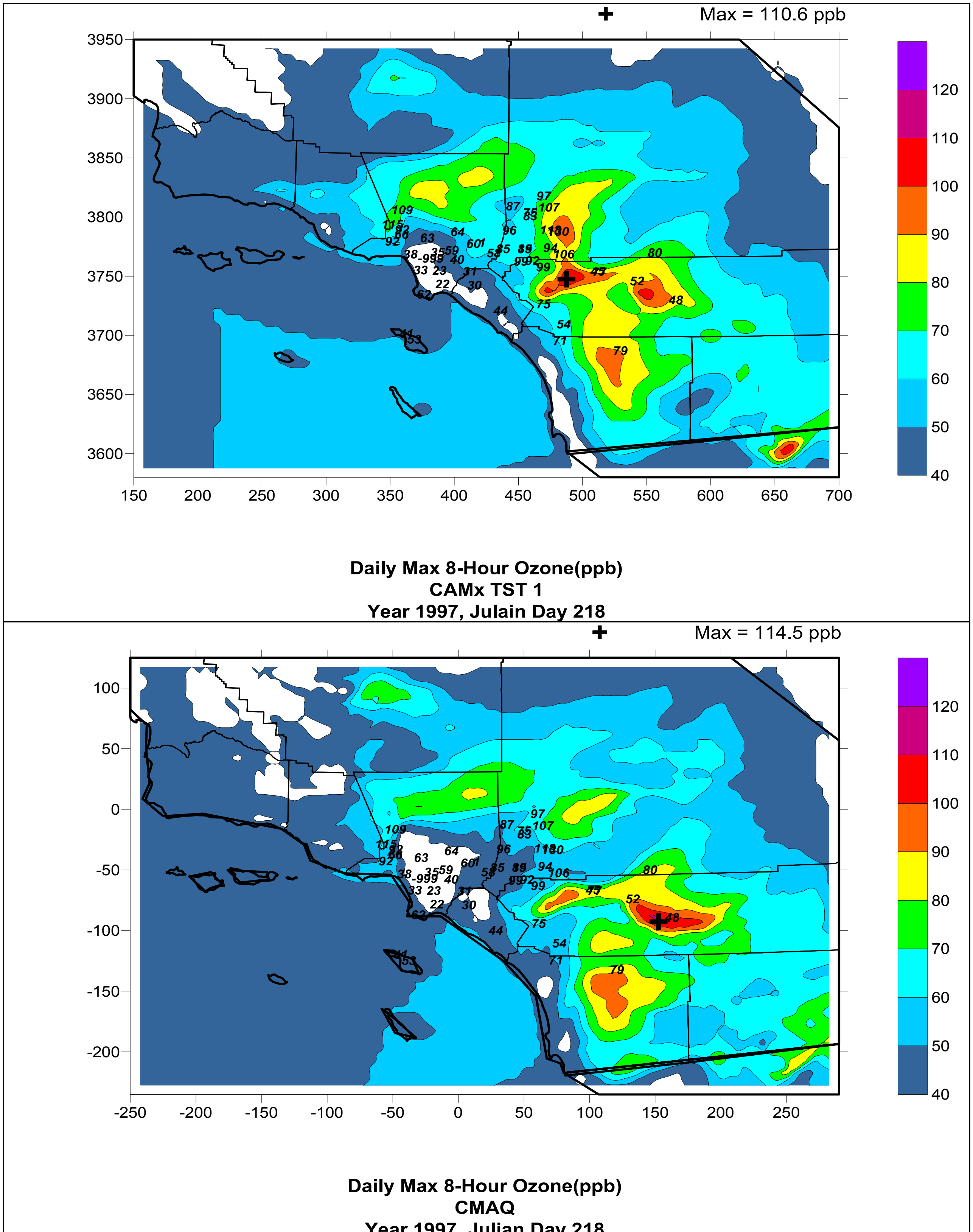
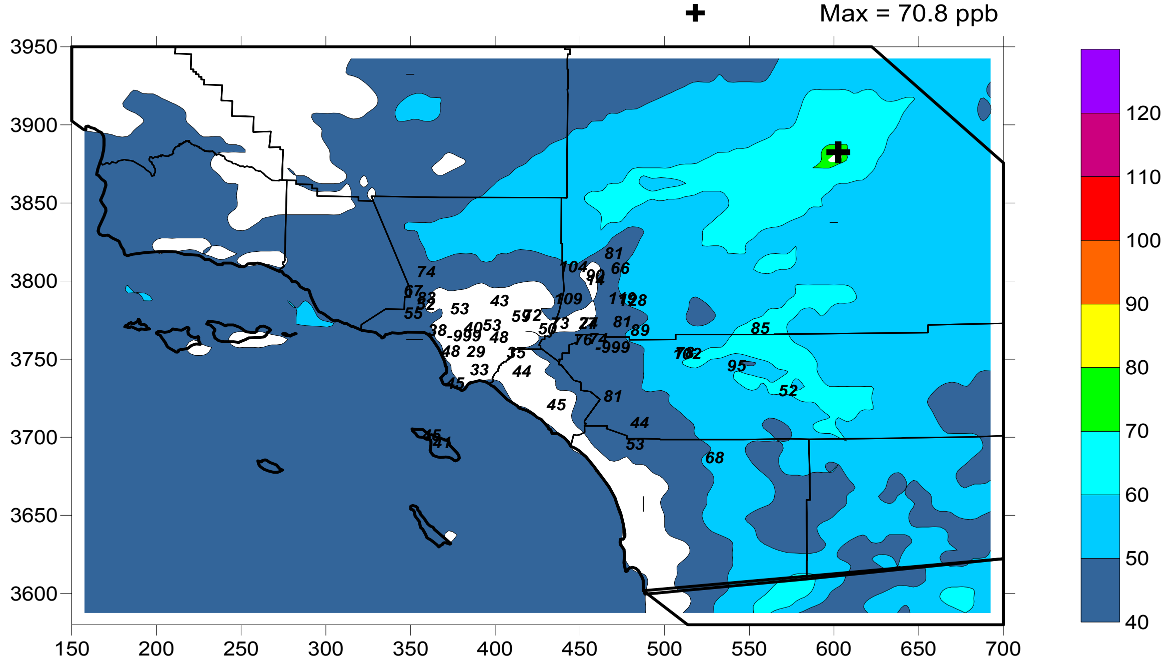
