

### 11.5 Meteorological Fields Needed for Model Evaluation

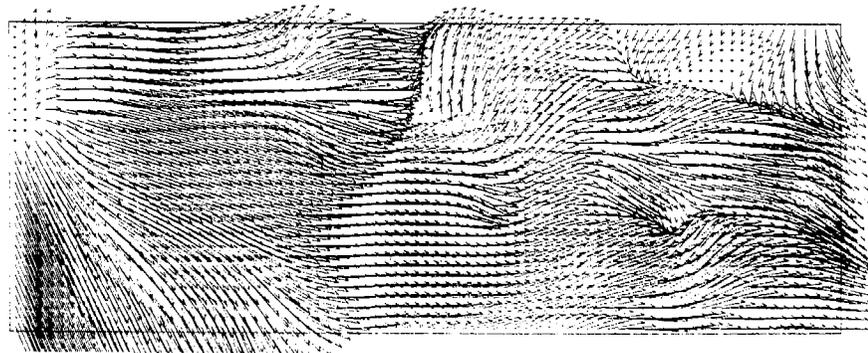
The basic meteorological inputs to the atmospheric diffusion equation are shown in Table 11.2. Two of the dominant processes that influence pollutant dispersion over the airshed are advective transport and turbulent mixing. In the model they are characterized by the velocity field, the height of the mixed layer, the surface aerodynamic roughness, solar insolation and vertical temperature structure. These fields were generated, for the period June 26-28, 1974 using the procedures described in Chapters 3 and 4. Figure 11.3 shows a typical surface wind field distribution and Figure 11.4 the spatial variation of the mixing height over the airshed. The basic meteorological input data needed for the model were derived primarily from the South Coast Air Quality Management District (SCAQMD) monitoring stations (APCD, 1974).

### 11.6 Emissions Inventory for South Coast Air Basin

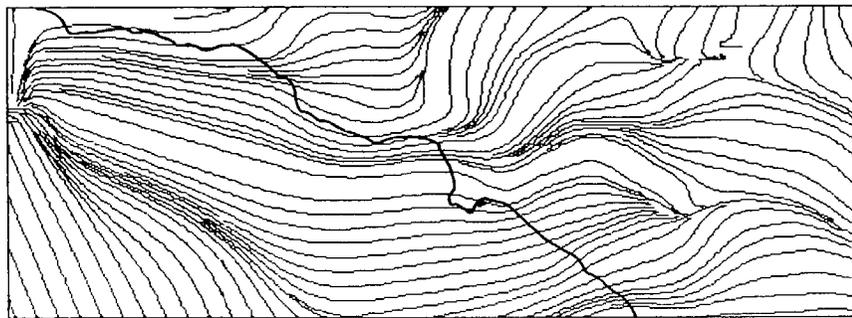
The most important input to any airshed model is a comprehensive detailed and accurate emission inventory, constructed at a level of detail consistent with the required spatial, temporal and chemical resolution of the model. In this study emissions from 130 different source categories were spatially distributed over the region shown in Figure 11.1. A summary of the daily totals and the distribution between mobile and stationary source classes is shown in Table 11.3, a more detailed breakdown is presented in Table 11.4. Diurnal variations in emission rates were resolved to within one hour in order that the



(a)



(b)



(c)

FIGURE 11.3

Typical Surface Wind Field Distribution for 27 June 1974

- (a) Direction and Magnitudes at Monitoring Sites
- (b) Generated Ground Level Flow Field
- (c) Streamlines for Generated Flow Field

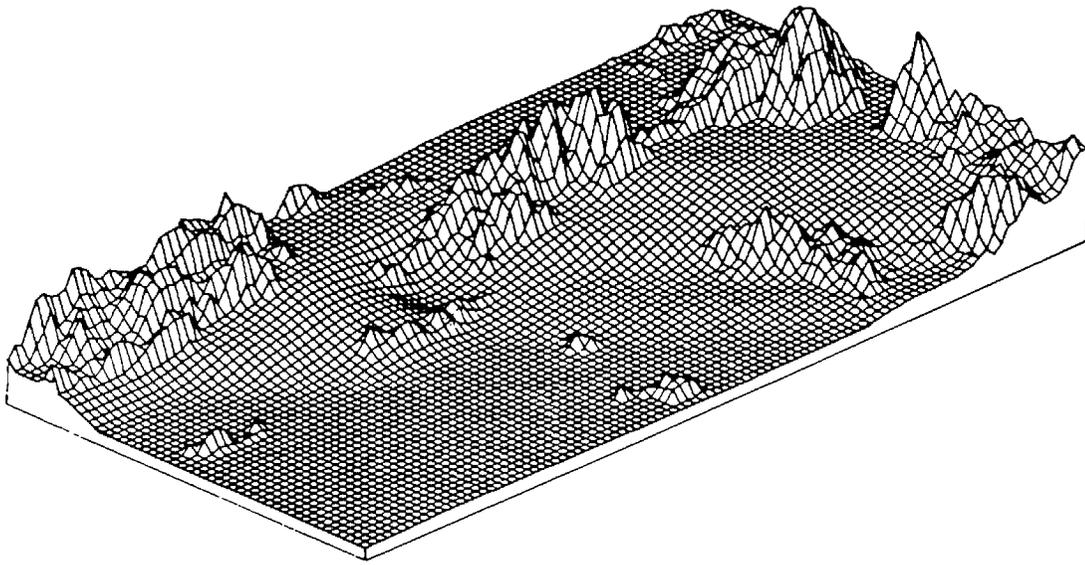


FIGURE 11.4

Mixing Height Distribution Above Sea Level  
(16:00 PST 26 June 1974)

TABLE 11.3

Summary of Total Emissions Into South Coast Air Basin\*

SPECIES	TOTAL EMISSIONS (Kg/day)	SOURCE CLASS CONTRIBUTION (%)	
		MOBILE	STATIONARY
Carbon Monoxide (CO)	8,610,000	98.8	1.2
Nitrogen Oxides (NO <sub>x</sub> )	1,320,000	62.3	37.7
Sulfur Oxides (SO <sub>x</sub> )	427,000	13.7	86.3
Reactive Hydrocarbons (RHC)	1,240,000	71.0	29.0

\* June 26, 1974

TABLE 11.4

## Emissions Inventory for South Coast Air Basin

CATEGORY OF EMISSIONS (CES)	CES NUMBER	CO	EMISSIONS (kg/day)			TOTAL HYDROCARBONS	REACTIVE HYDROCARBONS
			NO <sub>x</sub>	CO	NO <sub>x</sub>		
Emission	1	89	497		5,692	3,688	
Transportation	130	0	0		0	0	
Motor Vehicle	2	7,991,884	704,064		871,864	810,833	
Catalyst Gasoline Exhaust	14	0	0		0	0	
Non Catalyst Gasoline Exhaust	29	0	0		0	0	
Gasoline Evap. Loss Carb	23	0	0		0	0	
Gasoline Evap. Fuel Tank	122	0	0		52,461	52,461	
Gasoline Crankcase	21	0	0		0	0	
Diesel Exhaust	34	0	0		0	0	
Diesel Evaporative	37	0	0		0	0	
Motorcycle Exhaust	123	0	0		0	0	
Subtotals		7,991,973	704,561		930,016	866,982	
Off Road Motor Vehicle	38	265,643	7,103		19,204	16,861	
Industrial	58	0	0		0	0	
Construction	59	11,215	48,859		3,619	3,515	
Recreational	60	0	0		0	0	
Farm	61	0	0		0	0	
Subtotals		276,858	55,962		22,822	20,376	
Shipping	3	0	0		0	0	
Purging	30	0	0		0	0	
Off Loading	33	0	0		0	0	
Ballasting	28	0	0		814	731	
Transit	39	0	0		0	0	
Boilers Non Tankers	119	790	7,144		605	376	
Boilers Tankers	120	293	2,760		199	124	
Pleasure Craft	121	3,777	1,682		844	760	
Subtotals		4,859	11,568		2,462	1,991	

TABLE 11.4 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	CO	EMISSIONS (kg/day)			REACTIVE HYDROCARBONS
			NO <sub>x</sub>	TOTAL HYDROCARBONS		
Railroad	4	9,637	28,094	7,029	6,827	
Subtotals		9,637	28,094	7,029	6,827	
Aircraft	8	0	0	0	0	
Jet Exhaust	20	92,310	22,387	43,404	43,300	
Jet Fuel Evaporation	63	0	0	0	0	
Piston Exhaust	19	125,107	493	8,373	7,574	
Piston Fuel Evaporation	129	0	0	0	0	
Rocket	50	0	0	0	0	
Subtotals		217,417	22,880	51,777	50,873	
Stationary	65	0	0	0	0	
Petroleum	6	0	0	0	0	
Production	13	0	0	0	0	
Ext. Combustion Boilers	78	19	2,431	102	54	
Int. Combustion Engines	83	3,371	19,228	2,190	370	
Industrial Processes	87	2,283	33,271	42,819	27,370	
Seeps	118	0	0	9,947	8,057	
Crude Oil Evap. Fixed Roof	88	3,216	12	37,487	35,148	
Crude Oil Evap. Floating Roof	89	0	0	14	14	
Refining	12	0	0	0	0	
Ext. Combustion Boilers	77	0	0	0	0	
Boilers Residual Oil	73	22	982	41	25	
Boilers Distillate Oil	74	110	15,089	1,541	958	
Boilers Natural Gas	75	598	9,367	1,283	564	
Boilers Process Gas	76	91	7,982	432	399	
Internal Combustion Engines	84	3,334	20,616	3,023	725	
Industrial Processes	90	923	59,168	13,146	11,479	
Storage Evap.	91	0	0	5,974	3,870	
Crude Oil Evap. Fixed Roof	93	0	0	4,694	4,281	

TABLE 11.4 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	CO	NO <sub>x</sub>	EMISSIONS (kg/day)		REACTIVE HYDROCARBONS
				TOTAL HYDROCARBONS		
Crude Oil Evap. Float Rm	95	0	0	6,955		6,343
Gasoline Evap. Fixed Roof	92	0	0	1,673		1,673
Gasoline Evap. Float Roof	94	0	0	28,039		28,039
Marketing	10	0	213	81,877		13,403
Storage Evap.	100	0	0	4,569		3,100
Crude Oil Evap. Fixed Roof	97	0	0	1,495		1,456
Crude Oil Evap. Float Roof	99	0	0	984		958
Gasoline Evap. Fixed Roof	96	0	0	126		126
Gasoline Evap. Float Roof	98	0	0	3,218		3,218
Loading and Unloading	103	0	0	1,230		830
Gasoline Evap.	101	0	0	6,031		6,031
Crude Oil	102	26	190	3,092		2,777
Underground Storage at Sta.	40	0	0	32,102		32,105
Vehicle Refueling at Sta.	45	0	0	0		0
Subtotals		13,993	168,550	294,085		193,375
Commercial and Institutional	7	0	103	444		257
Internal Combustion Engines	82	1,034	7,498	1,173		1,000
Ext. Comb. Boilers & Space Heat	124	0	89	0		0
Residual Oil	125	88	1,471	44		8
Distillate Oil	126	91	12,544	439		226
Natural Gas	127	94	7,259	178		78
Process Gas	128	36	0	0		0
Printing	113	0	7	417		235
Flexigraphic	112	0	0	6,202		0
Gravure	114	0	0	14,536		11,607
Surface Coating Air Dried Achit.	16	0	0	0		0
Oil Base Incl. Solvent	110	0	0	73,562		39,356
Water Base	111	0	0	10,513		5,625
Dry Cleaning	22	0	0	0		0
Petroleum Base Perchloroethylene	46	0	142	3,668		0
Synthetic	43	0	2	3,112		2,260
Degreasing	11	0	0	186		0
Halogenated	42	2	26	4,912		0
Non-Halogenated	47	0	0	14,090		14,090
Subtotals		1,344	29,141	133,476		74,741

