

ATTACHMENT-7

Technical Report: CALGRID Ozone Simulations

Background

Regional photochemical simulation of ozone concentrations in the South Coast Air Basin (Basin) in the development of the 2003 Air Quality Management Plan (AQMP) ozone attainment demonstration was conducted using three modeling platforms and two chemical packages. These included the Urban Airshed Model (UAM), the California Photochemical Grid Model (CALGRID) and the Comprehensive Air Quality Model with Extensions (CALGRID). The chemical modules included Carbon Bond IV (CB-IV) and the State Air Pollution Research Center module (SAPRC99). Prior to the release of the Draft 2003 AQMP, the CAMx modeling platform was removed from the stable of regional simulation models due to its base-year performance in recreating peak observed ozone concentrations. Both UAM and CALGRID were retained for further evaluation for the Final AQMP and while UAM with CB-IV was selected as the modeling and chemical package for the Plan, CALGRID/SAPRC99 simulations continued to be conducted in support of the document and analysis.

This technical report briefly outlines the characteristics of the CALGRID model, and its application for the August 3-7, 1997 ozone simulation. Also discussed are the model input preparation, modifications made to accommodate meteorological model output and performance for the base and future year simulations. The discussion also provides an analysis of future year projections of carrying capacity that adjusts model output to account for under prediction of base-year ozone.

CALGRID Air Quality Model

The CALGRID model was developed under contract to the ARB (Yamartino, et. al., 1989; Scire, et. al., 1989). The model featured full compatibility with the CALMET meteorological model and it was the first regional air quality simulation model to incorporate the SAPRC chemical mechanism. Recent upgrades to the CALGRID model include the addition of the CB IV chemical mechanism (Kumar et. al, 1992) and the upgrade of the numerical advection solver (Earth Tech, 1996a). Since its release, the CALGRID model has been the subject of a number of peer reviews (eg., Yamartino, et. al., 1992; Kumar, et. al., 1994) and comparisons with other air quality models (Kumar, et. al. 1994; Earth Tech, 1996b; Jiang et. al., 1998; Schulman and Moore, 1998). CALGRID has been widely used in the United States and overseas because it is not dependent on resource-intensive prognostic meteorological models for air quality model inputs (Phinis, et. al., 1993; Jaing, et. al., 1997a; Jaing, et. al., 1997b; Silibello, et. al., 1998; Barna, et. al., 2000; Gimson, 2000; Vaughan and Lamb, 2002).

Adaptation of the CALGRID Air Quality Modeling System

CALGRID simulations were conducted using the Southern California Ozone Study (SCOS97) modeling domain and meteorological data. Prior to implementing CALGRID, three potential limitations of the air quality model were identified and addressed. CALGRID model supported the CB4 and SAPRC90 chemical mechanisms; however, it did not contain the most recent SAPRC99f mechanism. While CALGRID model was fully compatible with the CALMET meteorological model it was not formulated to directly use output from the MM5 mesoscale prognostic model. Thirdly, because CALGRID was developed to link diagnostic meteorological model there was concern that the model did not contain numerical corrections for mass-divergent flows.

By virtue of the accommodation of both the CB4 and the SAPRC chemical mechanisms, the chemical mechanism structure within the CALGRID code closely resembled the Flexible Chemical Mechanism of the UAM/FCM model. The UAM/FCM model (Kumar, et. al., 1995) was written to allow the inclusion or modification of any chemical mechanism. Because of this resemblance, it was relatively straightforward to create an interface between the UAM/FCM model and CALGRID allowing modifications to the chemical mechanisms within CALGRID. When this interface was completed, two upgrades of the CALGRID model were made. The first upgrade replaced the SAPRC90 mechanism with SAPRC99f. (Note: the versions of the SAPRC99 chemical mechanism was not subject to peer review). The second upgrade expanded the CB4 mechanism to include explicit representation of MTBE and inert tracer species. The inert species provided for the simulation of non-reactive trajectories.

A meteorological preprocessor was developed to marry the output of the MM5 prognostic model with the CALGRID/CALMET system. Meteorological products including the winds, temperature and diffusivity (vertical and horizontal) were converted from the MM5 output to the CALGRID input format. Vertical diffusivity was defined based on CALMET generated mixing heights.

To address the issue of mass divergence, CALGRID was modified to require a non-reactive chemical species designated as 'NONR'. Within CALGRID, the value of NONR is initialized with a concentration of 1 ppb and there are no emissions of NONR. After each one-half advection time step, all chemical species concentrations are normalized to NONR. In subsequent sensitivity tests of the modified CALGRID, the maximum mass divergence within the SCOS modeling domain was less than 10%.

Meteorological Model/Input Preparation

The CALGRID ozone simulations were driven by the MM5 recreation of the August 3-7, 1997 meteorological episode. Based on NOAA's NCEP-model initialization, MM5 was simulated using three grid domains (see Figure A-7-1) and using 4-

dimensional data assimilation. MM5 was based on a Lambert Conformal coordinate system. The four dimensional data assimilation benefited from the extensive surface monitoring and upper air radar wind and temperature-profiling network supporting the SCOS97 effort. The resolution of the model horizontal grid cell was 5-squared km in the inner domain.

As in many past mesoscale meteorological modeling efforts in southern California, the complexity of the terrain and the uniqueness of the initial conditions give rise to unusual wind flow patterns in the higher elevations. Nocturnal slope flows area often greatly exaggerated with down-slope flows occurring in gusts. Modifications to the terrain specification have been made to overcome this aspect of the prognostic simulation. In this application, the terrain file was reduced by two thirds.

Comparison of UAM and CALGRID Simulations

Table A-7-1 provides a comparison of the key components of the CALGRID and UAM simulations. In general, emissions, base meteorological data, background and initial conditions are identical between the applications. Major differences occur in the chemistry, advection schemes and the vertical layer structures. CALGRID is designed for pollutant transport over large domains. UAM was designed for an air basin application. Meteorological data input to CALGRID from MM5 required the development of preprocessor software to convert the hydrostatic prognostic data and diffusivity to fixed vertical layers. Based on the differences provided in the summary table it is easy to assume that the modeling applications will diverge greatly in their solution. However, model performance is remarkably similar.

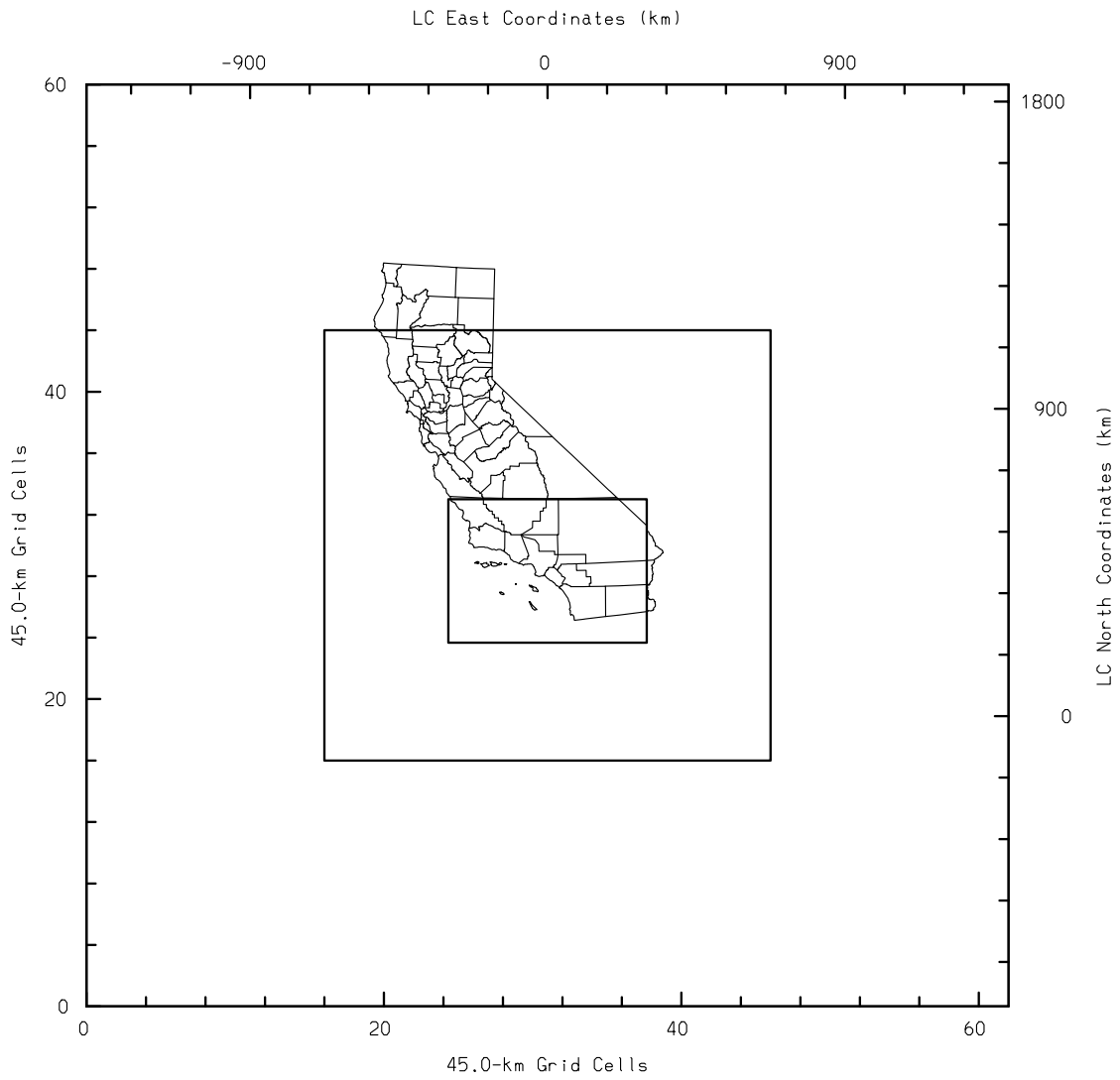


Figure A-7-1

Nested MM5 Domains:

The horizontal grid resolution of the outermost domain is 45 km, for the middle domain is 15 km, and for the fine scale domain is 5 km.

Table A-7-1

Comparison of CALGRID and UAM Modeling Systems

Parameter	CALGRID	UAM
<i>Modeling System</i>		
Domain Size	SCOS97	SCOS97
Grid Size	5-Km	5-Km
Vertical Layer Structure	Fixed 16 Layers	Variable 5-Layers
Region Top	5000 meters	2000 meters
Boundary/Top/Initial Conditions	Modified EPA Clean*	Modified EPA Clean*
Modeling Coordinate System	Lambert Conformal	UTM
<i>Emissions</i>		
Mobile Source	EMFAC2002/Offroad/DTM4	EMFAC2002/Offroad/DTM4
Area Source	Joint ARB/District	Joint ARB/District
Point Source	Local Districts Inventories	Local Districts Inventories
Emissions Allocation/Plume Rise	3-dimensional introduction	Layer-1 with Briggs plume rise
<i>Chemistry</i>		
Basic Module	SAPRC99	CB-IV
Chemical Solver	Quasi Steady States analysis (QSSA) or Hybrid Solver	quasi-steady state assumptions with Crank-Nicholson algorithm
Photolysis Rates	Radiation extinction as height above sea level.	One-dimensional based on Zenith angle
<i>Meteorology</i>		
Meteorological Data	SCOS97	SCOS97
Wind Model	MM5-4DDA	CALMET
Advection	Chapeau function based scheme with Forester filter	Forward-upstream diffusive-corrected algorithm of Smolarkewicz
Vertical Diffusivity/Diffusion	Horizontal diffusion- based on stability class with adjusted wind speed, (Smagorinsky method) Vertical diffusivity –Combination of various method depending on stability and layer height	Vertical diffusivity coefficient is calculated internally
Dry Deposition	Surface resistance model	Roughness length, stability, wind speed, deposition factor
Mixing Heights	CALMET	Holsworth
Cloud Cover	Yes	None
Mass Continuity Adjustment	NONR	O'Brien scheme

* Modified EPA Clean include NO - 0.0 ppb, NO₂ - 2 ppb, and VOC - 20 ppbv.

Base Year Model Performance

Table A-7-2 summarizes the base-year performance statistics for the CALGRID simulation for August 5th and August 6th. Performance criteria are outlined in Appendix V of the 1994 AQMP. Figures A-7-2 and A-7-3 provide the tile plots of predicted maximum concentration. Figures A-7-4a through A-7-4q provide the diurnal plots (dplots) of predicted and observed ozone concentrations.

The CALGRID simulation meets all of EPA's three-performance criteria in zones 3, 4 and 5 on August 5th and meets two criteria in zones 3 and 4 on the August 6th. The simulation under predicts the Basin peak concentration on both days with the ratios valuing 0.88 and 0.90 on the 5th and 6th respectively. Model performance for NO₂ in Zone 4, the primary ozone impact zone met criteria in five of six categories. NO₂ performance for the ratio of the unpaired peak concentrations and systematic bias met EPA criteria in each zone on August 6th. In general performance for NO indicated over prediction in zones 3 and 5 and under prediction in Zone 4. Overall, CO was under predicted in each zone, regardless of the day.

As depicted in Figure A-7-2, the August 5th CALGRID simulation predicts peak ozone concentrations in the Riverside area, near the location where the maximum concentration was observed. Impacts are predicted throughout the western portion of Riverside County and concentrations between 140 and 160 ppb occur along the foothill regions of eastern Los Angeles and western San Bernardino Counties. The primary impact zone shifts towards the northern portion of Los Angeles County and the desert portion of San Bernardino County on August 6th. This is consistent with the UAM simulations and reflects the development of the observed eddy circulation and southerly flow through the modeling domain.