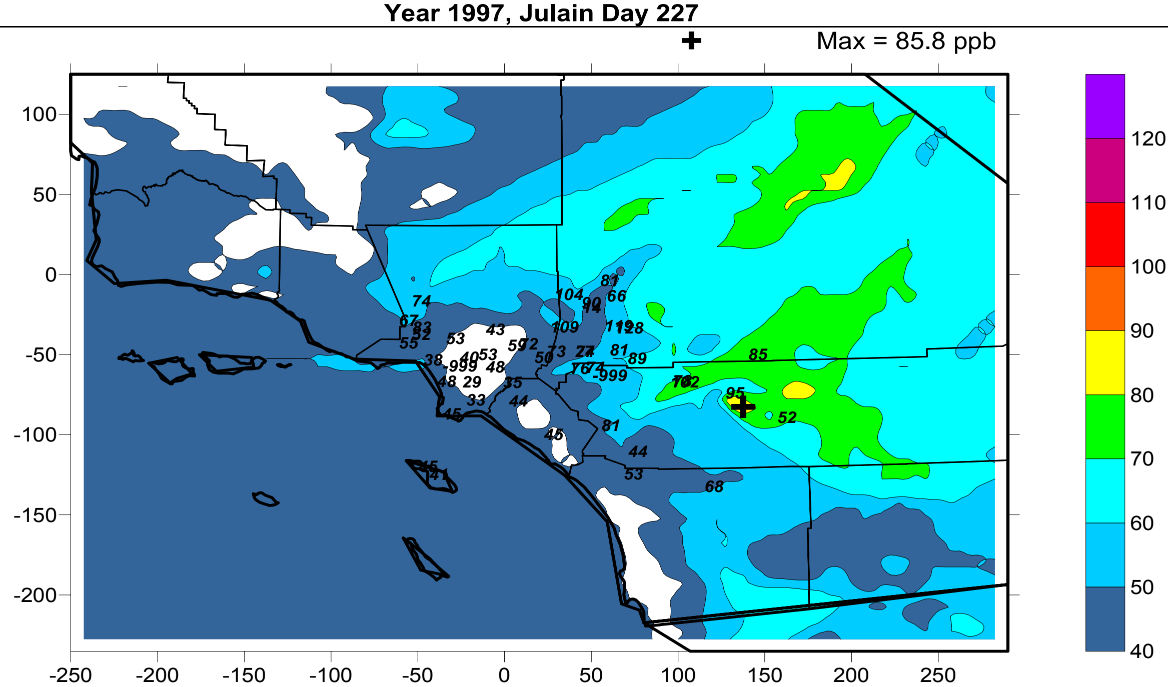