TABLE 11.4 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	EMISSIONS (kg/day)				
		CO	NO <sub>x</sub>	TOTAL HYDROCARBONS	REACTIVE HYDROCARBONS	
Industrial	5	1,831	9,049	4,159	1,277	
Internal Combustion Engines	81	2,006	13,308	0	493	
External Comb. Boilers & Heaters	49	0	0	0	0	
Residual Oil	69	286	1,060	21	4	
Distillate Oil	70	157	26,861	566	352	
Natural Gas	71	380	14,597	458	202	
Process Gas	72	4,310	1,416	703	650	
Chemical	15	0	17	2,722	1,484	
Metallurgical	35	0	0	0	0	
Primary Metals	85	54,232	15,713	10,325	4,337	
Secondary Metals	86	1,662	5,291	2,750	1,741	
Mineral	31	11,728	33,043	1,174	432	
Wood Processing	25	0	0	0	0	
Elec. Generation Boiler	18	0	0	0	0	
Residual Oil	56	7,236	121,409	6,513	4,051	
Distillate Oil	67	36	326	36	19	
Natural Gas	55	2,506	47,307	1,438	633	
Process Gas	68	0	0	0	0	
Coal	57	0	0	0	0	
Elec. Generation Inter. Comb.	79	677	7,134	549	468	
Surface Coating	44	2	6	440	147	
Heat Treated	48	303	396	6,432	2,155	
Air Dried	41	0	0	0	0	
Paint	80	0	349	10,348	7,706	
Varnish and Shellac	104	0	72	6,904	197	
Lacquer	105	17	183	15,371	3,949	
Enamel	106	0	137	13,941	8,984	
Primer	107	0	1	1,686	948	
Solvent	108	0	0	10,901	4,105	
Adhesives	109	26	7	7,887	5,331	
Incineration	51	23	127	172	17	
Land Fills	117	0	0	846,090	8,461	
Subtotals		87,408	297,808	953,594	58,142	

TABLE 11.4 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	EMISSIONS (kg/day)				TOTAL HYDROCARBONS	REACTIVE HYDROCARBONS
		CO	NO <sub>x</sub>				
Agricultural	9	0	0		0	0	
Agricultural Control Burn	17	0	0		0	0	
Vegetative Forest and Citrus	115	0	0		884,026	0	
Animal Wastes	116	0	0		65,715	13,143	
Pesticides	24	0	0		3,629	3,266	
Food Processing	32	30	895		2,467	186	
Orchard Heating	36	0	0		0	0	
Waste Burning or Wildfires	27	0	0		0	0	
Wine Processing	66	0	0		0	0	
Subtotals		30	895		955,837	16,595	
Domestic	54	0	0		0	0	
Solvent Use	26	0	0		27,491	2,859	
Utility Equipment 2 stroke	53	0	0		0	0	
Utility Equipment 4 stroke	52	0	0		0	0	
Fuel Combustion	62	5	1,214		998	0	
Structural Fires	64	0	0		0	0	
Subtotals		5	1,214		28,490	2,859	
TOTALS		8,603,526	1,320,691		3,379,587	1,292,760	

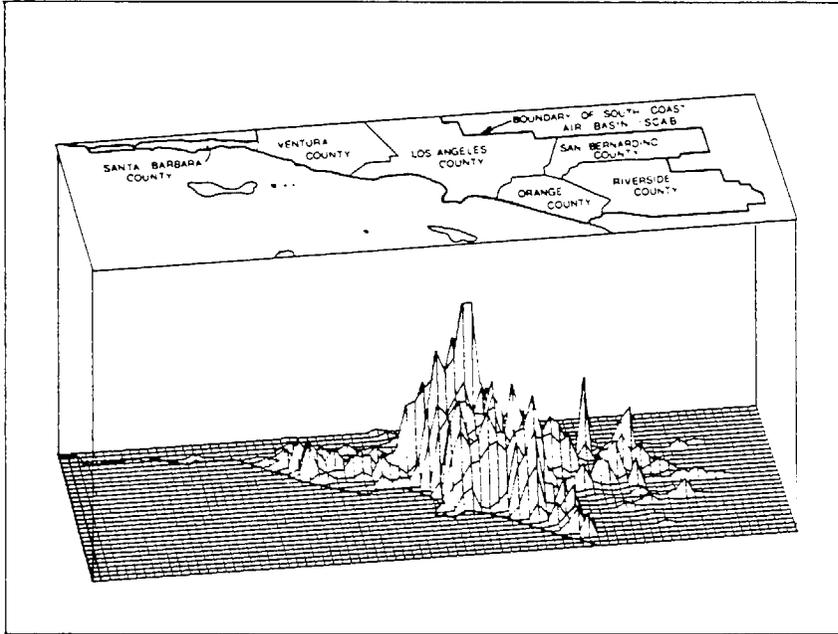
model predictions would be compatible with the averaging time used in making ambient air quality measurements. The spatial and temporal variations of pollutant emissions are shown in Figures 11.5-11.7. To avoid any ambiguity, all data times for input of information to the airshed model were defined in terms of the standard time (PST) of the region. For the South Coast Air Basin the standard time corresponds to time zone eight (8) which covers the longitudinal range 105-120°W. Table 11.5 gives the estimated 1974 composition of reactive hydrocarbon emissions in the SCAB grouped according to the chemical lumping scheme introduced in Chapter 8. The detailed hydrocarbon inventory is documented in Table 11.6. These results were derived from detailed composition profiles developed for each source category. For further details of the emission inventory the reader is referred to AQMP (1978).

#### 11.7 Assessment of the Accuracy of the Emissions Inventory

In order to become confident in making decisions based on an inventory, it is not sufficient merely to assemble the basic data. What is required is a quantitative evaluation of the likely errors.

The development of emissions data for a large urban area is an extremely complex undertaking and involves considerable resource commitments. From a practical point of view many simplifications and approximations must be invoked during the compilation of a spatially, chemically and temporally resolved inventory. The assessment of the level of uncertainty in a particular emission inventory is obviously a

CARBON MONOXIDE  
DAILY TOTAL EMISSIONS



DIURNAL VARIATION OF CARBON MONOXIDE EMISSIONS

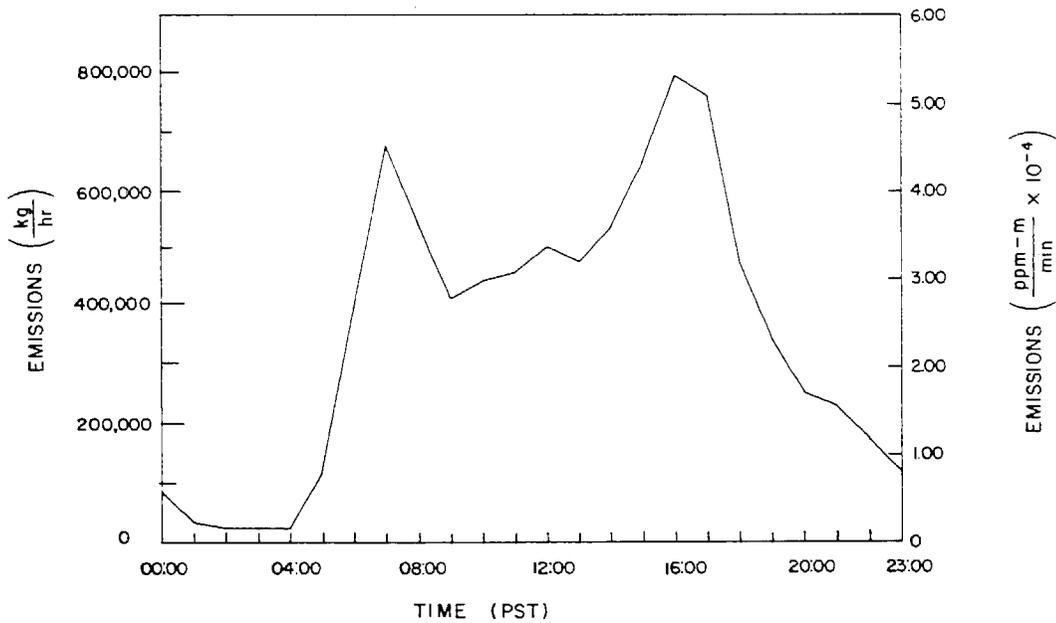
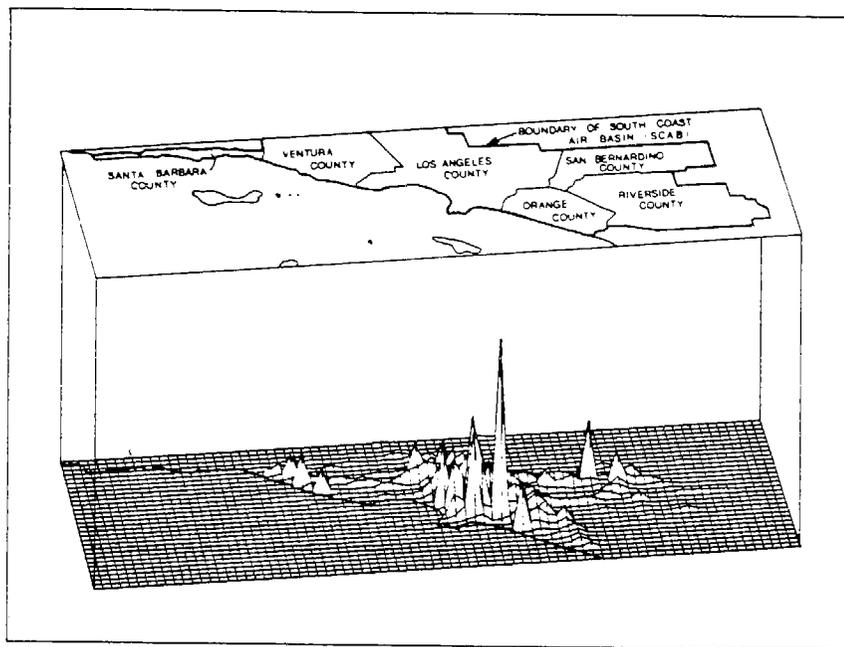


FIGURE 11.5

Spatial and Diurnal Variations in Carbon Monoxide (CO) Emissions

NITROGEN OXIDES  
DAILY TOTAL EMISSIONS



DIURNAL VARIATION OF NITROGEN OXIDES EMISSIONS

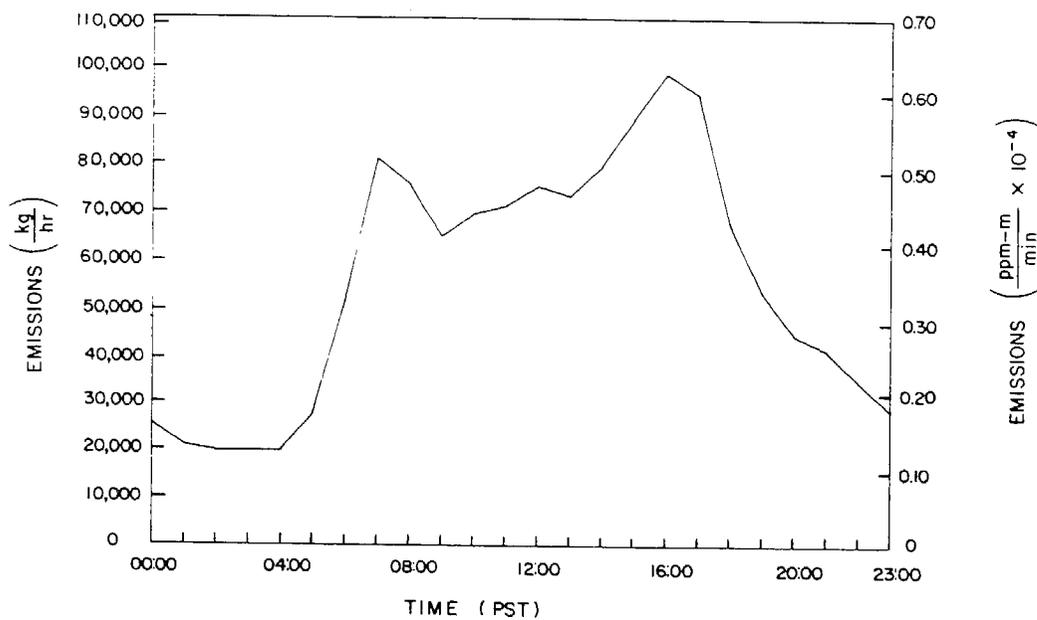
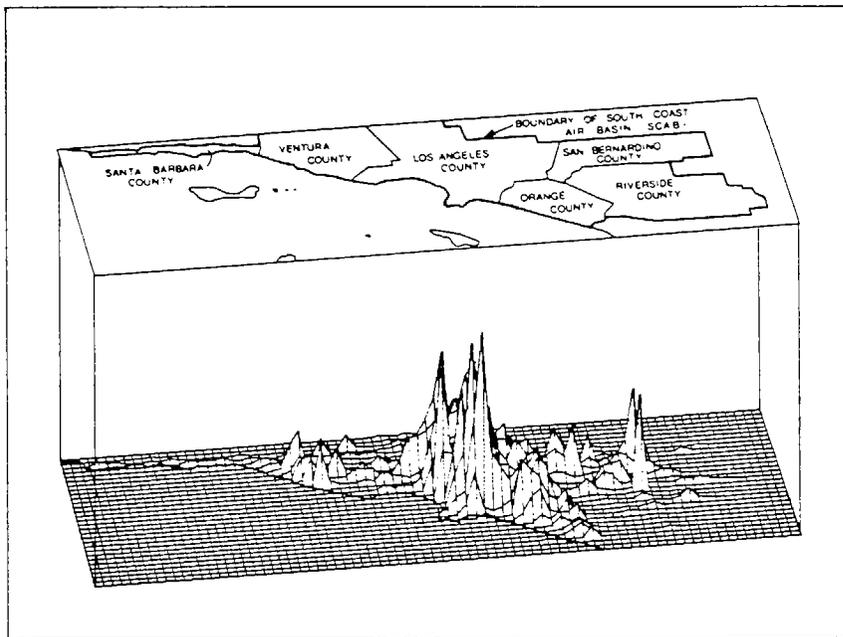