Figures A-7-4a through A-7-4q illustrate the capacity of the CALGRID simulation to recreate the temporal ozone distribution. The diurnal ozone plots indicate that ozone is slightly over predicted in the San Gabriel Valley and San Fernando Valley. In addition, the general tendency observed throughout the Basin is for over prediction of morning ozone concentrations. The morning tendency is clearly observed throughout Zone 4. This is in contrast to the tendency to lag late in the day observed by the UAM simulations.

Table A-7-3 provides an observational comparison of the performance of UAM and CALGRID for the base-year simulation. Also listed in the table are selected advantages and disadvantages of the use of either model.

TABLE A-7-2
Comparative Performance Statistics

<u>Statistic</u>	<u>Zone 3</u>		<u>Zone 4</u>		<u>Zone 5</u>	
	5 th	6 th	5 th	6 th	5 th	6 th
Ozone Threshold (pphm)	6.0	6.0	6.0	6.0	6.0	6.0
Ratio of Predicted Basin Peak to Peak Observed	0.88	0.90	0.88	0.90	0.88	0.90
Ratio of Unpaired Station Peaks	0.98	1.19	0.84	0.83	1.06	1.54
Systematic Bias (%)	5	25	11	9	-5	-3
Gross Error (%)	29	35	35	37	23	62
NO ₂ Threshold (pphm)	1.0	1.0	1.0	1.0	1.0	1.0
Ratio of Unpaired Station Peaks	0.44	0.82	0.58	0.75	0.49	0.92
Systematic Bias (%)	-59	-26	-42	-43	-24	-22
Gross Error (%)	64	49	47	65	41	59
NO Threshold (pphm)	1.0	1.0	1.0	1.0	1.0	1.0
Ratio of Unpaired Station Peaks	1.10	2.00	0.41	0.40	1.29	1.17
Systematic Bias (%)	-20	129	-32	-55	72	20
Gross Error (%)	90	208	72	87	142	123
CO Threshold (pptm)*	2.0	2.0	2.0	2.0	2.0	2.0
Ratio of Unpaired Station Peaks	0.79	1.75	0.68	0.62	0.85	0.93
Systematic Bias (%)	-51	-17	-27	-39	-12	-18
Gross Error (%)	61	60	49	52	54	60

Bold indicates numbers meeting performance goals.

* Note: No performance criteria for 1-hour average carbon monoxide and nitric oxide were available.

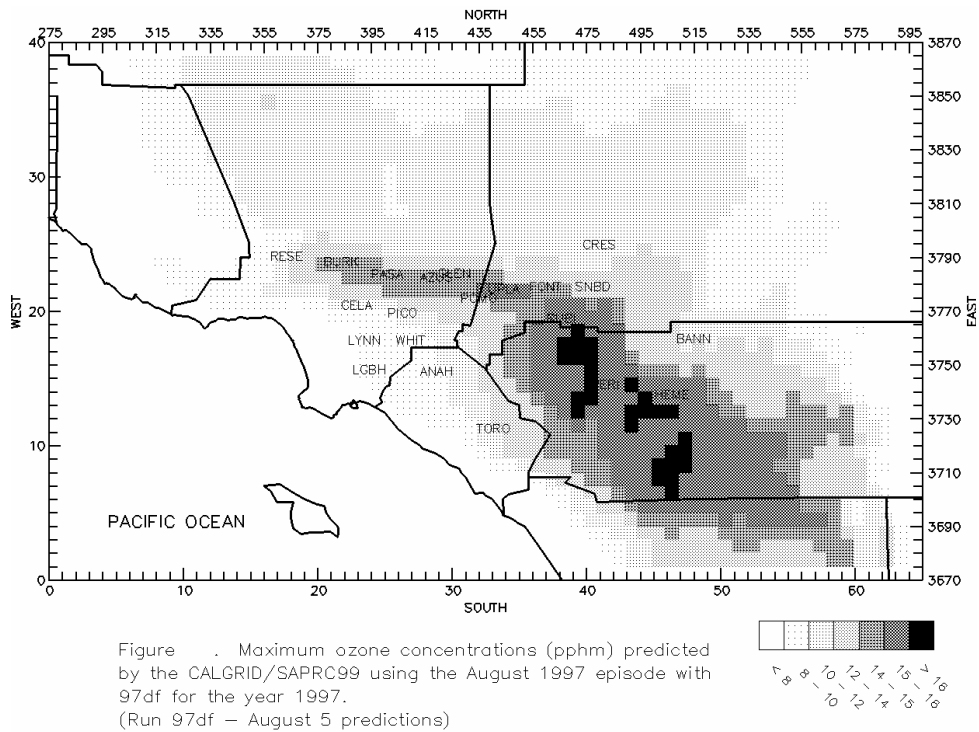


Figure A-7-2

Predicted Maximum 1-Hour Average Ozone Concentrations for August 5, 1997 Episode

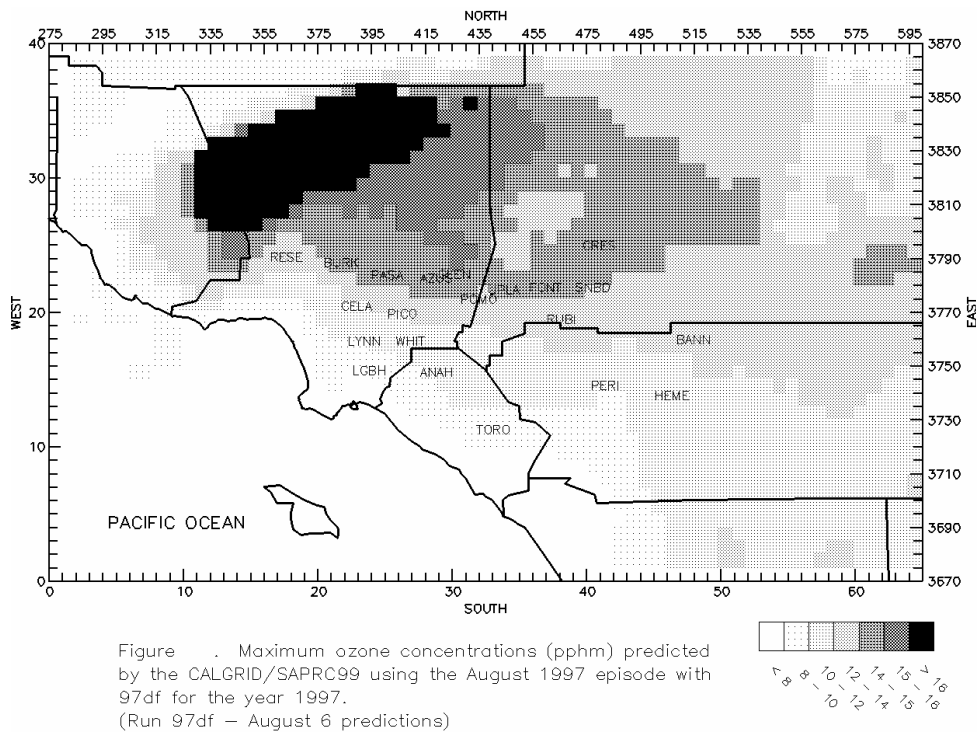
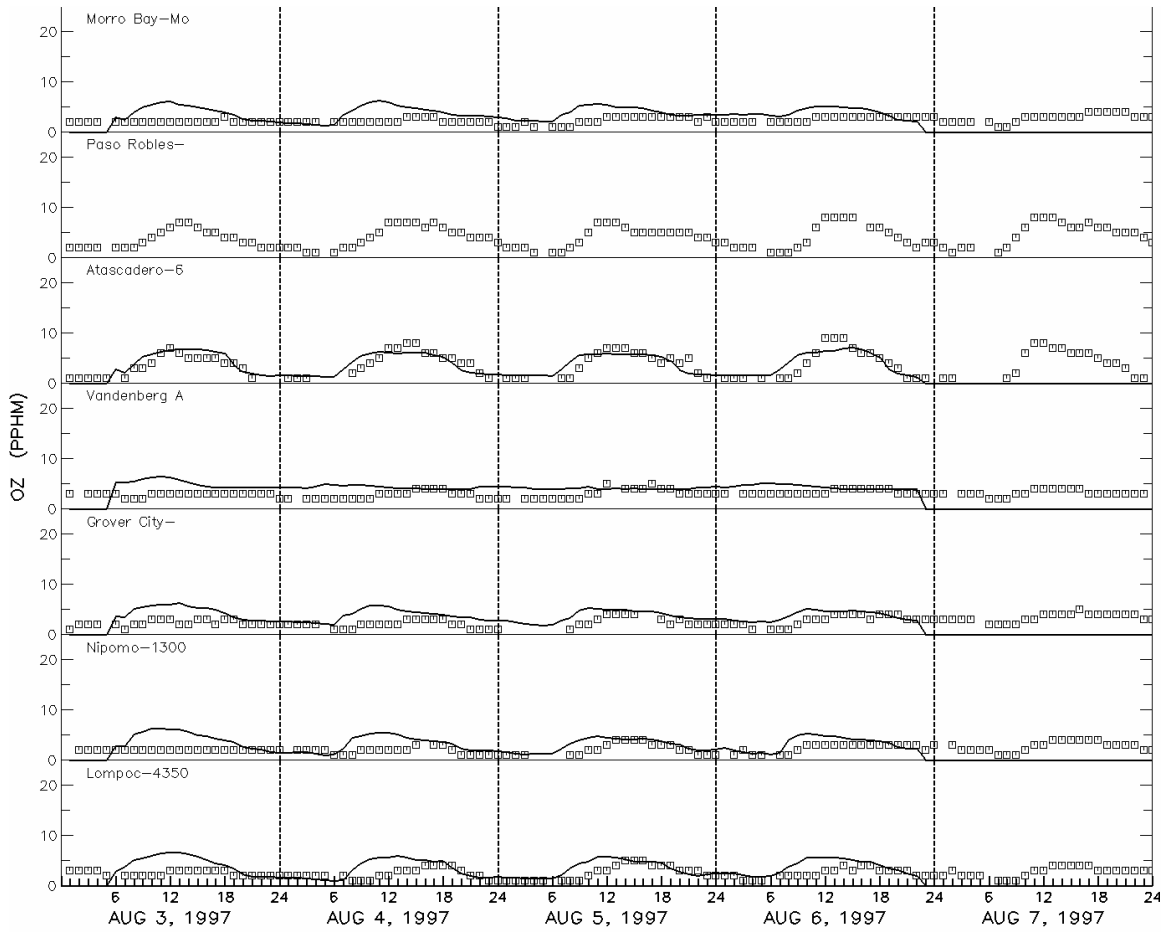


Figure A-7-3

Predicted Maximum 1-Hour Average Ozone Concentrations for August 6, 1997 Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4a

Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode

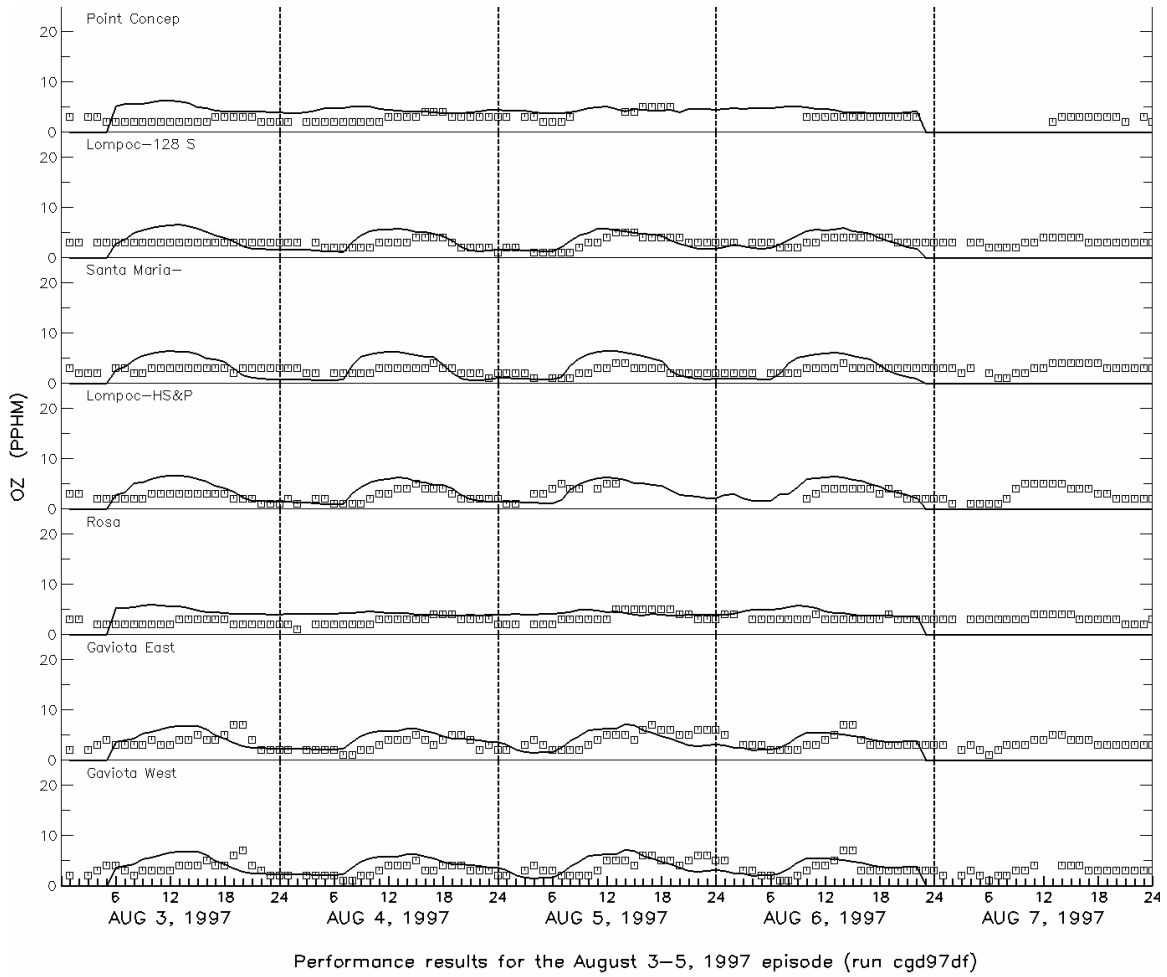
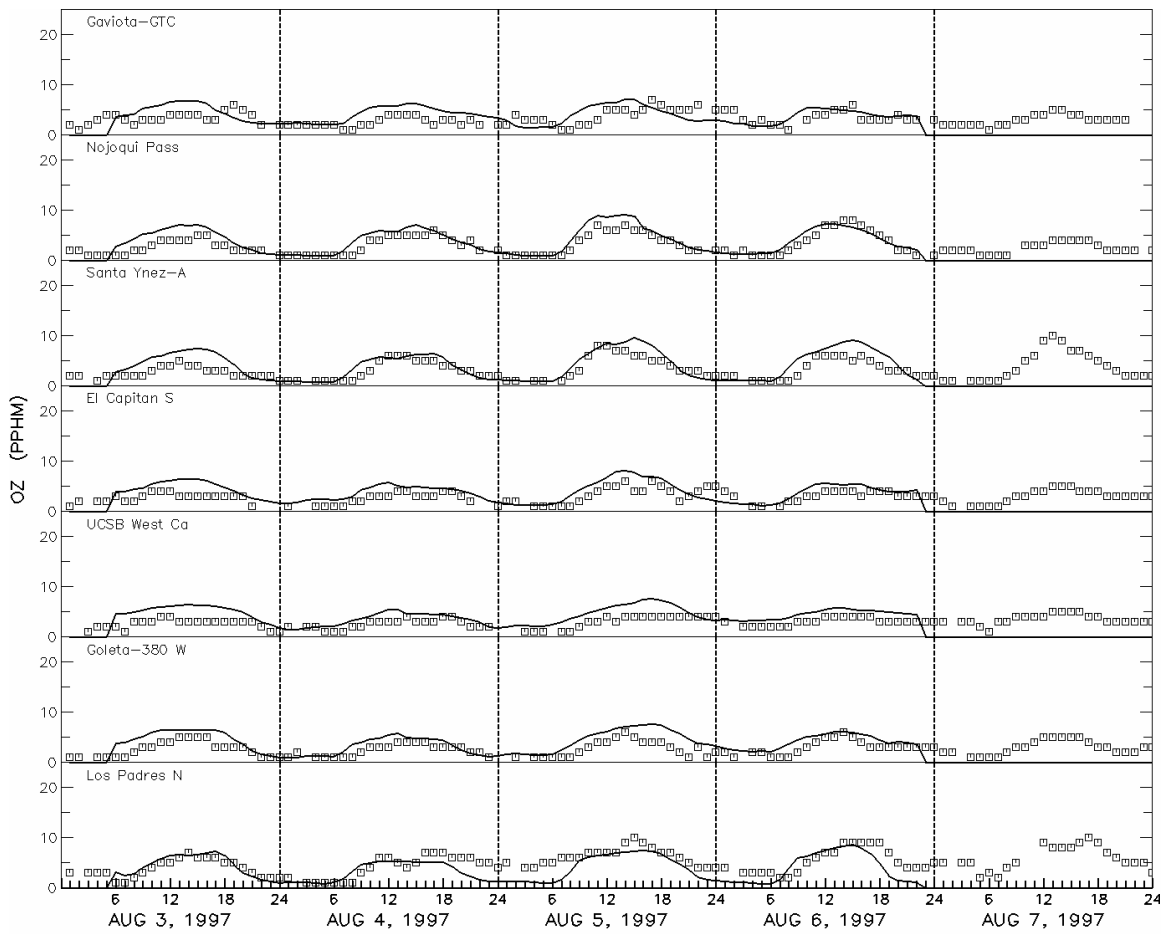


Figure A-7-4b

Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4c

Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode

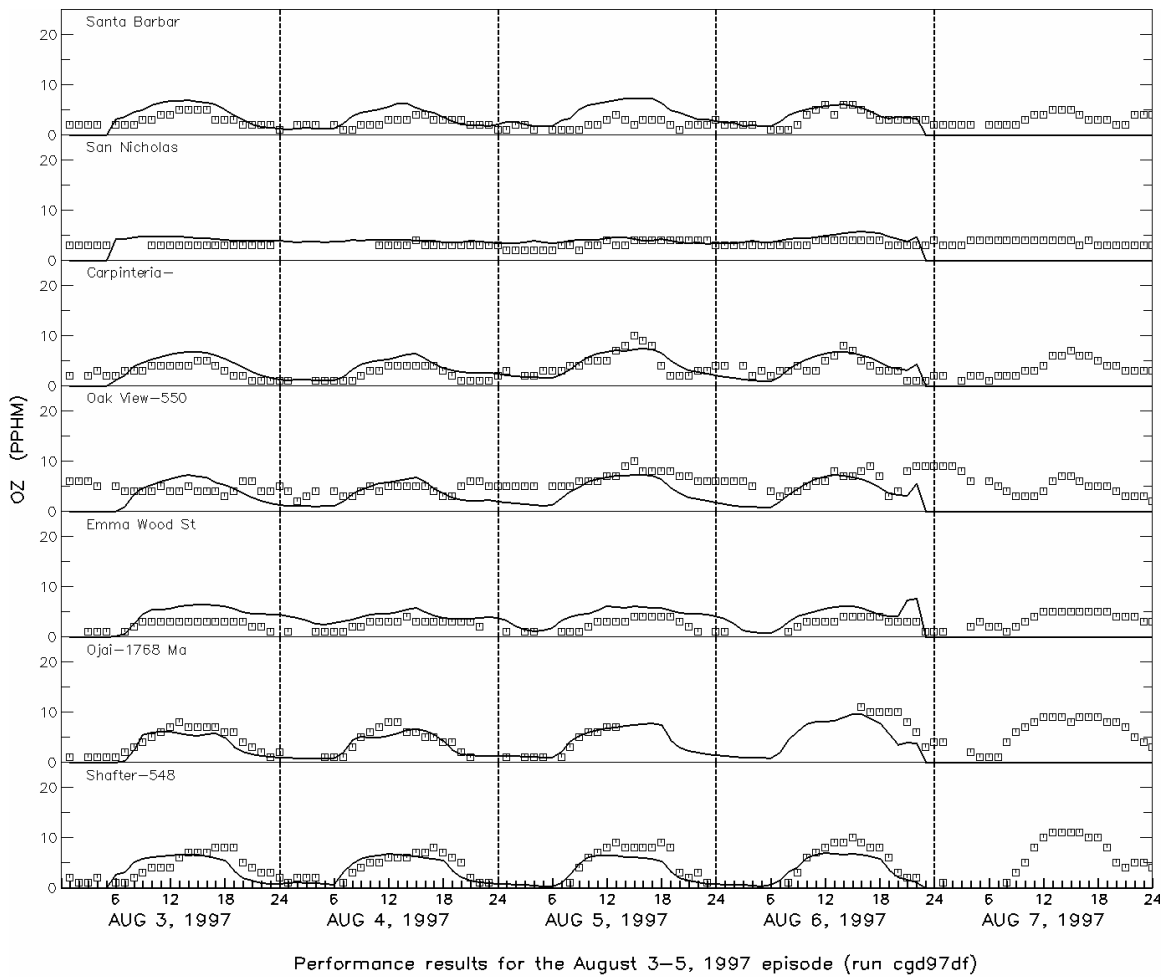
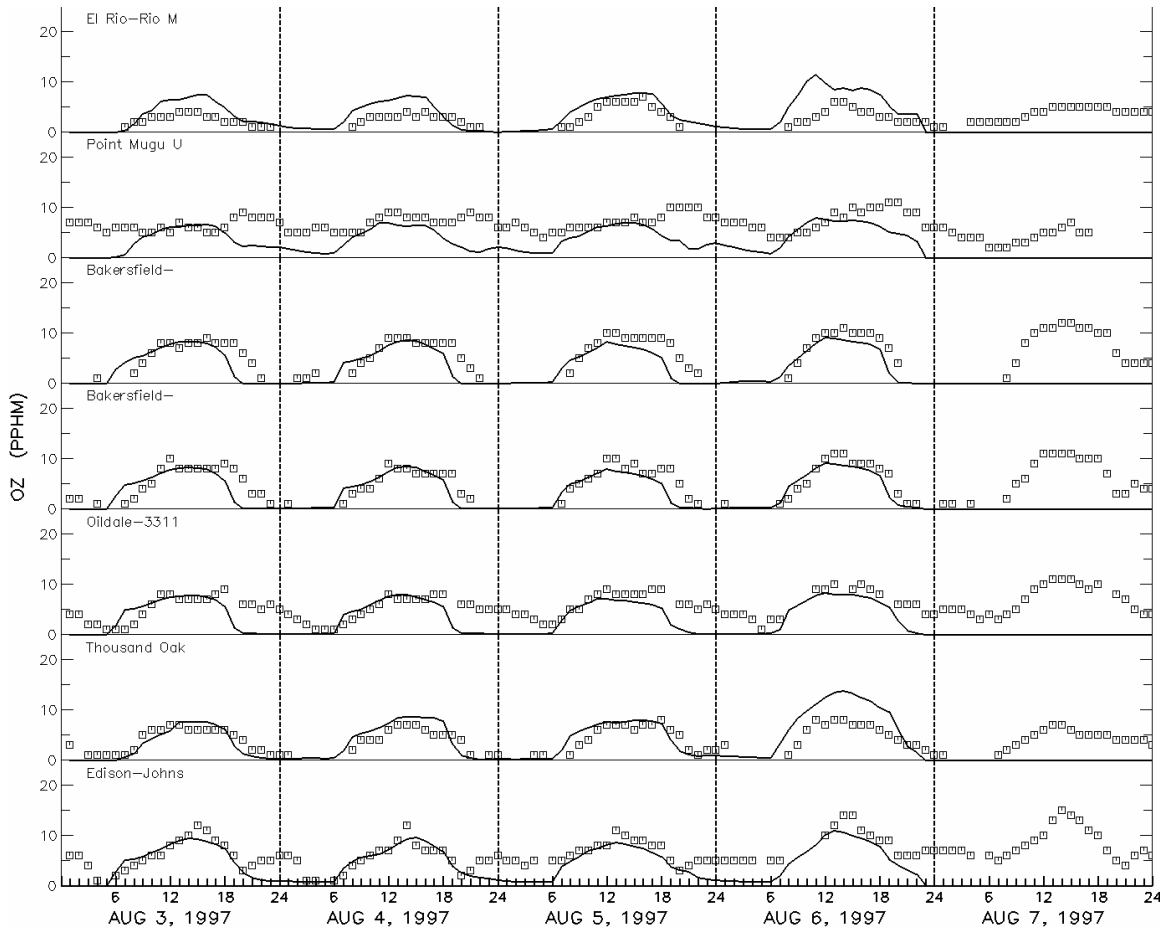


Figure A-7-4d

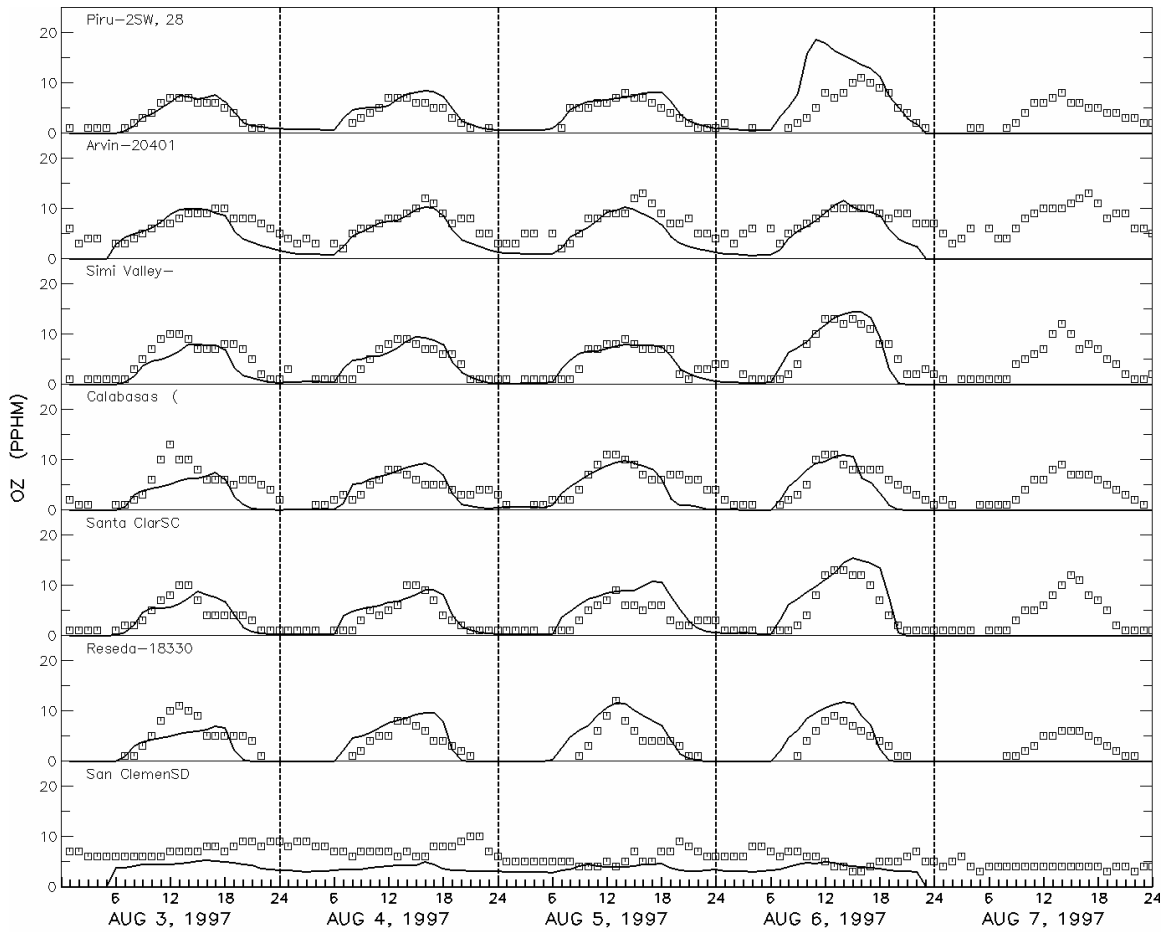
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4e