Figure B-2. Peak observed and CAMx (top) and CMAQ (bottom) estimated 8-hour ozone concentrations in the SoCAB on August 6, 1997.



Daily Max 8-Hour Ozone(ppb)
CAMx TST 1
Year 1997, Julain Day 227



Daily Max 8-Hour Ozone(ppb)
CMAQ
Year 1997, Julian Day 227

Figure B-3. Peak observed and CAMx (top) and CMAQ (bottom) estimated 8-hour ozone concentrations in the SoCAB on August 15, 1997.

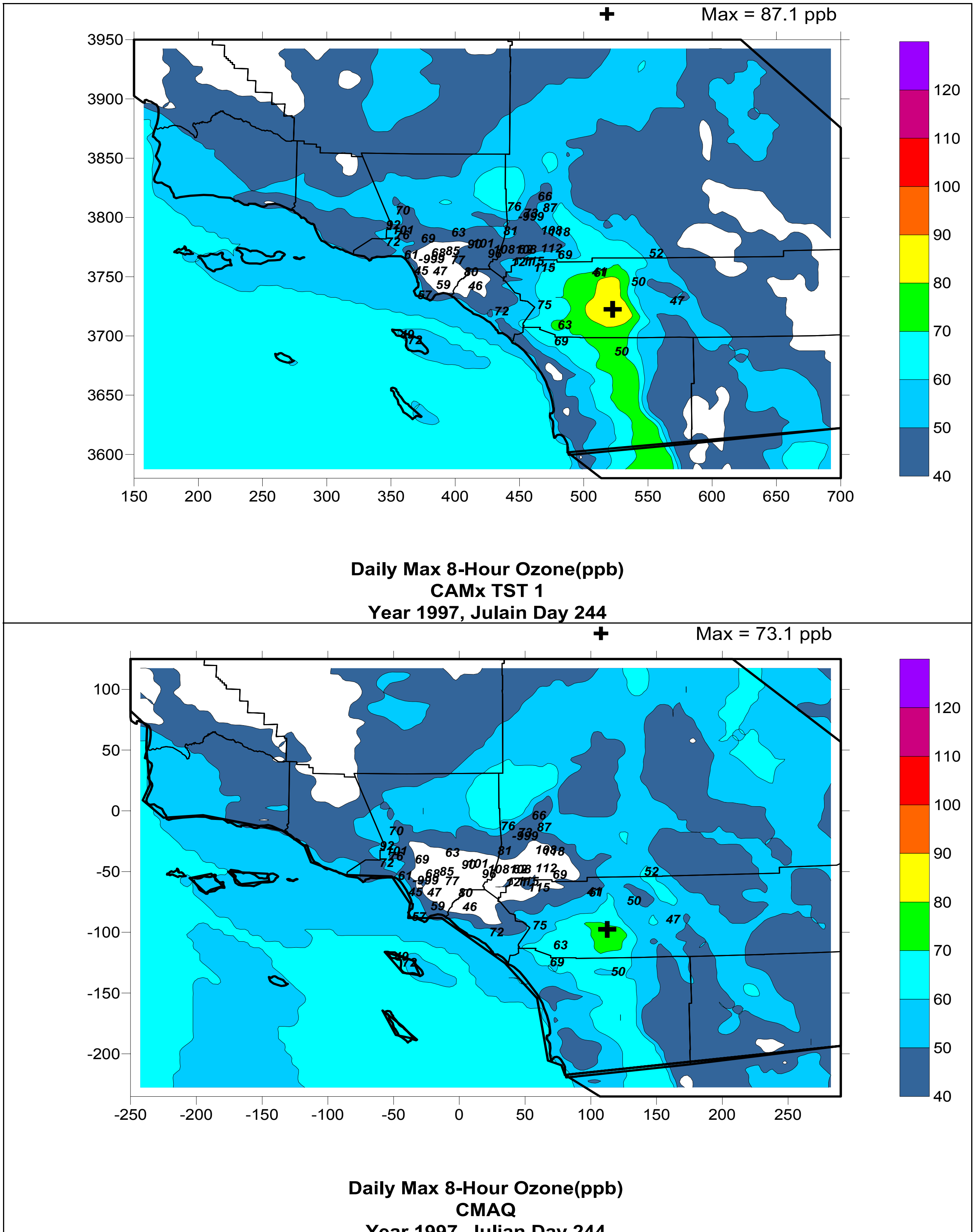


Figure B-4. Peak observed and CAMx (top) and CMAQ (bottom) estimated 8-hour ozone concentrations in the SoCAB on September 1, 1997.