FIGURE 11.6

Spatial and Diurnal Variations in Nitrogen Oxides (NO<sub>x</sub>) Emissions

REACTIVE HC  
DAILY TOTAL EMISSIONS



DIURNAL VARIATION OF REACTIVE HC EMISSIONS

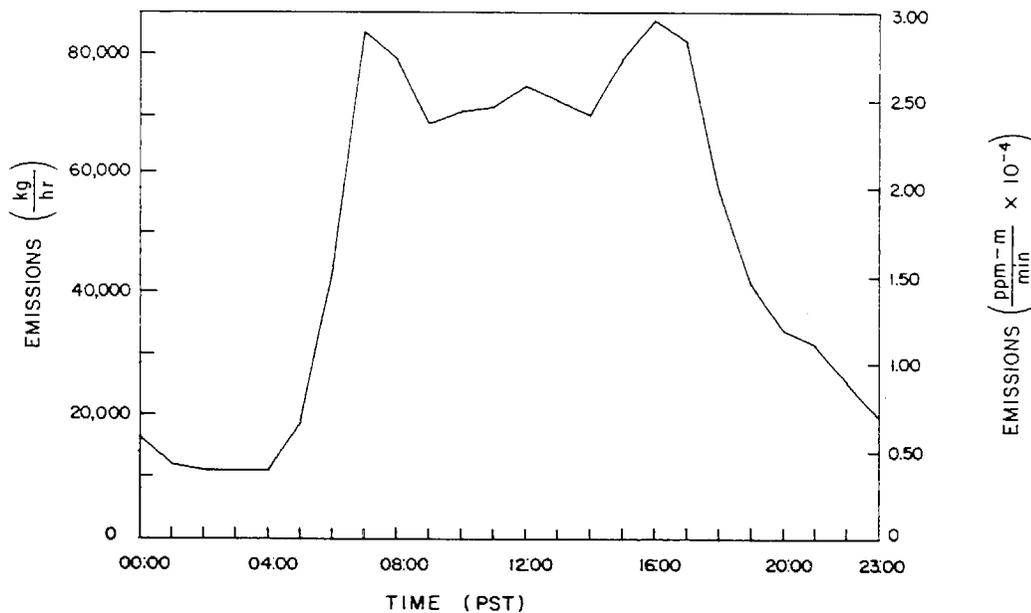


FIGURE 11.7

Spatial and Diurnal Variations in Reactive hydrocarbon (RHC) Emissions

TABLE 11.5  
Composition of Reactive Hydrocarbons in Inventory Region

SPECIES	EMISSIONS kg s <sup>-1</sup>	COMPOSITION(%)		MOLE WEIGHTED MOLECULAR WEIGHT	AVERAGE CARBON NUMBER
		WEIGHT	MOLE		
Formaldehyde (HCHO)	0.18	1.25	2.88	30.0	1.00
Other Aldehydes (RCHO)	0.25	1.74	2.22	63.1	3.36
Ethylene (C <sub>2</sub> H <sub>4</sub> )	0.82	5.73	13.4	28.0	2.00
Other Olefins (OLE)	1.98	13.8	14.2	67.4	4.83
Aromatics (ARO)	2.03	14.2	9.4	100.2	7.56
Alkanes (ALK)	9.04	63.3	57.9	83.5	5.82
TOTALS	14.30	100.0	100.0		

TABLE 11.6

## Reactive Hydrocarbon Emissions for the South Coast Air Basin

CATEGORY OF EMISSIONS (CES)	CES NUMBER	REACTIVE HYDROCARBONS (kg/day)							ALKANES
		FORMAL-DEHYDE	OTHER ALDEHYDES	AROMATICS	ETHYLENE	OLEFINS			
Emission	1	0	0	0	2,100	438	1,150		
Transportation	130	0	0	0	0	0	0		
Motor Vehicle	2	22,668	15,693	212,735	91,546	150,832	317,358		
Catalyst Gasoline Exhaust	14	0	0	0	0	0	0		
Non Catalyst Gasoline Exhaust	29	0	0	0	0	0	0		
Gasoline Evap. Loss Carb	23	0	0	0	0	0	0		
Gasoline Evap. Fuel Tank	122	0	0	7,607	0	7,659	37,195		
Gasoline Crankcase	21	0	0	0	0	0	0		
Diesel Exhaust	34	0	0	0	0	0	0		
Diesel Evaporative	37	0	0	0	0	0	0		
Motorcycle Exhaust	123	0	0	0	0	0	0		
Subtotals		22,668	15,694	220,341	93,646	158,930	355,703	510	
Off Road Motor Vehicle	38	595	403	4,263	2,362	3,399	5,838		
Industrial	58	0	0	0	0	0	0		
Construction	59	186	536	431	223	231	1,908		
Recreational	60	0	0	0	0	0	0		
Farm	61	0	0	0	0	0	0		
Subtotals		782	939	4,694	2,585	3,630	7,746		
Shipping	3	0	0	0	0	0	0		
Purging	30	0	0	0	0	0	0		
Off Loading	33	0	0	0	0	0	0		
Ballasting	28	0	0	0	0	0	731		
Transit	39	0	0	0	0	0	0		
Boilers Non-Tankers	119	1	0	24	65	24	262		
Boilers Tankers	120	0	0	8	21	8	86		
Pleasure Craft	121	0	0	211	40	149	360		
Subtotals		1	0	243	126	181	1,440		

TABLE 11.6 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	FORMAL-DEHYDE	REACTIVE HYDROCARBONS (kg/day)					OLEFINS	ALKANES
			OTHER ALDEHYDES	AROMATICS	ETHYLENE				
Railroad	4	362	1,040	836	432	449	3,706		
Subtotals		362	1,040	836	432	449	3,706		
Aircraft	8	0	0	0	0	0	0	0	
Jet Exhaust	20	0	4,926	18,099	0	8,624	11,650	0	
Jet Fuel Evaporation	63	0	0	0	0	0	0	0	
Piston Exhaust	19	571	1,130	2,003	0	0	3,870	0	
Piston Fuel Evaporation	129	0	0	0	0	0	0	0	
Rocket	50	0	0	0	0	0	0	0	
Subtotals		571	6,056	20,102	0	8,624	15,520	0	
Stationary	65	0	0	0	0	0	0	0	
Petroleum	6	0	0	0	0	0	0	0	
Production	13	0	0	0	0	0	0	0	
Ext. Comb. Boilers	78	15	0	5	0	0	34	0	
Int. Comb. Engines	83	0	0	0	160	11	199	511	
Industrial Processes	87	0	0	5,117	3,250	0	19,003	0	
Seeps	118	0	0	0	0	0	8,057	0	
Crude Oil Evap. Fixed Roof	88	0	0	41	0	0	35,107	0	
Crude Oil Evap. Floating Roof	89	0	0	0	1	0	13	0	
Refining	12	0	0	0	0	0	0	0	
Ext. Combustion Boilers	77	0	0	0	0	0	0	0	
Boilers Residual Oil	73	0	0	2	4	2	18	0	
Boilers Distillate Oil	74	2	0	62	165	62	669	0	
Boilers Natural Gas	75	103	0	77	0	0	385	0	
Boilers Process Gas	76	33	0	0	0	76	291	0	
Internal Combustion Engines	84	30	0	0	30	0	665	0	
Industrial Processes	90	1,484	0	51	17	1,572	8,354	0	
Storage Evap.	91	3	0	725	1	14	3,127	0	
Crude Oil Evap. Fixed Roof	93	0	0	178	127	0	3,976	0	
Crude Oil Evap. Floating Roof	95	0	0	264	188	0	5,891	0	
Gasoline Evap. Fixed Roof	92	0	0	243	0	244	1,186	0	
Gasoline Evap. Floating Roof	94	0	0	4,066	0	4,094	19,880	0	

TABLE 11.6 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	REACTIVE HYDROCARBONS (kg/day)						
		FORMAL- DEHYDE	OTHER ALDEHYDES	AROMATICS	ETHYLENE	OLEFINS	ALKANES	
Marketing	10	24	0	16	25	0	13,338	
Storage Evap.	100	6	0	361	4	10	2,719	
Crude Oil Evap. Fixed Roof	97	0	0	0	0	0	1,456	
Crude Oil Evap. Floating Roof	99	0	0	0	0	0	958	
Gasoline Evap. Fixed Roof	96	0	0	18	0	18	89	
Gasoline Evap. Floating Roof	98	0	0	467	0	470	2,282	
Loading and Unloading	103	0	0	57	0	0	773	
Gasoline Evap.	101	0	0	344	0	483	5,205	
Crude Oil	102	0	0	0	111	0	2,665	
Underground Storage at Sta.	40	0	0	2,520	0	2,472	27,113	
Vehicle Refueling at Sta.	45	0	0	0	0	0	0	
Subtotals		1,700	0	14,613	4,083	9,526	163,453	
Commercial and Institutional	7	0	0	144	0	0	113	
Internal Combustion Engines	82	41	122	52	144	54	587	
Ext. Comb. Boilers & Space Heat	124	0	0	0	0	0	0	
Residual Oil	125	0	0	0	0	0	8	
Distillate Oil	126	1	0	0	0	0	225	
Natural Gas	127	14	0	11	0	0	53	
Process Gas	128	0	0	0	0	0	0	
Printing	113	38	0	0	5	104	87	
Flexigraphic	112	0	0	0	0	0	0	
Gravure	114	0	0	5,774	0	0	5,833	
Surface Coating Air Dried	16	0	0	0	0	0	0	
Oil Base Incl. Solvent	110	0	0	8,901	0	0	30,455	
Water Base	111	0	0	1,272	0	0	4,352	
Dry Cleaning	22	0	0	0	0	0	0	
Petroleum Base Perchloroethylene	46	0	0	0	0	0	0	
Synthetic	43	0	0	0	0	0	2,260	
Degreasing	11	0	0	0	0	0	0	
Halogenated	42	0	0	0	0	0	0	
Non Halogenated	47	0	0	0	0	0	14,090	
Subtotals		94	122	16,154	149	158	58,064	

TABLE 11.6 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	REACTIVE HYDROCARBONS (kg/day)							
		FORMAL-DEHYDE	OTHER ALDEHYDES	AROMATICS	ETHYLENE	OLEFINS	ALKANES		
Industrial	5	389	0	79	0	393	415		
Internal Combustion Engines	81	36	0	0	20	0	437		
External Comb. Boilers & Heaters	49	0	0	0	0	0	0		
Residual Oil	69	0	0	0	0	0	4		
Distillate Oil	70	0	0	23	61	23	246		
Natural Gas	71	37	0	28	0	0	137		
Process Gas	72	53	0	0	0	123	473		
Chemical	15	13	12	524	166	202	567		
Metallurgical	35	0	0	0	0	0	0		
Primary Metals	85	6	0	1,397	1,859	281	794		
Secondary Metals	86	494	0	73	0	0	1,173		
Mineral	31	5	0	47	18	41	321		
Wood Processing	25	0	0	0	0	0	0		
Elec. Generation Boiler	18	0	0	0	0	0	0		513
Residual Oil	56	7	0	261	697	261	2,827		
Distillate Oil	67	0	0	0	0	0	18		
Natural Gas	55	115	0	86	0	0	431		
Process Gas	68	0	0	0	0	0	0		
Coal	57	0	0	0	0	0	0		
Elec. Generation Inter. Comb.	79	19	57	24	68	25	275		
Surface Coating	44	0	0	0	9	0	139		
Heat Treated	48	0	0	0	128	0	2,026		
Air Dried	41	0	0	0	0	0	0		
Paint	80	0	0	7,275	0	0	430		
Varnish and Shellac	104	0	0	188	0	0	9		
Lacquer	105	0	0	1,911	0	0	2,038		
Enamel	106	0	0	1,646	0	0	7,337		
Primer	107	0	0	539	0	0	408		
Solvent	108	0	0	2,276	0	0	1,829		
Adhesives	109	0	0	4,337	0	0	994		
Incineration	51	0	0	3	3	5	7		
Land Fills	117	0	0	1,692	0	0	6,769		
Subtotals		1,175	69	22,410	3,028	1,354	30,106		