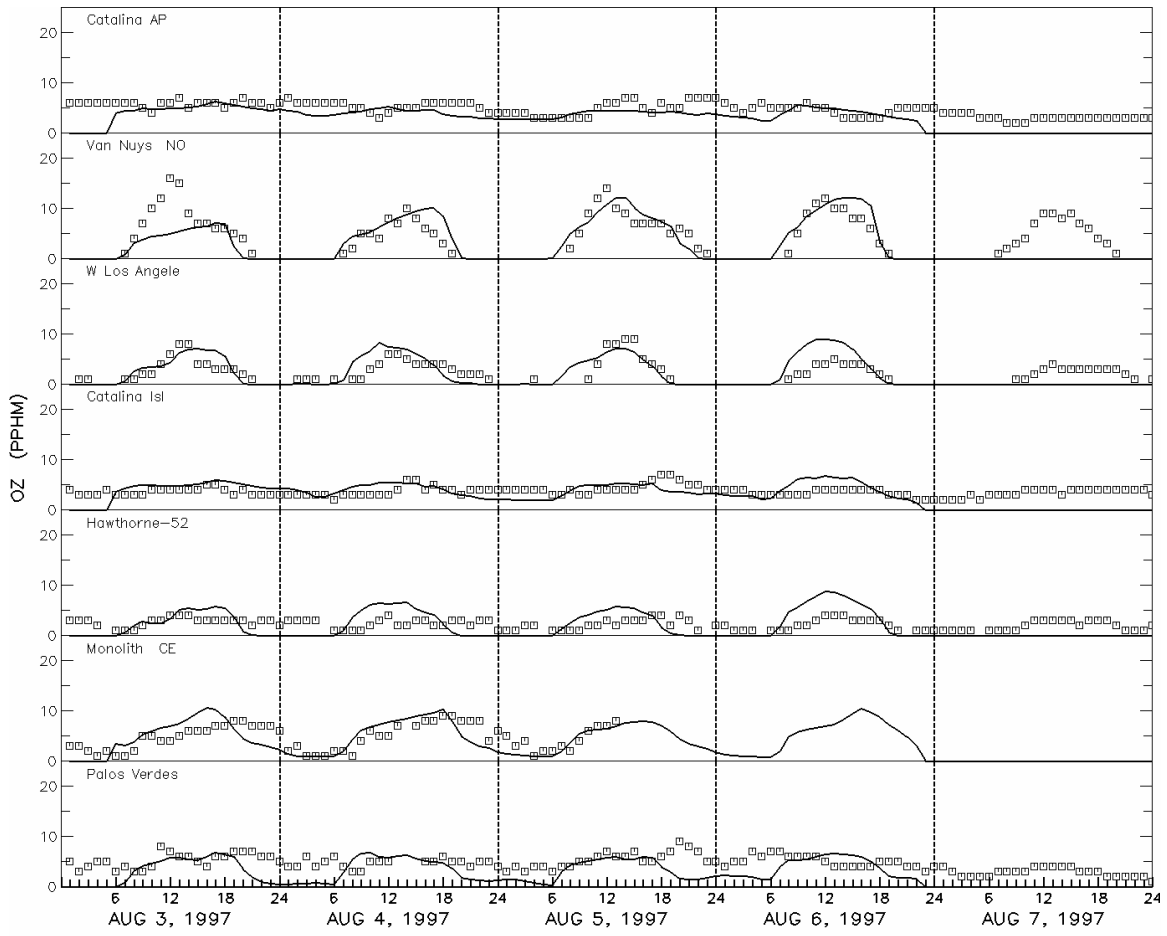
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4f

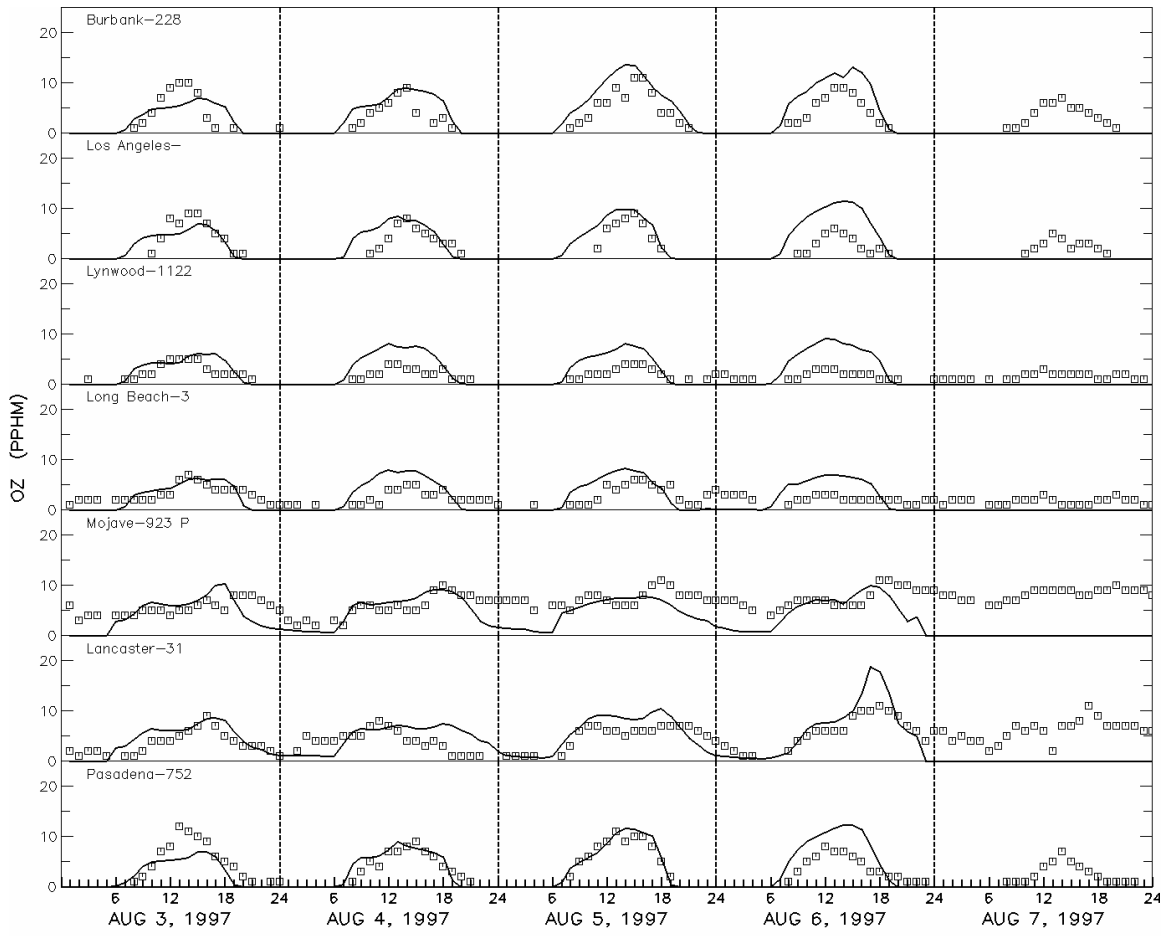
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4g

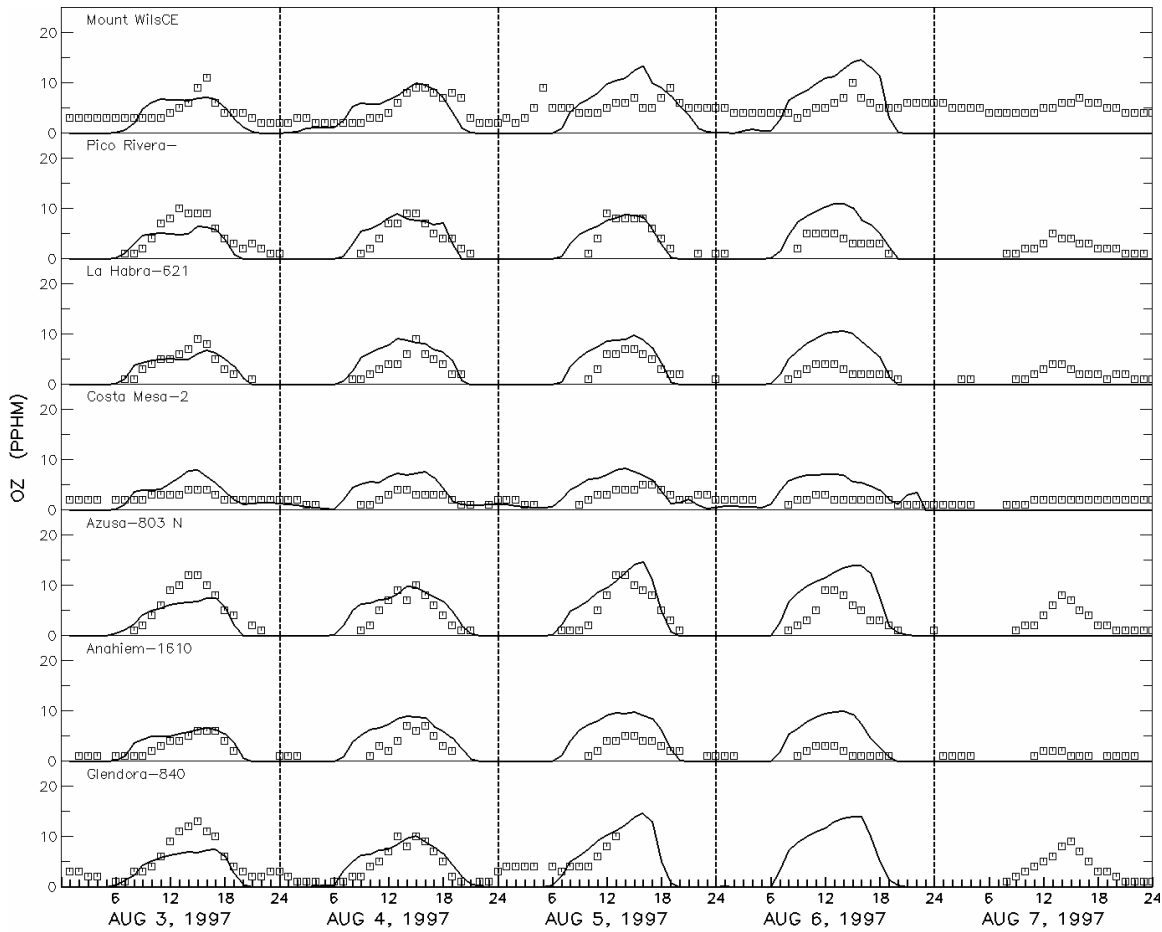
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4h

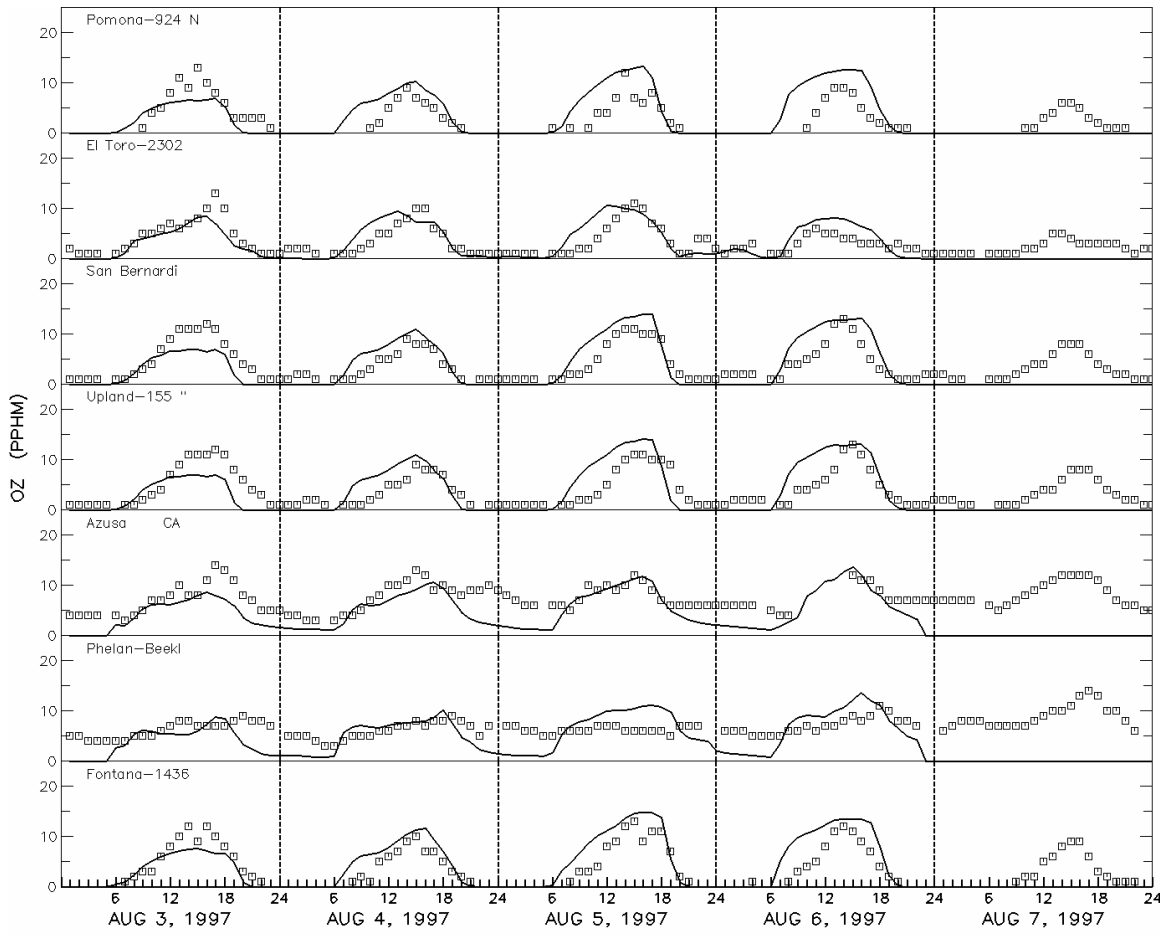
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4i