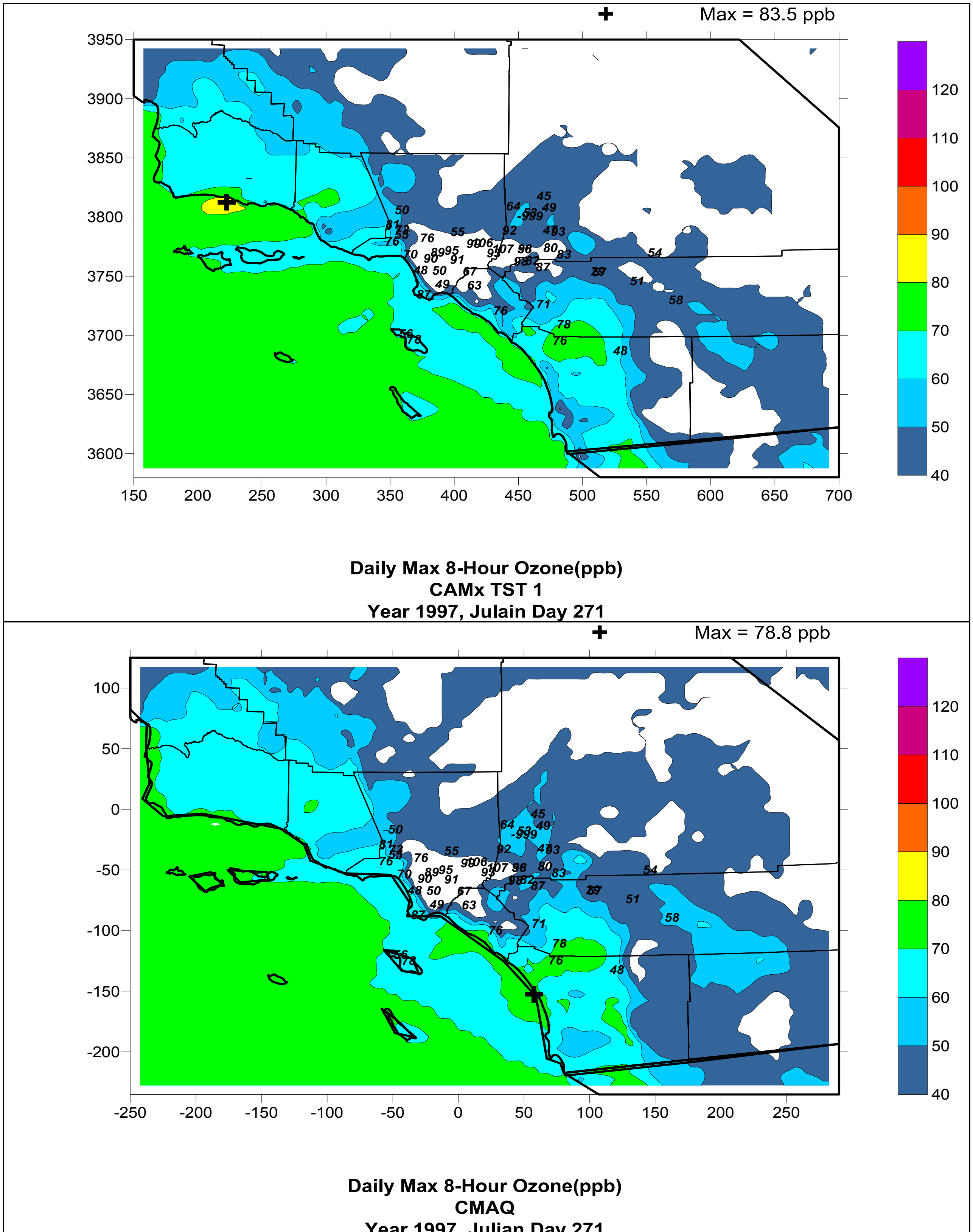


Figure B-5. Peak observed and CAMx (top) and CMAQ (bottom) estimated 8-hour ozone concentrations in the SoCAB on September 28, 1997.