TABLE 11.6 (continued)

CATEGORY OF EMISSIONS (CES)	CES NUMBER	REACTIVE HYDROCARBONS (kg/day)						
		FORMAL- DEHYDE	ALDEHYDES	AROMATICS	ETHYLENE	OLEFINS	ALKANES	
Agricultural	9	0	0	0	0	0	0	
Agricultural Control Burn	17	0	0	0	0	0	0	
Vegetative Forest and Citrus	115	0	0	0	0	0	0	
Animal Wastes	116	0	0	0	0	0	13,143	
Pesticides	24	0	0	1,172	0	0	2,094	
Food Processing	32	3	0	2	34	52	95	
Orchard Heating	36	0	0	0	0	0	0	
Waste Burning or Wildfires	27	0	0	0	0	0	0	
Wine Processing	66	0	0	0	0	0	0	
Subtotals		3	0	1,174	34	52	15,332	
Domestic	54	0	0	0	0	0	0	
Solvent Use	26	165	0	1,237	0	0	1,457	
Utility Equipment 2 Stroke	53	0	0	0	0	0	0	
Utility Equipment 4 Stroke	52	0	0	0	0	0	0	
Fuel Combustion	62	0	0	0	0	0	0	
Structural Fires	64	0	0	0	0	0	0	
Subtotals		165	0	1,237	0	0	1,457	
TOTALS		27,522	23,919	301,805	104,083	182,904	652,526	

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substantial undertaking and, most properly, should be carried out when the inventory itself is compiled. The objective of this section is to present a methodology for assessing the accuracy of existing emission inventories given estimates of errors in individual source categories. The procedure uses chemically weighted sensitivity analysis methods that distribute both percentage and physical errors in accordance to their total contribution to photochemical oxidant production. By applying the techniques to the present inventory, those sources contributing most to the uncertainty in total emissions can be identified. This information can then be used to help design field and source test programs that will provide improved data bases for control strategy development.

Emissions from each source class can be characterized according to level of spatial resolution, level of temporal resolution, and source activity or emission factor. The level of spatial resolution achievable is in principle as fine as one desires since the locations of all sources can presumably be specified (although traffic count data may not be available on a street-by-street basis). Temporal emission rates will fluctuate some from day to day and the output from some stationary sources may vary with ambient temperature. Even with these variations the major problem in properly specifying source emissions is still the uncertainty in emissions quantities derived from source activities and emission factors. Goklany (1980) presents a detailed discussion of emission inventory errors and suggests various engineering checks that

can be made to insure that the basic data are reliable, accurate and self consistent.

Two basic factors are involved in emission specification, the quantity emitted and its composition. Emission compositions are typically estimated from engineering or source tests. Recent studies aimed at establishing  $\text{NO}_x$  and  $\text{SO}_x$  emission inventories for stationary sources in the South Coast Air Basin have presented estimates of the level of accuracy of the overall inventories (Bartz et al., 1974). These reports estimate that a  $\pm 20\%$  uncertainty in the total emissions is reasonable, whereas, uncertainties in individual source emissions can range as high as  $\pm 300\%$ . A compensating factor is that generally the large uncertainties are associated with small absolute emission levels. Probably the most serious emission inventory problems are those associated with hydrocarbon emissions. Given the existence of uncertainties in the inventory, one must develop methodologies for identifying the major errors.

The basic goal of this analysis is to develop a procedure that will place error bounds on emissions of reactive hydrocarbons (RHC), nitrogen oxides ( $\text{NO}_x$ ) and carbon monoxide (CO). With the exception of CO, these groupings represent the sum of many individual species. In order to generalize the methodology consider a chemical grouping,  $j$ , composed of emissions of  $n_j$  species. If there are  $m$  source classes in the emissions inventory then the total emissions from group  $j$ ,  $E_T^j$ , is given by

$$E_T^j = \sum_{k=1}^m \sum_{i=1}^{n_j} w_i E_i^k \quad (11.1)$$

where  $D_T^k$  is the emission of species  $i$  from source class  $k$  and  $w_i$  is a weighting factor that can be used to account for differences in chemical reactivity of the individual species. The choice of suitable forms for  $w_i$  is discussed subsequently. In (11.1), for example,  $n_j = 1$  for CO and  $n_j = 2$  for  $\text{NO}_x$  since  $E_{\text{NO}_x} = E_{\text{NO}} + E_{\text{NO}_2}$ . If the  $E_i^k$  are considered to be statistically independent then the variance of the total emissions,  $(\sigma_T^j)^2$ , for a linear model is simply the sum of the individual components  $\sigma_{E_i}^2$  (Feller, 1968)

$$(\sigma_T^j)^2 = \sum_{k=1}^m \sum_{i=1}^{n_j} w_i^2 (\sigma_{E_i^k}^2) \quad (11.2)$$

In practice the standard deviation of the emissions from a particular source is normally expressed as some fraction  $f_i^k$  of the total, i.e.  $\sigma_{E_i^k} = f_i^k E_i^k$ . If a further assumption is made that each source class  $k$  contributes to the total error an amount proportional to the total emissions then the right hand side of (2) can be manipulated to give the fractional uncertainty  $f_T^j$  in emission group  $j$  as

$$f_T^j = \left\{ \sum_{k=1}^m \sum_{i=1}^{n_j} w_i^2 \left[ f_i^k \frac{E_i^k}{E_T^j} \right]^2 \right\}^{1/2} \quad (11.3)$$

One obvious conclusion that can be drawn from this analysis is that the fractional error in the total emissions is less than the sum of the

errors associated with the individual components. Ditto et al. (1976) present a similar analysis including a generalization that accounts for the case when one or more of the  $\sigma_{E_i^k}$  are fixed.

In the above derivation the only assumption made about each of the  $E_i^k$  was that they were independent and so the uncertainty bounds on  $E_T^j$  are simply  $E_T^j(1 \pm f_T^j)$ . In developing the fractions  $f_j$  for each source type it is important to consider the types of errors that might be involved in calculating the emission data.

When error distributions deviate significantly from normality a theorem due to Chebyshev (Feller, 1968) can be used to estimate upper bounds on the confidence intervals. This theorem states that for a random variable  $E_T^j$  that has a mean  $\bar{E}_T^j$ , and standard derivation  $(f_T^j \bar{E}_T^j)$ , the probability that  $|E_T^j - \bar{E}_T^j| > r(f_T^j \bar{E}_T^j)$  is less than  $1/r^2$ . Thus a  $(1-s) \times 100\%$  confidence interval is given by  $(\bar{E}_T^j (1 \pm rf_T^j))$  where  $r(f_T^j) = 1/s$ . An important feature of the theorem is that it is independent of the distribution of the random variable  $\bar{E}_T^j$ . While the inequality is true for any value of  $r > 1$ , the bounds are not sharp, and, as a result, the estimate of the confidence intervals is conservative.

One of the most important reasons for incorporating the weightings  $w_i$  in (11.1) is to account for differences in the chemical reactivity of individual species. The need for weighting can be illustrated by considering the emissions of methane from landfills. While there are typically very large uncertainties associated with estimating the mass fluxes, the contribution of methane to oxidant production within an

urban airshed is small. Unless the methane emissions are appropriately weighted, the uncertainties place unrealistically large error bounds on the hydrocarbon inventory. Given this situation it is clearly desirable to develop a weighting scheme that accounts for differences in chemical reactivity. From a practical view point there are two important considerations that any proposed scheme must satisfy. First it must be able to be applied in an a priori manner and secondly, the procedure should not require the numerical solution of kinetic rate equations. Primary attention in this section will be given to characterizing the weighting scheme for the reactive hydrocarbon grouping (RHC).

As might be expected there are many different ways to characterize the chemical reactivity of hydrocarbons including: organic consumption rate, peak oxidant levels, NO<sub>2</sub> formation rate and the time to the ozone peak (Dimitriades, 1974; Trijonis and Arledge, 1975; CARB, 1976; Darnall et al., 1976; and Bufalini et al., 1976). The scheme adopted here is to weight the emissions of individual hydrocarbon species on the basis of their rate of removal by reactions involving the hydroxyl radical (OH) (Darnall et al., 1976).

The normalized weighting factors in (11.1) for the hydrocarbon group are given by

$$w_i = \frac{\sum_{p=1}^{n_j} \frac{r_{p,p} k_{p,p}(\text{OH})}{\text{MW}_p}}{\sum_{j=1}^m \sum_{p=1}^{n_j} \frac{r_{p,p} k_{p,p}(\text{OH})}{\text{MW}_p}} \quad (11.4)$$

where  $k_p(\text{OH})$  is the rate constant for the reaction  $\text{HC}_p + \text{OH}$ .  $\text{MW}_p$  is

the molecular weight of hydrocarbon species  $p$  and  $r_p$  is the weight fraction; together  $MW_p$  and  $r_p$  convert the emissions from a mass to a molar basis. The reactivity weights for some different source classes are shown in Table 11.7.

Now consider the 1974 SCAB emissions inventory, a summary version of which is shown in Figure 11.8. Estimates of source class errors derived from engineering analyses and personal interviews (Grisinger, 1981); Bradley, 1981) were used to derive the  $f$  fractions. The error in the total emissions were derived using equation (11.3). One of the most striking results from Table 11.7 is the difference between class rankings based on mass emissions and net chemical reactivity.

This section has introduced a technique for establishing overall uncertainty limits on the emissions for a region such as the South Coast Air Basin. For the particular case studied the calculations suggest the following ranges: CO  $\pm$  20%, NO<sub>x</sub>  $\pm$  15%, Reactive Hydrocarbons  $\pm$  25% and Total Hydrocarbons  $\pm$  120%.

### 11.8 Initial and Boundary Conditions for Model Evaluation

The initial concentration field was established using the procedures described in Goodin et al. (1979a, 1981). Hourly averaged data from the monitoring sites (APCD, 1974) shown in Figure 11.9, were interpolated to the computational grid. Since most of these monitoring sites did not report ozone concentrations, but rather oxidant levels, the air quality data were converted to the form required by the model using:  $[O_3] = [OX] - 0.2[NO_2] + [S_2]$  (Eldon and Trijonis, 1977). In

TABLE 11.7

Reactivity Weighted Inventory of Emissions from Major Hydrocarbon Source Categories in the South Coast Air Basin

RANK ON A REACTIVITY BASIS	CATEGORY OF EMISSIONS (CES)	CES NUM--BER	TOTAL HYDROCARBON EMISSIONS (kg/day)	REACTIVE HYDROCARBON EMISSIONS (kg/day)	REACTIVITY WEIGHT	WEIGHTED EMISSIONS	RANK ON MASS BASIS
1	Motor Vehicle	2	871,864	810,833	0.03464	30,203	1
2	Jet Exhaust	20	43,404	43,300	0.07426	3,223	7
3	Gasoline Evap. (Fuel Tank)	122	52,461	52,461	0.02845	1,492	6
4	Gasoline Evap. (Floating Roof)	94	28,039	28,039	0.02845	798	11
5	Off Road Motor Vehicle	38	19,204	16,861	0.03563	684	13
6	Underground Storage at Stations	40	32,102	32,105	0.01632	524	10
7	Oil Base Including Solvent	110	73,562	39,356	0.00582	428	4
8	Industrial Processes (Pet. Refining)	87	42,819	27,370	0.00811	347	8
9	Industrial Processes (Pet. Refining)	90	13,146	11,479	0.02103	276	18
10	Crude Oil Evap. (Fixed Roof)	88	37,487	35,148	0.00696	261	9
11	Railroad	4	7,029	6,827	0.03127	220	26
12	Piston Exhaust	19	8,373	7,574	0.02199	184	24
13	Land Fills	117	846,090	8,461	0.00018	149	2
TOTALS (% Contribution to the total SCAB emission Inventory)			2,075,580 (61%)	1,119,814 (87%)		38,789 (95%)	