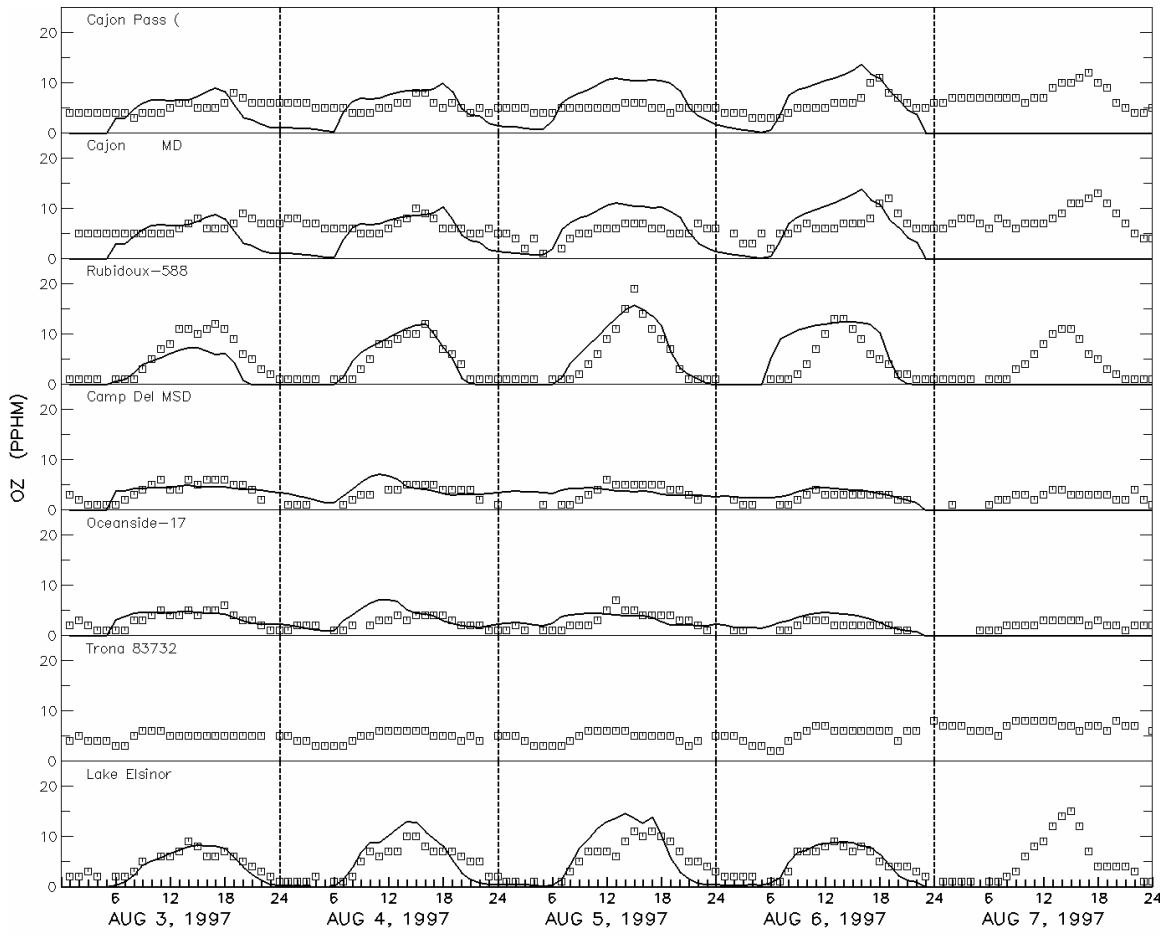
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4j

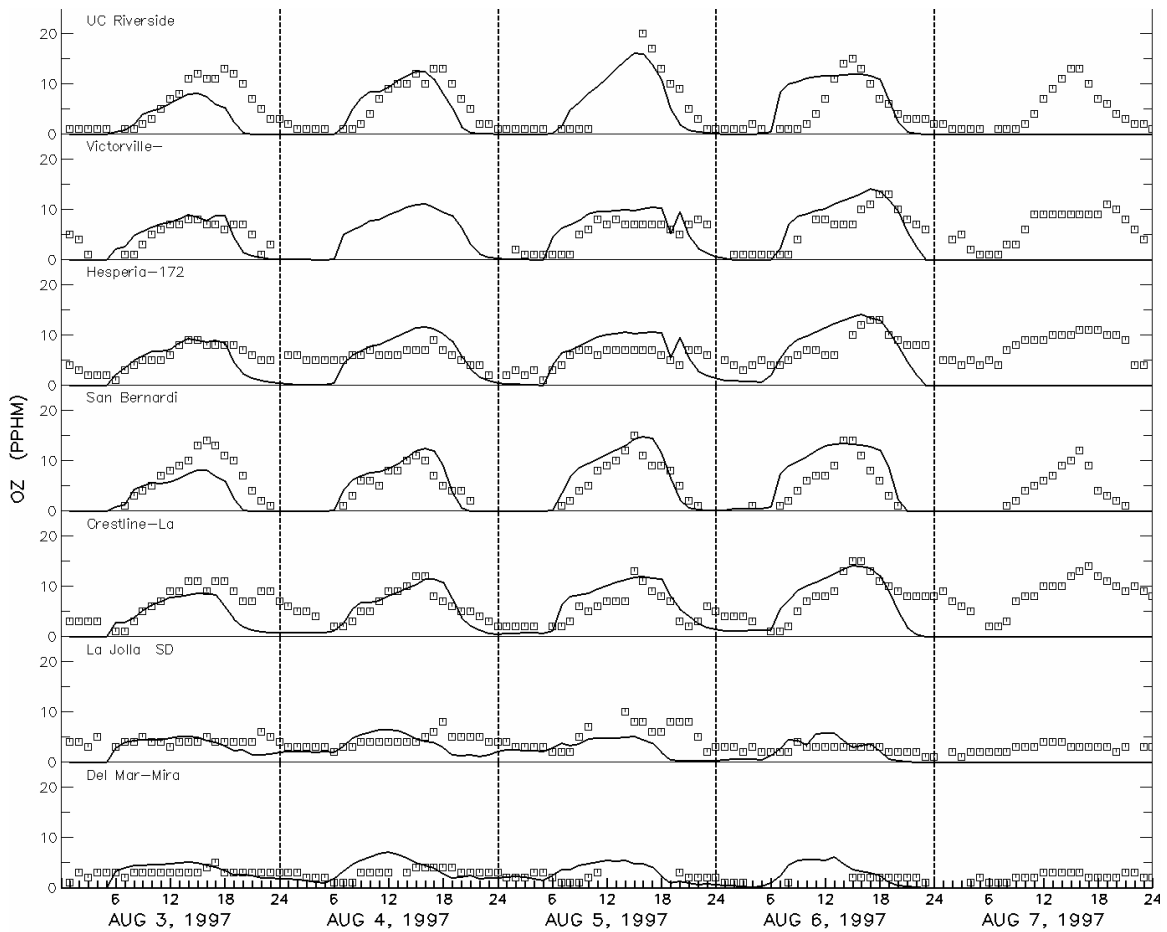
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August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-74k

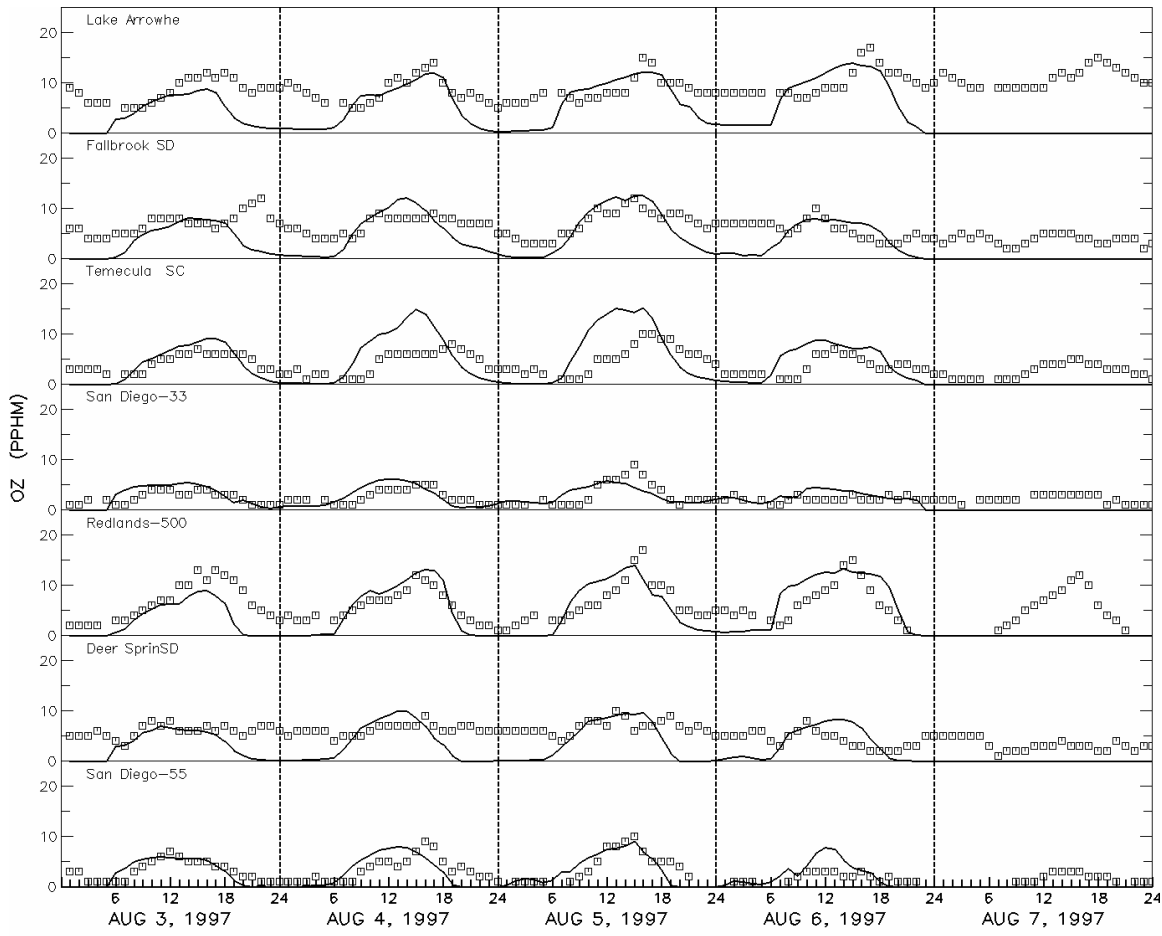
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4I