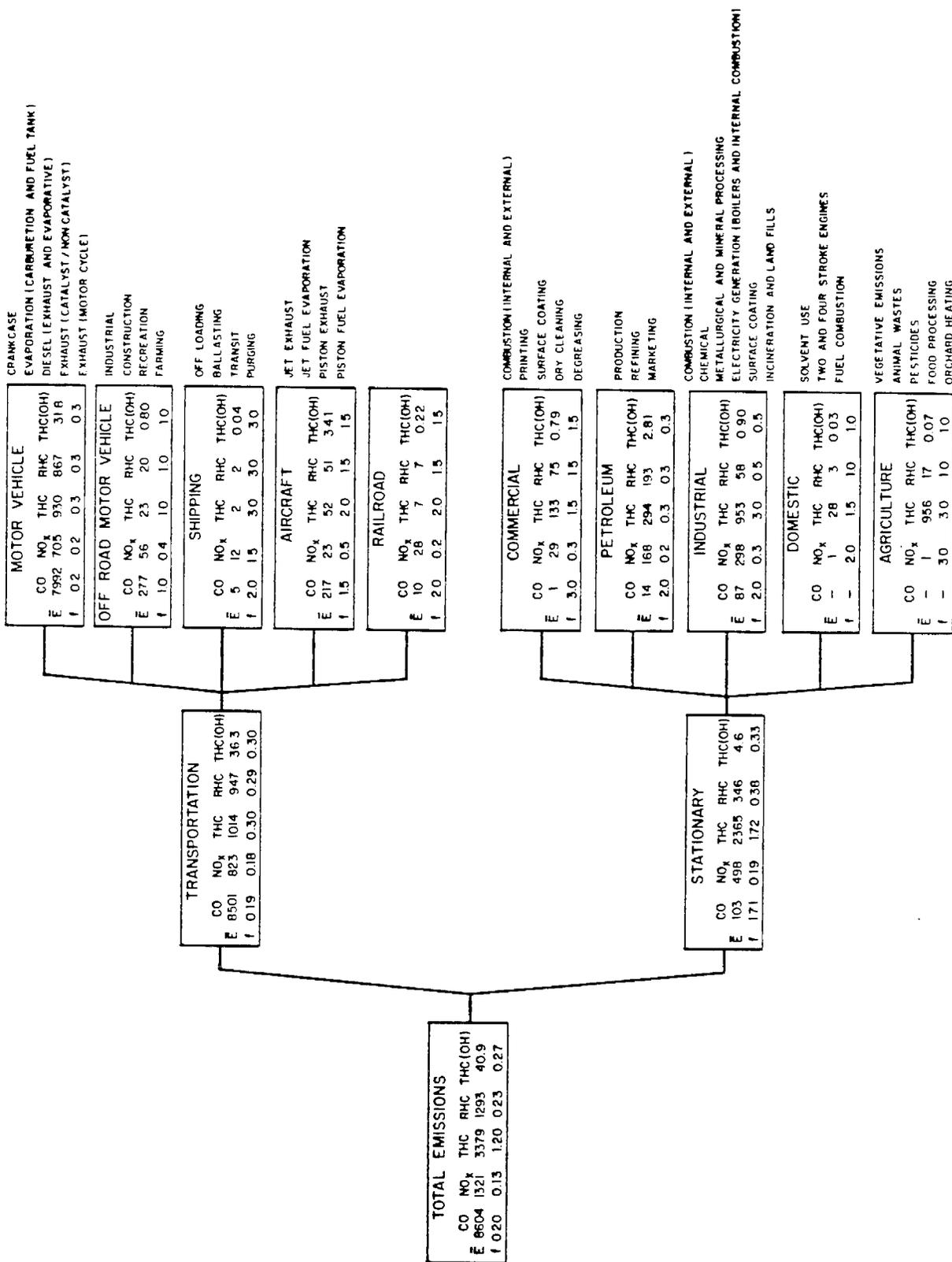


FIGURE 11.8

Simplified Structure of the Inventory Used in this Study Together with an Assessment of the Uncertainty of Pollutant Emissions from Different Source Categories (E is the pollutant emission rate in kg day<sup>-1</sup>x10<sup>-3</sup> and f is the fractional uncertainty in the inventory category).



this expression [OX] is the oxidant concentration corrected for any calibration errors. (0.8 for data outside of Los Angeles County). The remaining terms in the conversion formula correct for the effects of interferences. Because of the poor quality of most reactive hydrocarbon measurements, a set of splitting factors was developed for converting total hydrocarbon readings into the components needed for the chemical mechanism. These factors were derived from emissions data and from the results of detailed field measurements reported in Altshuller et al. (1974), Cavanagh et al. (1969), Kopczynski et al. (1972), Lamb et al. (1980), Mayrsohn and Crabtree (1976), and Stephens and Burleson (1969). Given a total hydrocarbon measurement, expressed in ppmC, the factors shown in Table 11.8 enables the partitioning of this value into the equivalent ppmv amounts needed for the reaction mechanism.

A three-dimensional model requires initial and boundary concentrations aloft. Unfortunately, few pollutant concentration measurements have been taken above urban regions. One of the most comprehensive measurement programs conducted over the Los Angeles basin was that performed by Blumenthal et al. (1978). The results of that study indicated that on days with light winds aloft, polluted air that has been carried into the inversion layer can remain there overnight to be mixed down the following day. Figure 11.10 shows the measured ozone concentrations from Burbank and Mt. Lee, which are only 5 km apart but differ in elevation by about 300 m. The ozone concentration at Mt. Lee remains high during the night since little of the NO released at the surface is able to mix vertically under nighttime stable conditions.

TABLE 11.8

Splitting Factors for Converting Total Hydrocarbon Measurements  
into Hydrocarbon Classes for Chemical Mechanism\*

CLASS	URBAN CONDITIONS	RURAL CONDITIONS
Ethylene	0.0247	0.0057
Paraffins	0.0419	0.00967
Olefins	0.0110	0.00253
Aromatics	0.0075	0.00173
Formaldehyde	0.0433	0.0100
Aldehydes	0.0118	0.00273

\*  
ppmv of individual class = Splitting factor x THC in ppmC

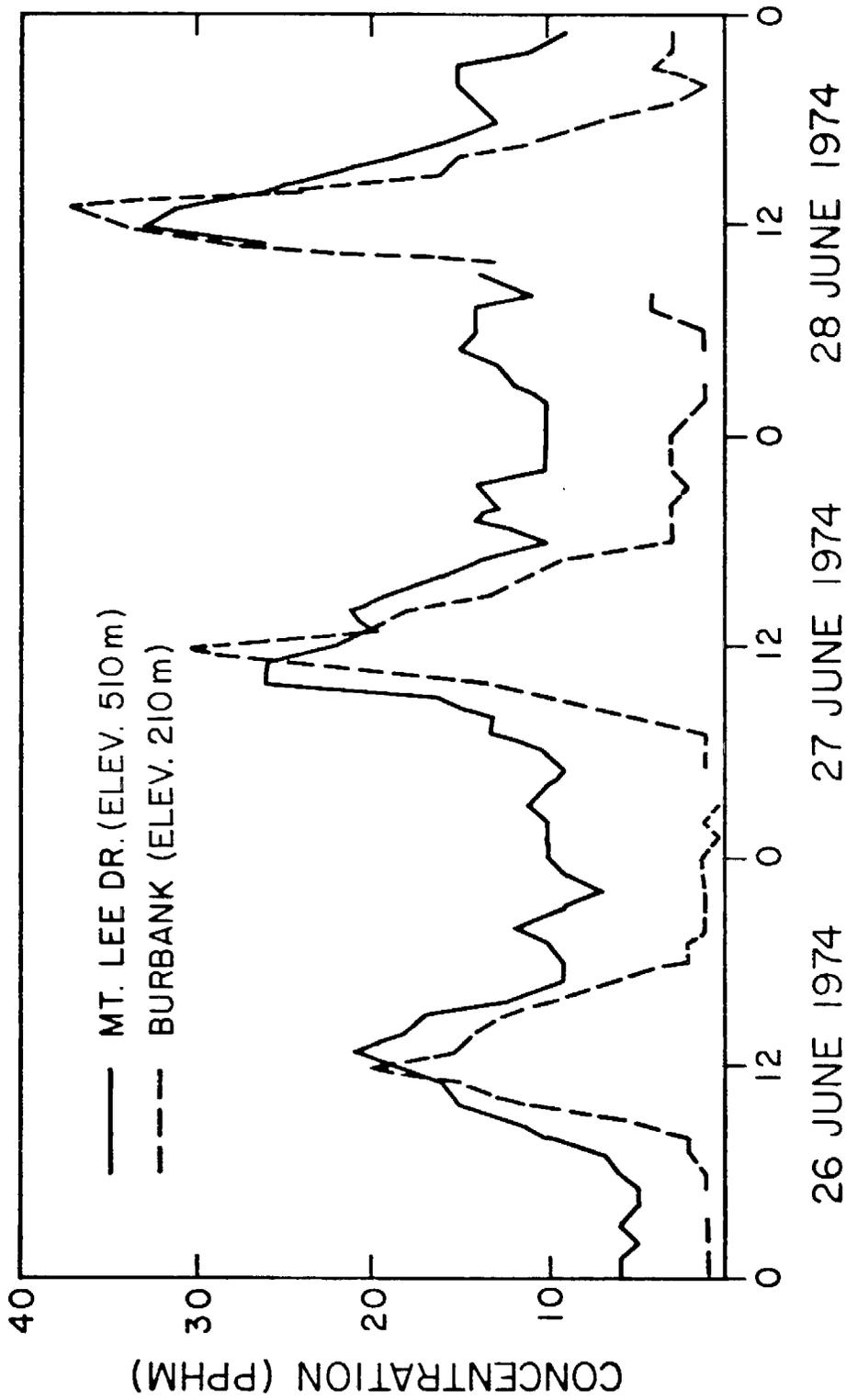


FIGURE 11.10

Measured Ozone Concentrations at Mt. Lee (elevation 510 m) and Burbank (elevation 210 m) During the Period 26-28 June 1974

The maximum hourly averaged concentration at Burbank increased from 0.20 ppm to 0.37 ppm during the episode. This increase of about 0.10 ppm on successive days is approximately the same magnitude as the overnight level at Mt. Lee, indicating that the downward mixing of polluted air from the inversion layer could account in part for the increased pollutant levels observed during this episode.

The procedure adopted in this study for constructing initial and boundary concentrations aloft is to assume a uniform value within the mixed layer using the surface concentration. The concentration then is assumed to decrease linearly to the background value at the top of the modeling region. Table 11.9 summarizes the results of a literature survey carried out to establish background levels and it also presents the values used in the present study. One of the major reasons for carrying out multi-day simulations was to minimize the influence, on the second day, of assumptions about initial conditions on the first day. The initial conditions for the second and subsequent days are simply the model outputs from the preceding day.

#### 11.9 Location of the Airshed Boundaries of the Modeling Region

When choosing the location of the boundary of a modeling region, tradeoffs must be made among factors such as computer storage, computational costs and the accuracy of the results. Important physical phenomena that occur near the edge of the current study region are the land-sea breeze and mountain-valley flow regimes. Polluted air masses carried out to sea by the night time land breeze often return the next

TABLE 11.9

## Natural (Unpolluted), Rural and Airshed Background Concentrations

SPECIES	NATURAL BACKGROUND CONCENTRATION (ppm)	REFERENCE	RURAL BACKGROUND CONCENTRATION (ppm)	REFERENCE	VALUE USED FOR BACKGROUND CONDITIONS
CH <sub>4</sub>	1.5	Robinson and Robbins (1968)	>1.4	Rasmussen et al. (1977)	1.0 (THC)
	1.4	Rasmussen et al. (1974)			
Reactive HC	<0.002	Rasmussen et al. (1974)	0.05-	Rasmussen et al. (1977)	
	ppmC		0.18ppmC		
CO	0.1	Robinson and Robbins (1968)	0.2-0.7	RTI (1975)	0.1
	0.01-	Cavanaugh et al. (1969)			
	0.26	Junge (1963)			
O <sub>3</sub>	0.04-	Chatfield and Harrison (1976)	0.0-0.2	RTI (1975)	0.04*
	0.055				
	0.01	Jerskey et al. (1976)			
NO	0.001	Robinson and Robbins (1968)	<0.05	Spicer et al. (1975)	0.01*
	0.0002-	Rasmussen et al. (1974)	<0.01	RTI (1975)	
	0.002				
NO <sub>2</sub>	0.001	Robinson and Robbins (1968)	<0.05	Spicer et al. (1975)	0.01*
	0.0009-	Rasmussen et al. (1974)	0.005-0.01	RTI (1975)	
	0.0013				

\* During daylight hours NO, NO<sub>2</sub> and O<sub>3</sub> are in photolytic equilibrium.

day with the sea breeze as shown in Chapter 5. Upslope flows caused by heating of mountain slopes can inject pollutant-laden air into the inversion layer, to be subsequently fumigated down to the surface. At night, downslope or drainage flows can bring contaminated air, which is different from the surrounding surface air, into the basin. Since Eulerian or fixed-grid numerical procedures do not follow material that leaves the airshed, it is desirable to locate the grid boundary farther from the main calculation area than the greatest extent of significant return flows. In view of the importance of these flows, trajectory studies were conducted to locate suitable boundaries for the airshed model.