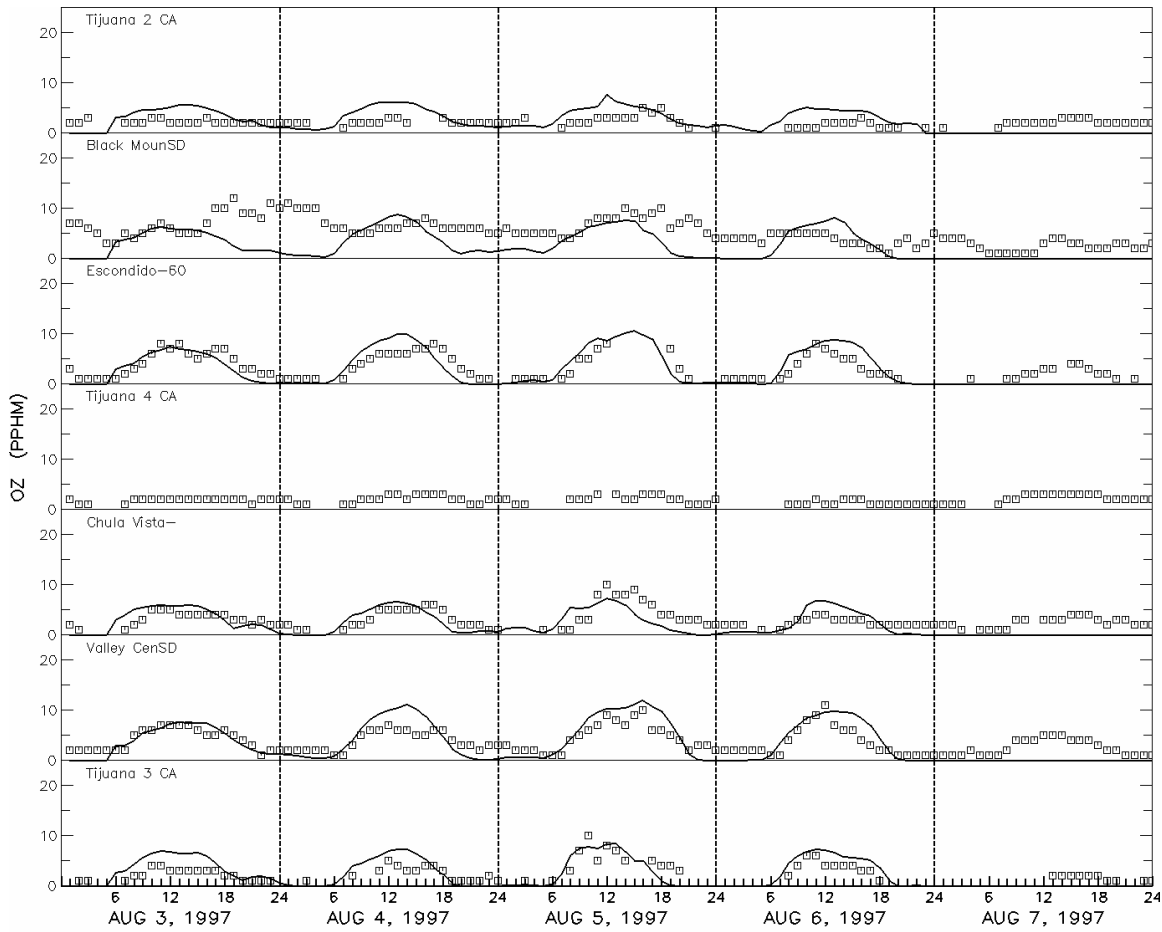
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4m

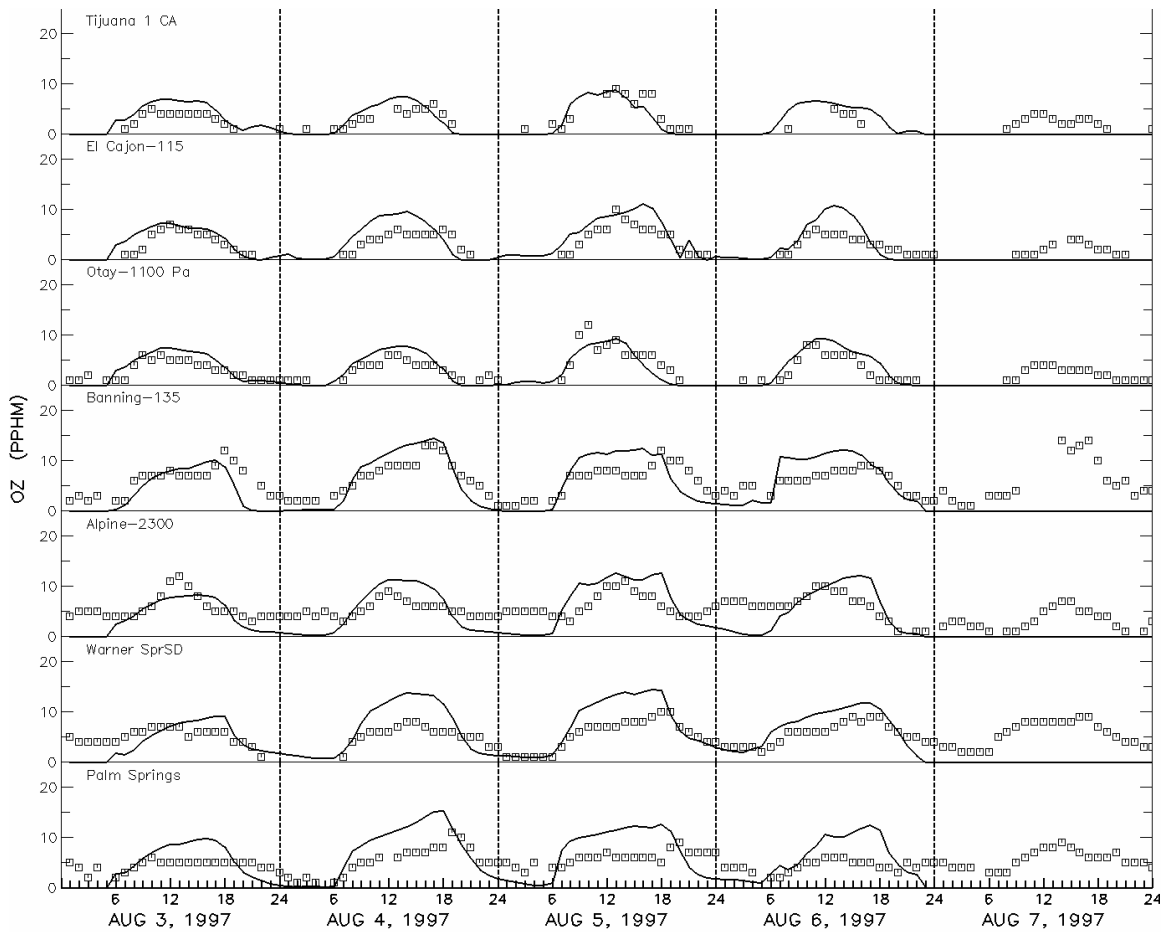
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4n

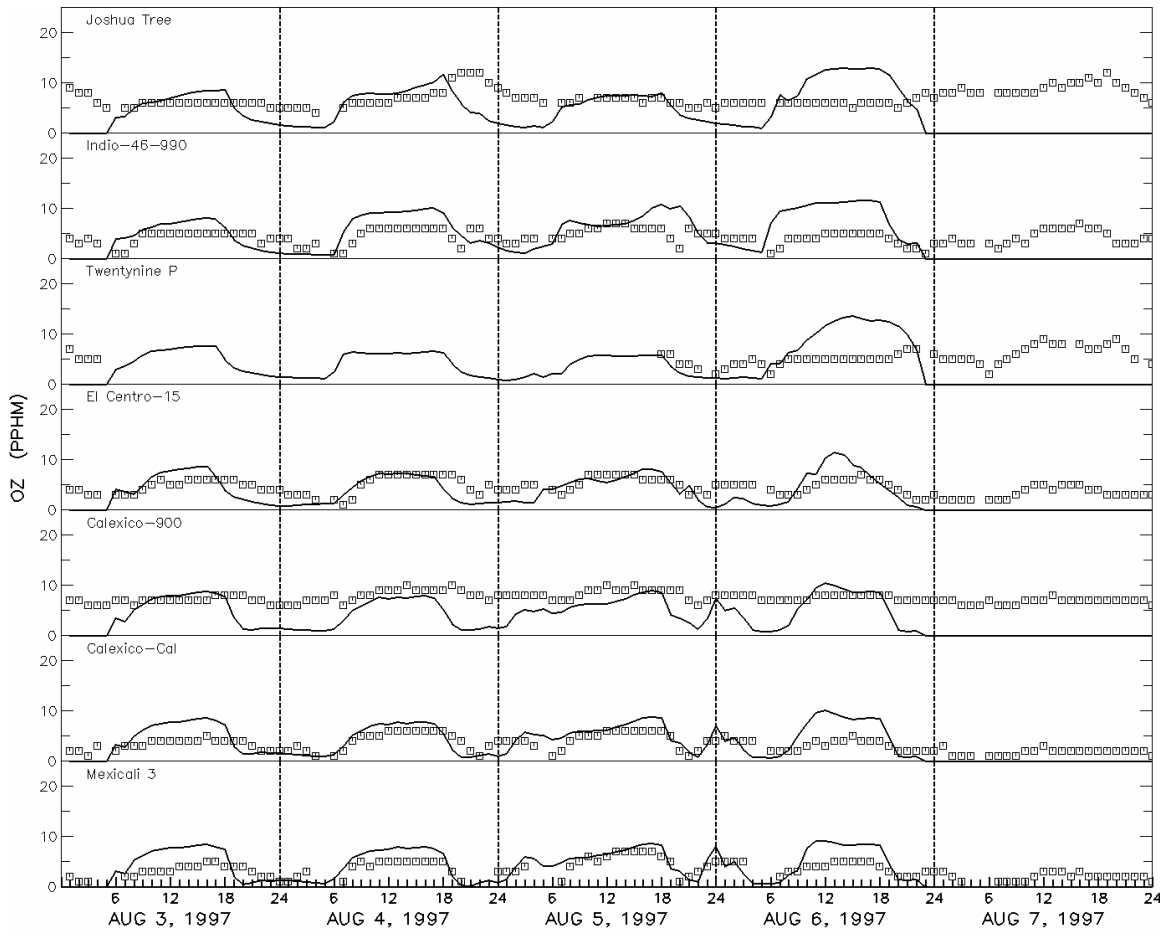
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4o

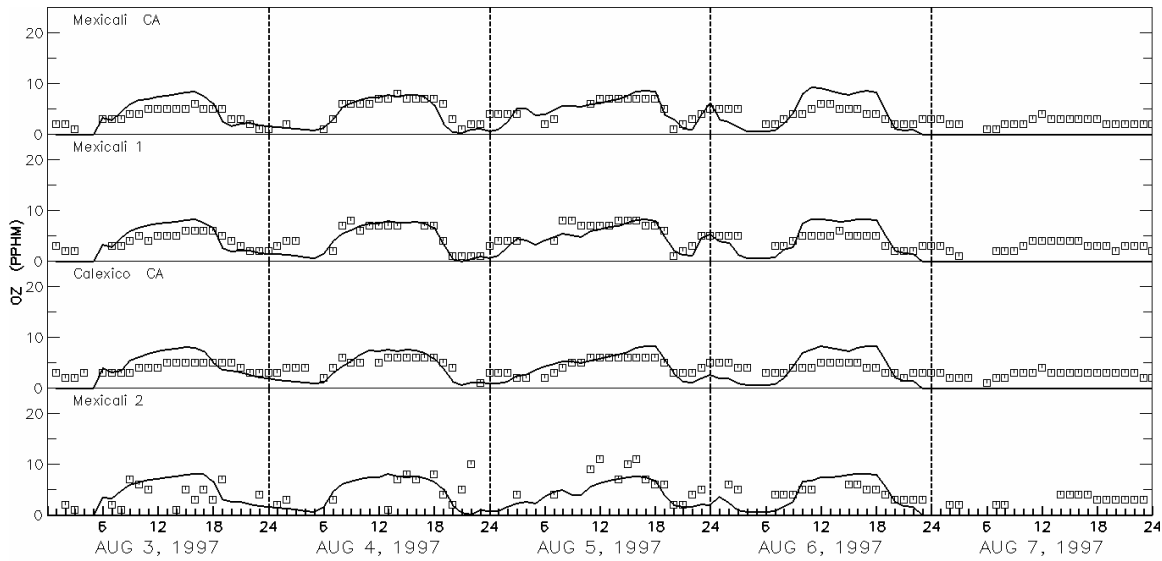
Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3-5, 1997 episode (run cgd97df)

Figure A-7-4p

Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode



Performance results for the August 3–5, 1997 episode (run cgd97df)

Figure A-7-4q

Simulated Maximum 1-Hour Average Ozone (Solid Line) Vs. Observed (Squares):
August 3-7, 1997 Ozone Meteorological Episode

Table A-7-3
General Observations

Model	Base Year Simulation Observations	Model Advantages	Model Disadvantages
UAM	<ul style="list-style-type: none"> (a) Peak concentration is south of observed (b) San Gabriel Valley generally under- predicted (c) NO_x and CO reasonably well predicted in Zone 5 source area (d) Peak concentration consistent with observations 	<ul style="list-style-type: none"> (a) Urban Application (b) Extensive Experience (c) Ease of use 	<ul style="list-style-type: none"> (a) Older advection schemes (b) Variable grid cell height based on mixing height (c) Mass continuity issues (d) Limited number of vertical layers
CALGRID	<ul style="list-style-type: none"> (a) Timing of peak and location well simulated (a) Broader area of ozone impact with morning peaks (b) Slight over-prediction of NO_x in Zone 5 source areas (d) Peak concentration 88 percent of observations 	<ul style="list-style-type: none"> (a) Urban/Regional Application (b) Coupled with CALMET Meteorological model (c) Fixed layers (d) advection designed for longer range transport 	<ul style="list-style-type: none"> (a) Minimal Experience in Modeling Community (b) Diagnostic meteorological model mass continuity issues (c) Requires MM5 interface (d) More complex application

CALGRID 2002 Mid-Course Evaluation

Table A-7-4 summarizes the 2002 CALGRID mid-course simulations compared to observed ozone air quality in 2002 while Figures A-7-5 and A-7-6 provide the 2002 predicted spatial distribution of ozone. As discussed in Chapter 3, observed ozone on days having similar meteorological characteristics as August 5, 1997, ranged from 140 to 170 ppb with an average of 150 ppb. The CALGRID simulation for August 5th reached 141 ppb, within the 2002 observed range but far below the 169 ppb peak observed concentration. CALGRID predictions for August 6th fell below the range of observed ozone concentrations.