Numerical experiments were performed for 27 June 1974, in order to choose the location of the boundary of a subgrid area to be analyzed within the 400 x 150 km study area. Parcels of air leaving the coast with the land breeze were followed to determine their seaward extent. Figure 11.11 illustrates the problem in a simple manner. These trajectory calculations were begun at 00:00 PST on 27 June, the approximate start of the land breeze. The calculations were performed using the surface wind fields generated from measured data. Six parcels were tracked from coastal origins between Santa Barbara and San Juan Capistrano. The seaward extent of polluted air leaving the coastline on this day ranged from 0 to 25 km. Thus, if a western boundary for a subgrid region were to be established parallel to the coastline, it should be set approximately 25 km offshore in order to avoid loss of polluted air that might return following a flow reversal. Similar

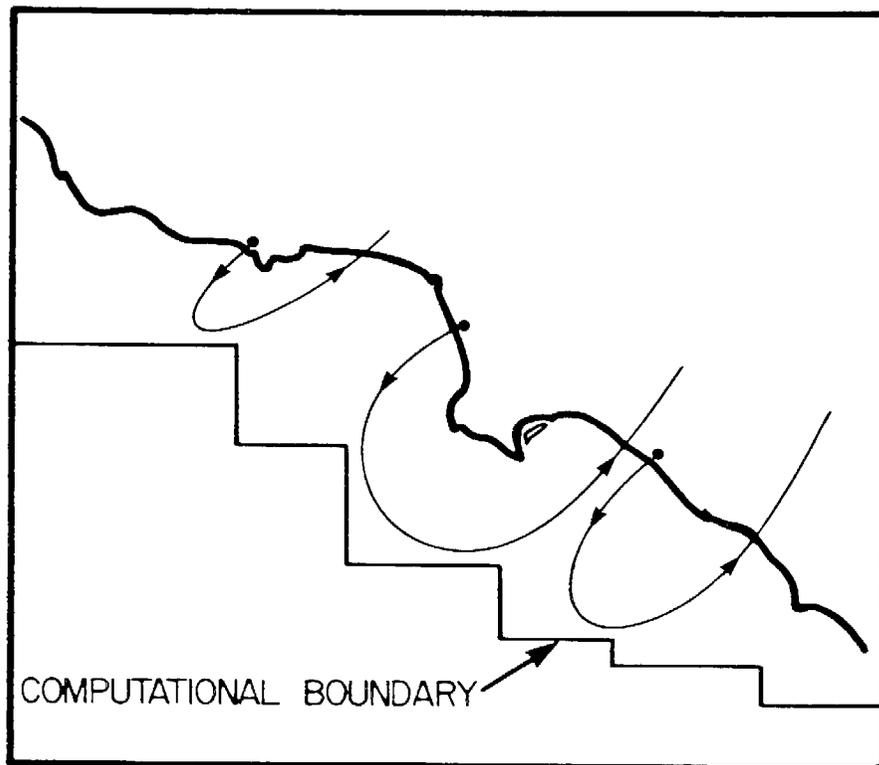


FIGURE 11.11

Illustration of Procedure Used to Define Computational Region  
that Minimizes the Effects of Inflow Boundary Conditions

calculations were performed to study inland flow patterns. Trajectories were initiated at Newhall, San Bernardino, Pomona and Perris at 00:00 at 27 June 1974. These studies indicated that during the night, air travels only a short distance (2 to 10 km) toward downtown Los Angeles from these locations. The horizontal extent of the computational domain employed is shown as the shaded region in Figure 11.12.

After an examination of mixing depth and vertical temperature structure data for the 26-28 June 1974 episode, the height of the top of the modeling region was set at 1525 m above the terrain. When a mixed layer existed, it was less than 1100 m deep at all points in the basin and so material trapped aloft could be satisfactorily tracked. On those occasions when the mixed layer was destroyed by heating, its depth was assumed to be 1100 m. After a series of detailed calculations the number of computational cells in the vertical direction was set equal to 5, representing a compromise between computational cost and the ability to resolve vertical concentration gradients.

#### 11.10 Summary

Table 11.10 shows a summary of aerometric and emissions information available for 26-28 June 1974 for the study region.

#### 11.11 Predicted and Observed Concentrations for 26-27 June 1974

The model was applied to simulate the two-day period 26-27 June 1974 in the SCAB. The concentrations of 15 species (NO, NO<sub>2</sub>, O<sub>3</sub>, CO, PAN, HONO, RO<sub>2</sub>NO<sub>2</sub>, RONO, H<sub>2</sub>O<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, OLE, ALK, ARO, HCHO and RCHO) are

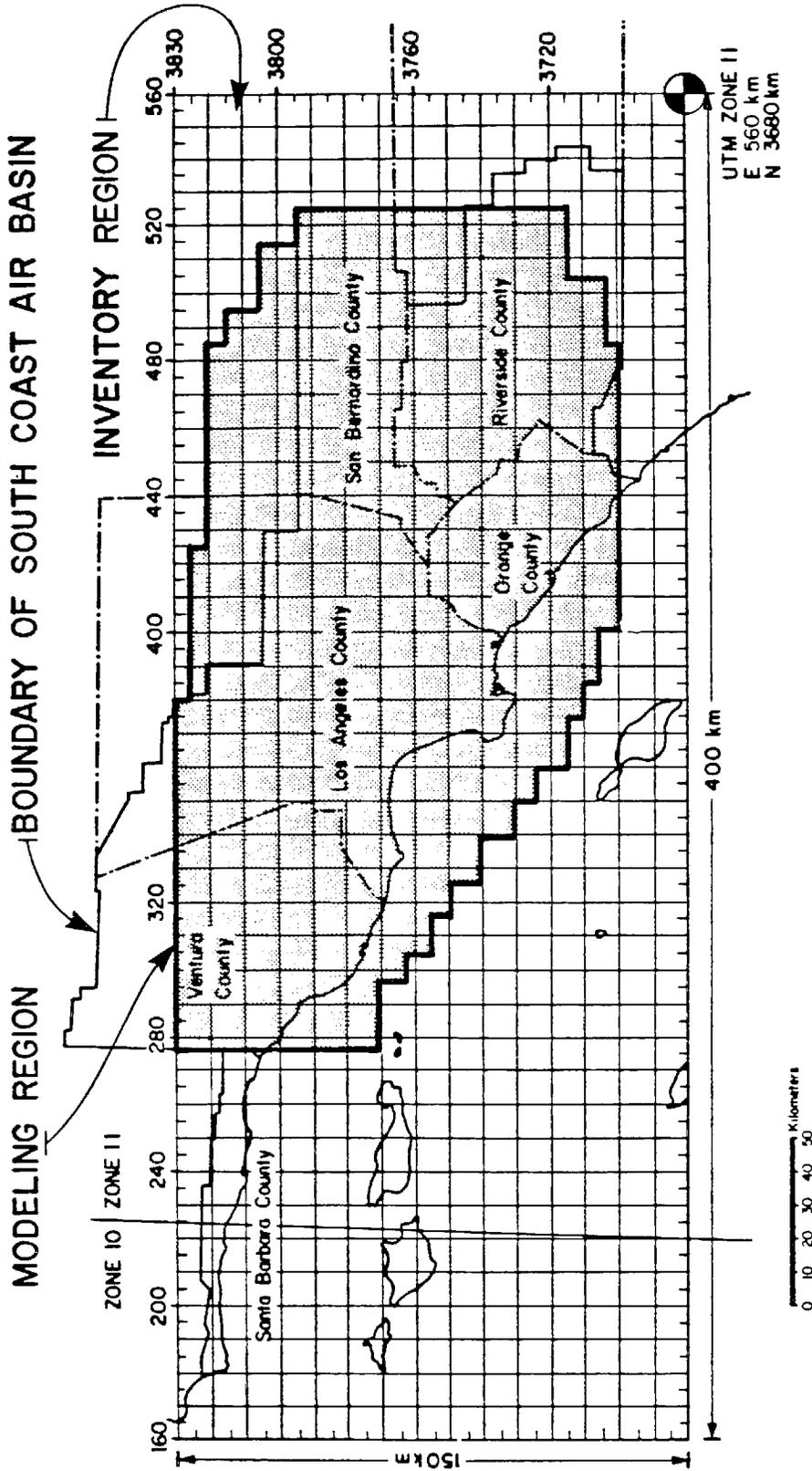


FIGURE 11.12

Definition of Computational Grid System Over the South Coast Air Basin  
The shaded portion corresponds to the area used  
in the model performance evaluation.

TABLE 11.10 Summary of Aerometric and Emissions Information Available for 26-28 June 1974 for the South Coast Air Basin

TYPE OF DATA	NATURE OF DATA COLLECTED	REMARKS	SOURCE OR ORGANIZATION(S) COLLECTING DATA
<b>AIR QUALITY DATA</b>			
Surface pollution concentration	55 air quality monitoring stations	Data are hourly averaged and include measurements of CO, NO, NO <sub>2</sub> , O <sub>3</sub> , THC, RHC and SO <sub>2</sub> .	SCAQMD, ARB, CALTRANS, USFS
Pollution concentrations aloft	None	Estimates of vertical concentration profiles were derived from detailed field measurements collected from different periods.	
<b>METEOROLOGICAL DATA</b>			
Surface Winds	63 surface wind monitoring stations	Data include hourly averaged and instantaneous values.	SCAQMD, ARB, NWS, USN, USAF
Upper level winds	Radiosondes at Edwards AFB (0400 PST), Pt. Mugu (0400, 1000, and 1500 PST), and San Nicholas Island (0930 and 1500 PST). Pibal balloons at LAX (0530 and 1130 PST) and El Monte (0600 and 1230 PST). Aircraft spiral at Riverside (0600 PST).		SCAQMD, USN, USAF, NWS
Mixing depths	Aircraft spiral at Riverside (0600 PST). Radiosondes at LAX (0530, 1030 PST), El Monte (0600, 1230 PST), Pt. Mugu (0400, 1000, 1500 PST), and San Nicholas Island (0930, 1500 PST), and Edwards AFB (0400 PST). Continuous acoustic sounder at El Monte.	Data are instantaneous except for continuous acoustic sounder at El Monte.	ARB, NWS, USN, USAF
Surface temperatures	Temperatures at 14 stations.	Data are hourly averaged values.	NWS, SCAQMD
Solar radiation	Radiation measurements at UCLA and LAX.	Data are hourly averaged and daily averaged values.	NWS, SCAQMD
Humidity	Humidity at 14 stations	Data are hourly averaged values	NWS, SCAQMD
Cloud cover	Cloud cover at 7 airports and 2 other locations.	Data are instantaneous values recorded every hour.	NWS, SCAQMD
<b>EMISSIONS DATA</b>			
Traffic	Emissions estimates derived from the LARTS transportation model and the ARB FVY011 emissions model.	Peak, off-peak and total emissions rates for THC, SO <sub>2</sub> , NO <sub>x</sub> and CO are available. Percentage of hot and cold starts are included in the inventory, but they are not spatially or temporally distributed; vehicle speed distributions and types (four classes) are included.	ARB, CALTRANS
Refinery	Emissions for organic gases, NO <sub>x</sub> , CO and particulates estimated for 28 facilities		SCAQMD

TABLE 11.10 Summary of Aerometric and Emissions Information Available for 26-28 June 1974 for the South Coast Air Basin (Continued)

TYPE OF DATA	NATURE OF DATA COLLECTED	REMARKS	SOURCE OR ORGANIZATION(S) COLLECTING DATA
EMISSIONS DATA (Cont)			
Aircraft	Gridded emissions estimates for all major airports in inventory region.		CALTRANS, SCAQMD
Power plants	Emissions estimates of NO, NO <sub>2</sub> and CO for each plant in inventory region.	Diurnal distribution of emissions based on inspection of daily operating logs.	SCE, LADWP
Distributed area sources	Emissions estimates for organic gases, NO <sub>x</sub> and CO.		SCAQMD
Other stationary sources	Emissions estimates for organic gases, NO <sub>x</sub> and CO.		SCAQMD

predicted in each of the grid cells as a function of time commencing at 0:00 hours 26 June. Of the 15 species calculated, two for which there exist both monitoring data and National Ambient Air Quality Standards, and the two that provide the most stringent test of a model to simulate photochemical air pollution, are  $\text{NO}_2$  and  $\text{O}_3$ . Therefore, we confine our attention here to these two species.

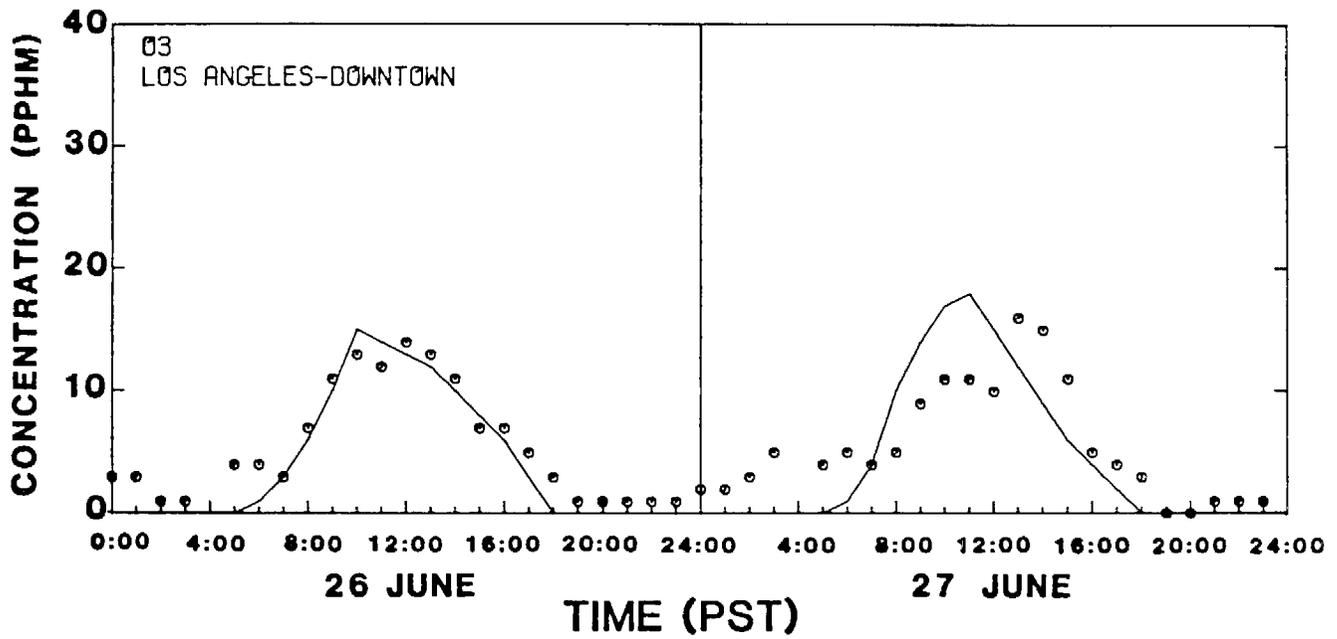
The computed concentration field may be presented in several ways:

1. One-hour-average ground-level concentration fields at each hour
2. Isopleths (contour lines of constant concentrations) at each hour
3. Concentrations as a function of time for various grid cells, in particular those containing a monitoring station.

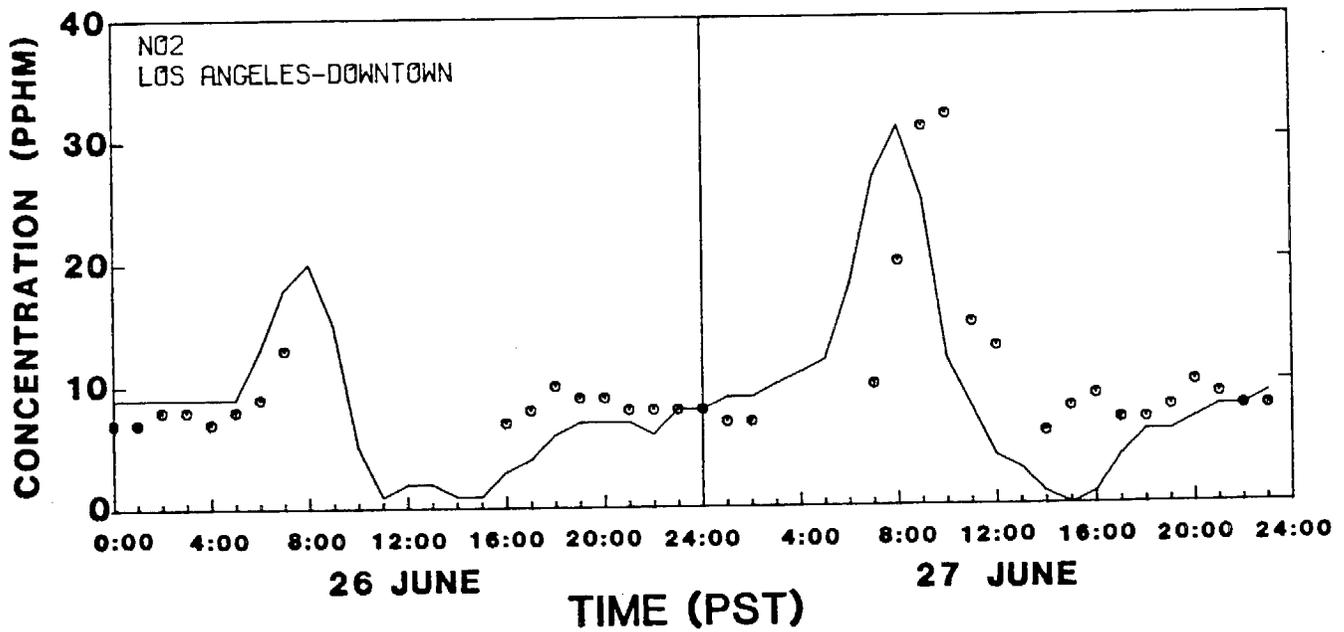
Each of these three ways of presenting predicted concentrations is useful and informative. For economy of space and because we are especially interested in comparisons with observations, we only show here the temporal behavior of the concentrations in the grid cells containing monitoring stations.

Figures 11.13-11.17 show predicted and observed concentrations of  $\text{NO}_2$  and  $\text{O}_3$  during 26-27 June 1974 at several monitoring stations in the SCAB. Results at all the monitoring sites are shown in Appendix C.

In the early morning both  $\text{NO}$  and reactive hydrocarbons peak due to traffic emissions. The  $\text{NO}_2$  peak concentrations are delayed a few hours, consistent with the time required to oxidize  $\text{NO}$ . Observed and predicted ozone concentrations increase with distance toward the east. Ozone concentrations gradually increase until the time of the peak



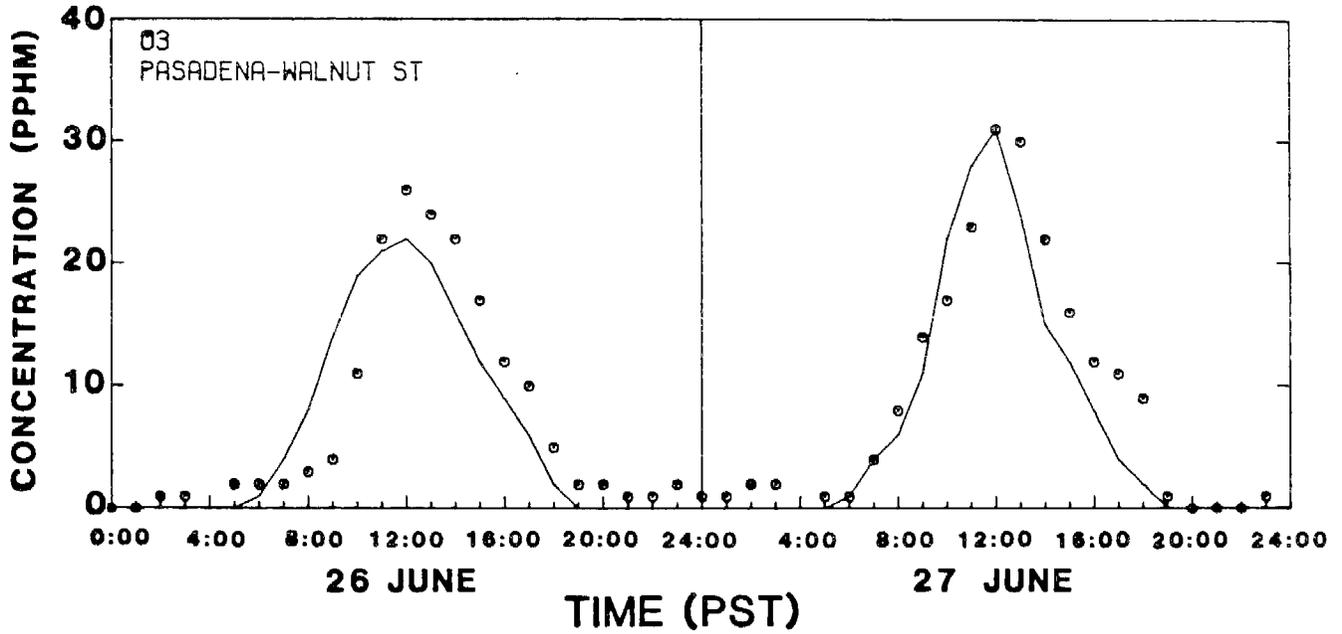
(a)



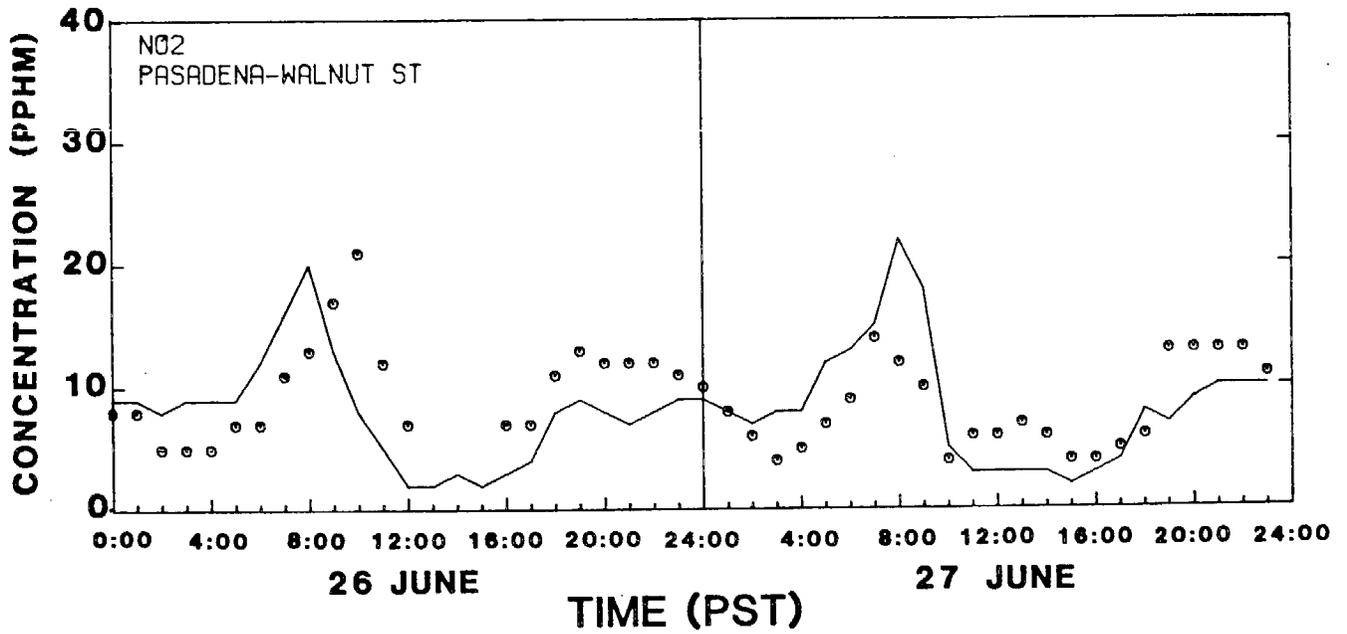
(b)