TABLE A-7-4

CALGRID 2002 Projected Maximum 1-Hour Ozone Concentrations (ppb)

Episode Day	CALGRID Predicted (ppb)	4-Day 2002 Historical Average Ozone (ppb)	Range of Observations for Comparable days in 2002 (ppb)
August 5, 1997	141	150	140 - 169
August 6, 1997	126	140	130 - 150

2007 CALGRID Simulations

One major component of the 2003 AQMP modeling attainment demonstration addresses the issue of transport of ozone and precursor pollutants into the Coachella Valley, Antelope Valley, South Central Coast and Mojave Desert. The attainment year for each of these areas is 2007.

CALGRID predicted maximum ozone concentration maps for the year 2007 are presented in Figures A-7-7 and A-7-8 for the August 5th and August 6th 1997 episodes. Controlled emissions are used for equivalent the 2007 projection. Emission reductions through 2007 are expected to take place through exiting established control measures and reductions in mobile source emissions as projected by EMFAC2002. Table A-7-5 lists the 2007 predicted ozone air quality for the Basin and its neighboring transport partners.

While projected ozone concentrations in the Basin will exceed 124 ppb, by 2007 all areas of the Coachella Valley demonstrate attainment of the federal ozone standard.

CALGRID projections of the 2007 one-hour maximum ozone concentrations for Ventura County (South Central Coast Air Basin), the Antelope Valley, and the San Bernardino County portion of the Mojave Desert indicate that all three areas will meet the federal standard. Also presented in Table A-7-5 Valley is an adjusted prediction for one-hour maximum ozone for the Antelope Valley and Mojave Desert. Both CALGRID and UAM over predicted ozone concentrations in the high desert for the August 6th base year simulation. For the UAM simulation, Hesperia and Victorville were over predicted by an average of 33 percent while Lancaster was over predicted by 43 percent. For the CALGRID simulation, Hesperia and Victorville were over predicted by 9 percent while Lancaster was over predicted by 71 percent. By adjusting the 2007 UAM simulation in the local area for the base-year over prediction the estimated Antelope Valley and Mojave Desert impacts are lowered to 72 and 112 ppb, respectively. This correction is consistent with the projected is consistent with the direct CALGRID simulation for August 5th.

TABLE A-7-4

CALGRID 2007 Projected Maximum 1-Hour Ozone Concentrations (ppb)

Episode Day	Basin	Coachella Valley	Antelope Valley	Mojave Desert	Ventura-South Central Coast
August 5, 1997	135	121	107	105	95
August 6, 1997	123	117	123 (72)*	122(112)*	112

* Concentration for the high desert inside the brackets is the scaled value to adjust for systematic over prediction in the base year

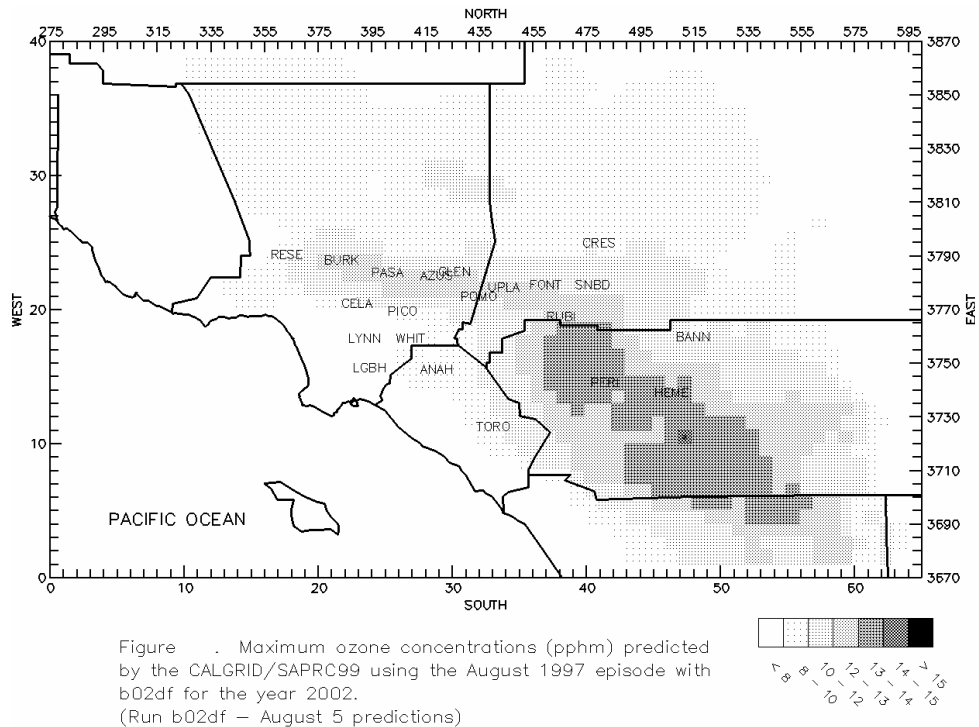


Figure A-7-5

Predicted 2002 Maximum 1-Hour Average Ozone for August 5, 1997 Episode

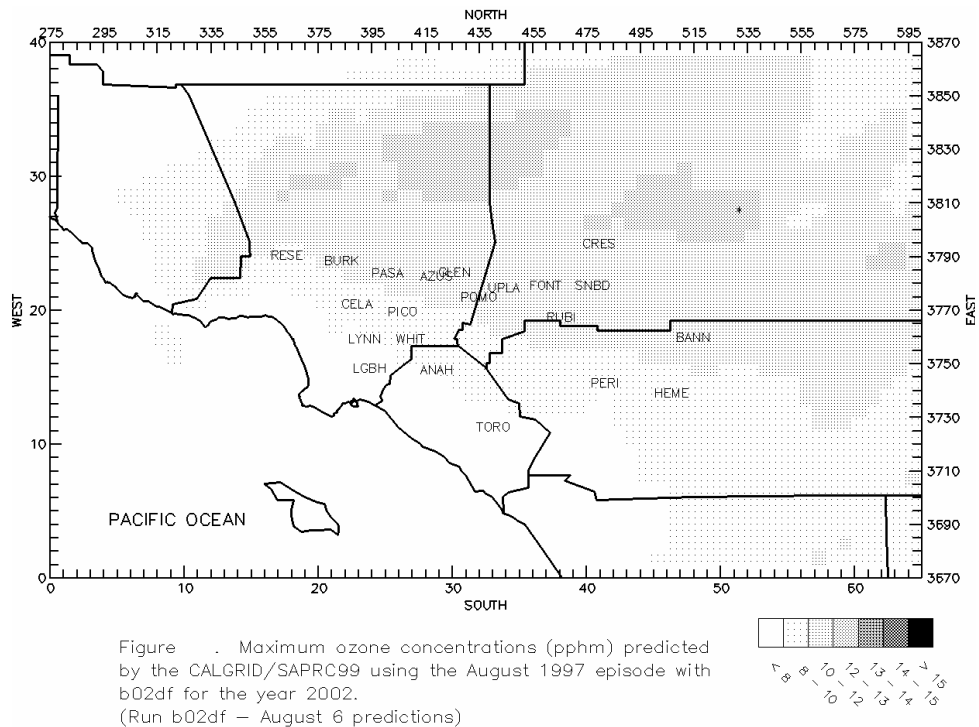


Figure A-7-6

Predicted 2002 Maximum 1-Hour Average Ozone for August 6, 1997 Episode

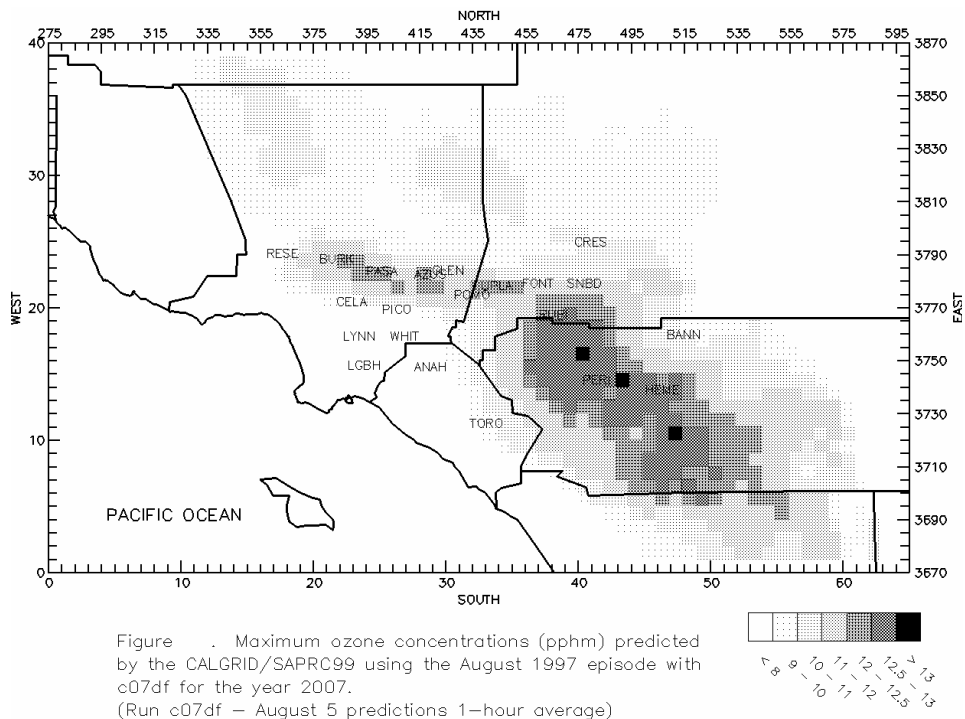


Figure A-7-7

Predicted 2007 Maximum 1-Hour Average Ozone for August 5, 1997 Episode

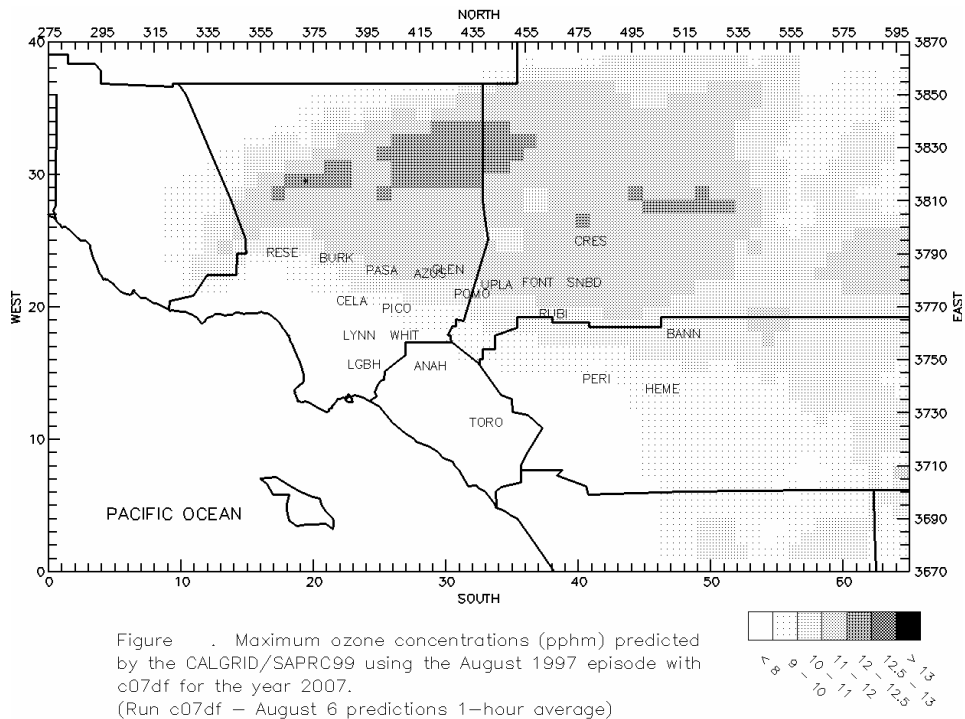


Figure A-7-8

Predicted 2007 Maximum 1-Hour Average Ozone for August 6, 1997 Episode

2010 CALGRID BASE-YEAR AND CONTROLLED SIMULATIONS

Table A-7-6 presents the results of the CALGRID 2010 simulations for the base-year and control options 1 and 2. Figures A-7-9 through A-7-14 provide the tile plots of predicted maximum ozone from the base-year and controlled scenarios.

The 2010 base-year predicted peak concentrations predicted by CALGRID indicate that the both August 5th and August 6th will exceed the federal 1-hour standard if no further controls are implemented. The Basin will meet the federal standard with implementation of either control option-1 or control option-2. Again, it is important to note that the 1997 base-year simulations under predicted the maximum ozone concentrations and scaling of the modeled results will result in higher ozone impacts for both the controlled and baseline emissions scenarios.

TABLE A-7-6

CALGRID 2010 Projected Maximum 1-hour Ozone Concentrations (ppb)

Episode Day	2010 Baseline	2010 Control Option-1	2010 Control Option-1
August 5, 1997	134	112	112
August 6, 1997	127	109	108

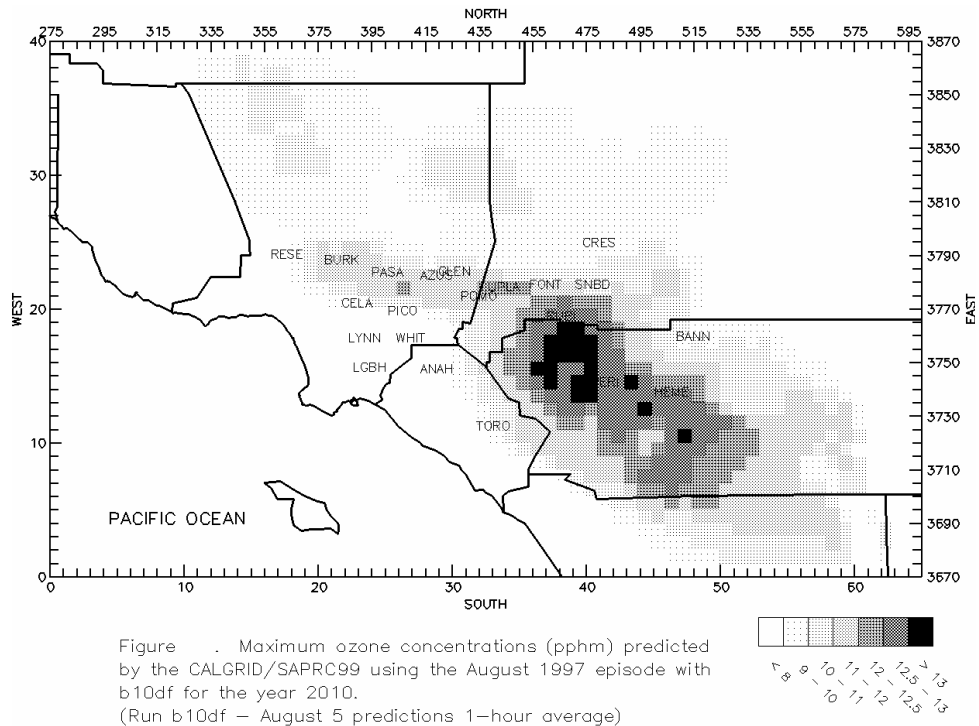


Figure A-7-9
 Predicted 2010 Baseline 1-Hour Average Ozone Concentrations for August 5, 1997

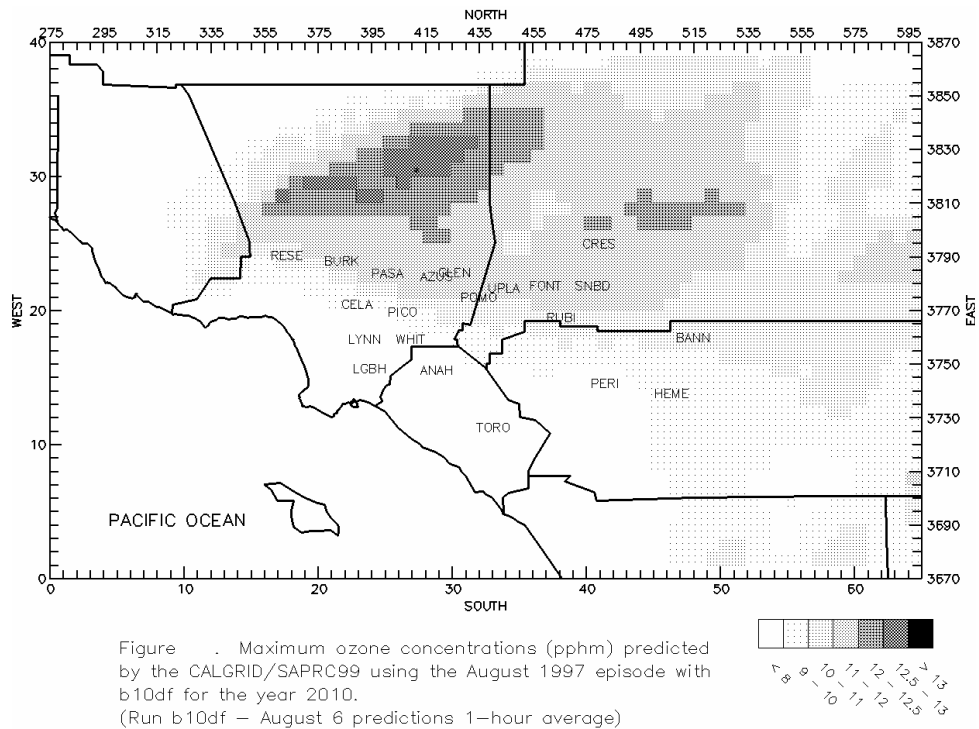


Figure A-7-10
 Predicted 2010 Baseline 1-Hour Average Ozone Concentrations for August 6, 1997

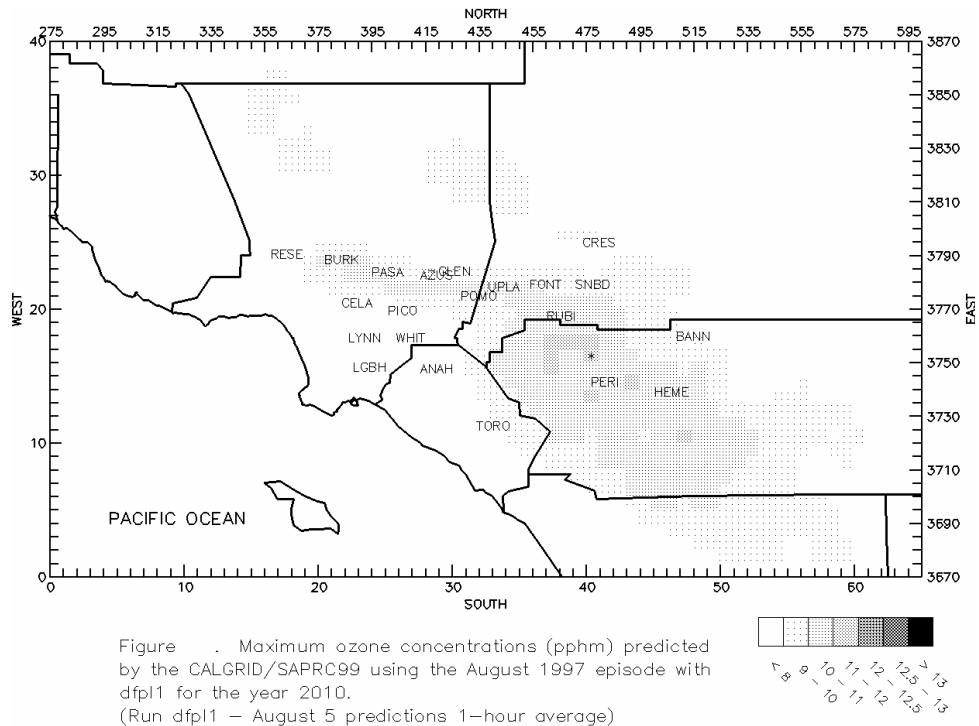


Figure A-7-11

Predicted 2010 Maximum 1-Hour Average Ozone for August 5, 1997 Episode Option-1

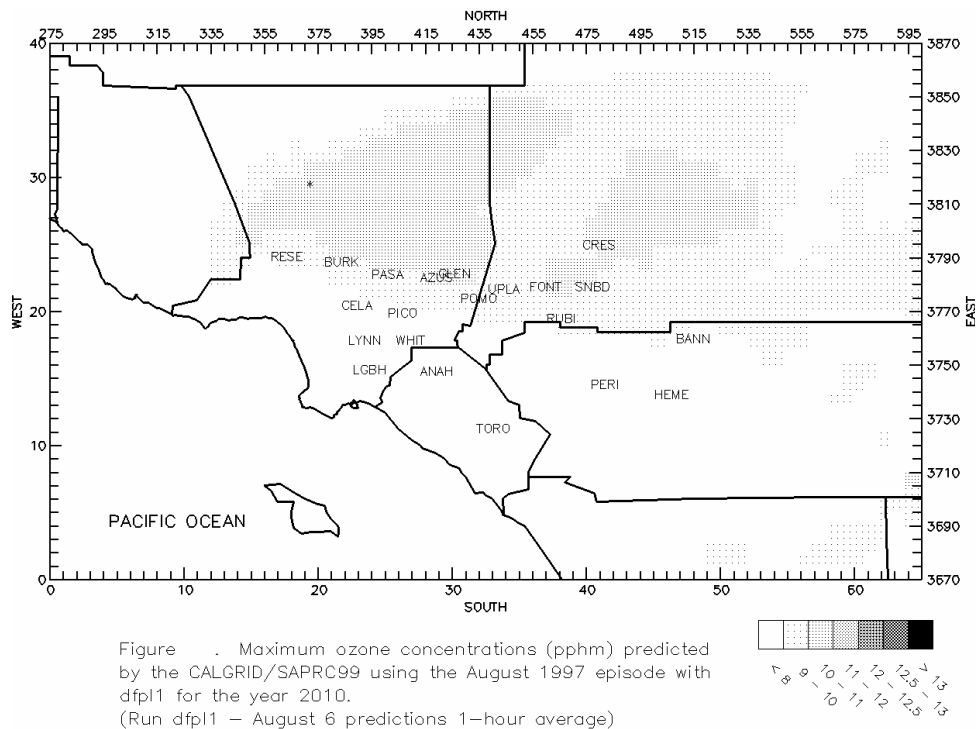


Figure A-7-12

Predicted 2010 Maximum 1-Hour Average Ozone for August 6, 1997 Episode Option-1

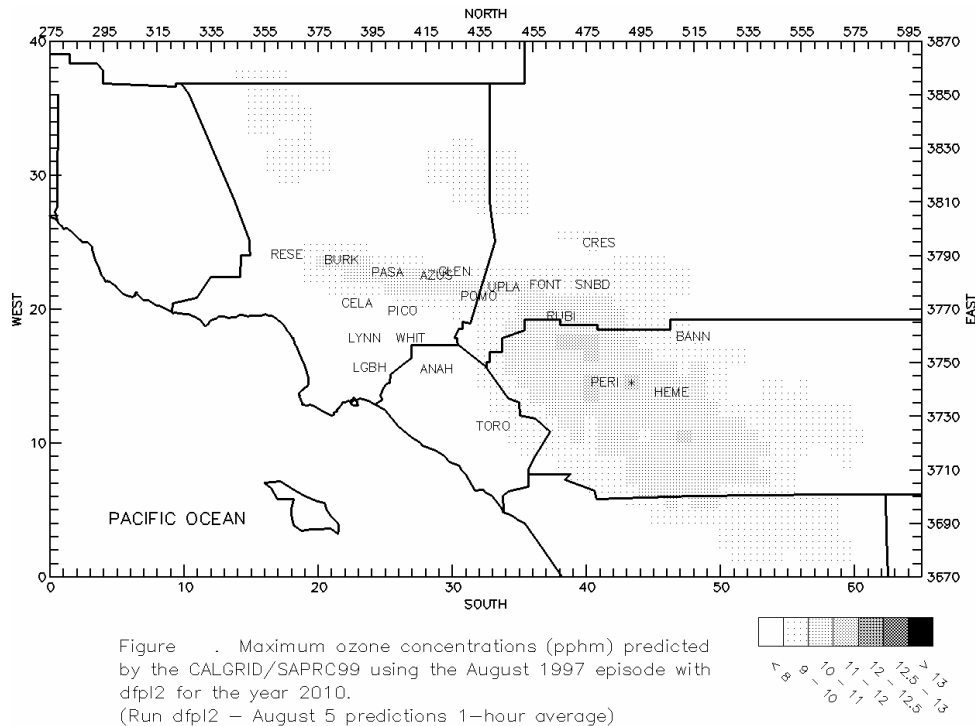


Figure A-7-13

Predicted 2010 Maximum 1-Hour Average Ozone for August 5, 1997 Episode Option-2

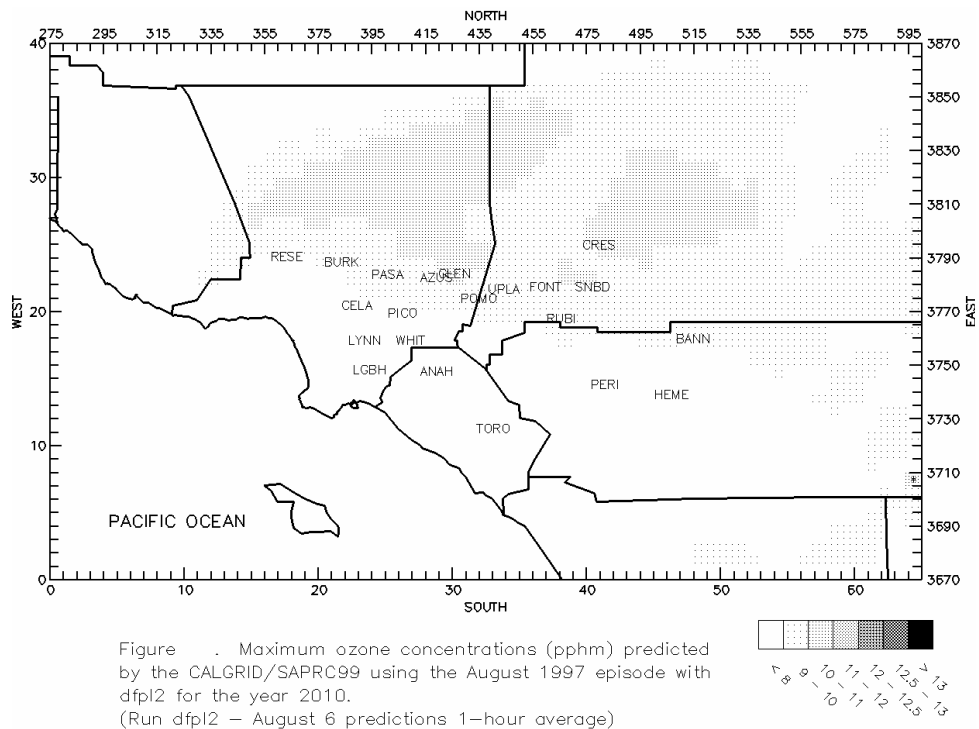


Figure A-7-14

Predicted 2010 Maximum 1-Hour Average Ozone for August 6, 1997 Episode Option-2

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