FIGURE 11.13

Predicted and Observed Concentrations of:  
 (a) Ozone and (b) Nitrogen Dioxide at Downtown Los Angeles  
 (- predicted, o observed)



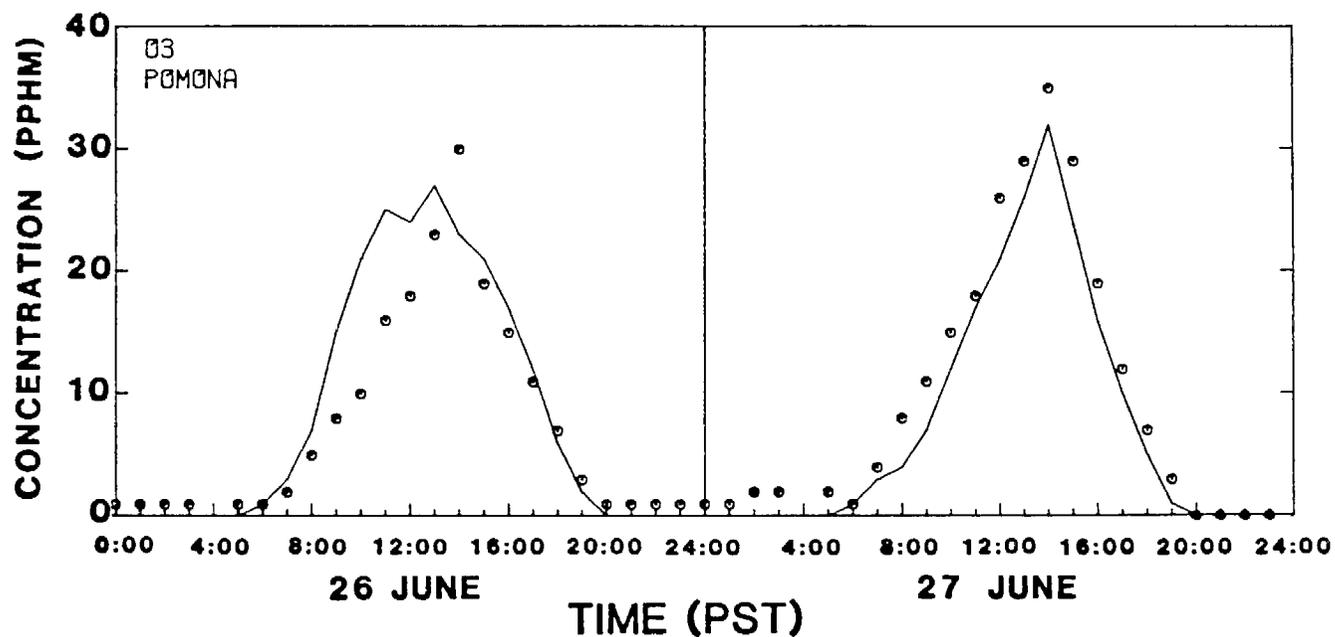
(a)



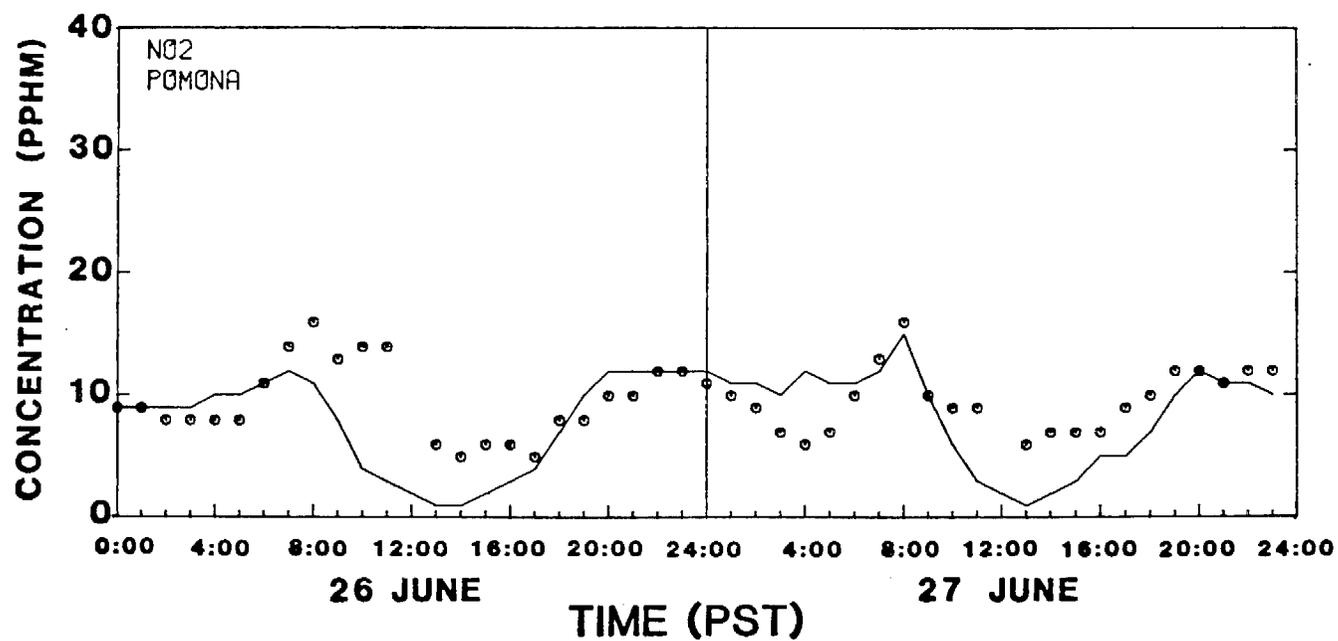
(b)

FIGURE 11.14

Predicted and Observed Concentrations of:  
 (a) Ozone and (b) Nitrogen Dioxide at Pasadena  
 (- predicted, o observed)



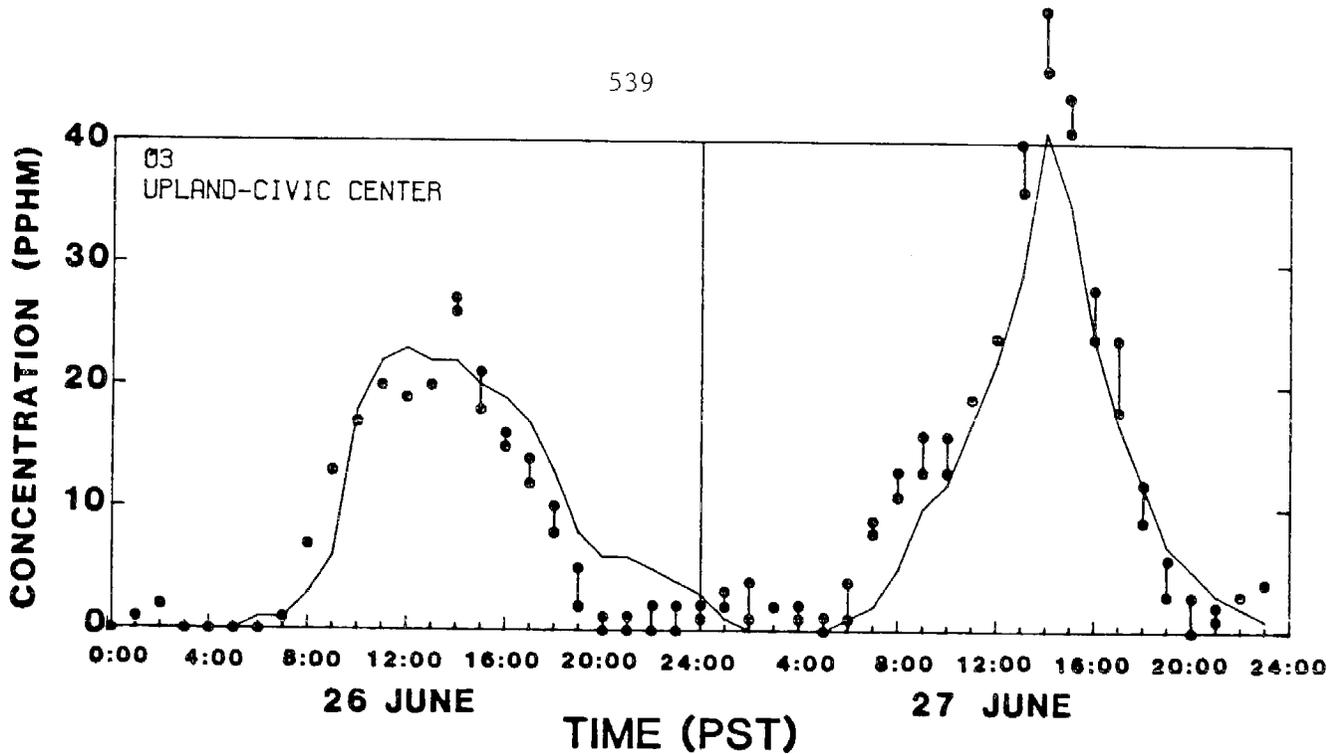
(a)



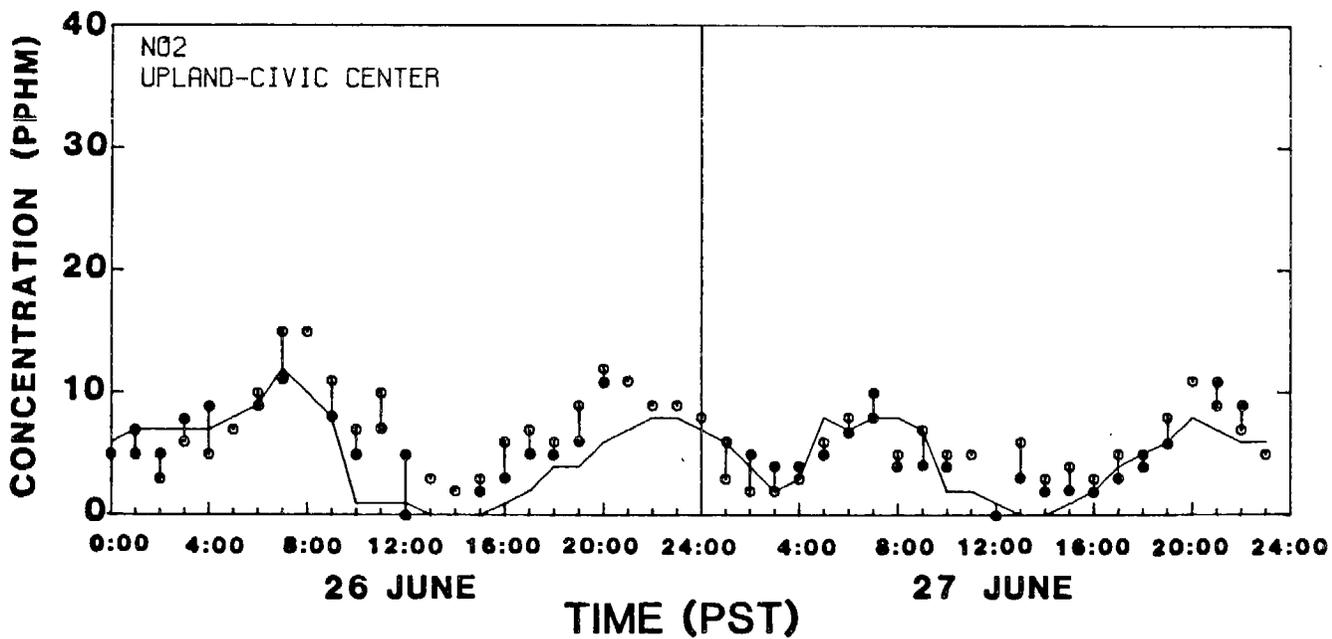
(b)

FIGURE 11.15

Predicted and Observed Concentrations of:  
 (a) Ozone and (b) Nitrogen Dioxide at Pomona  
 (- predicted, o observed)



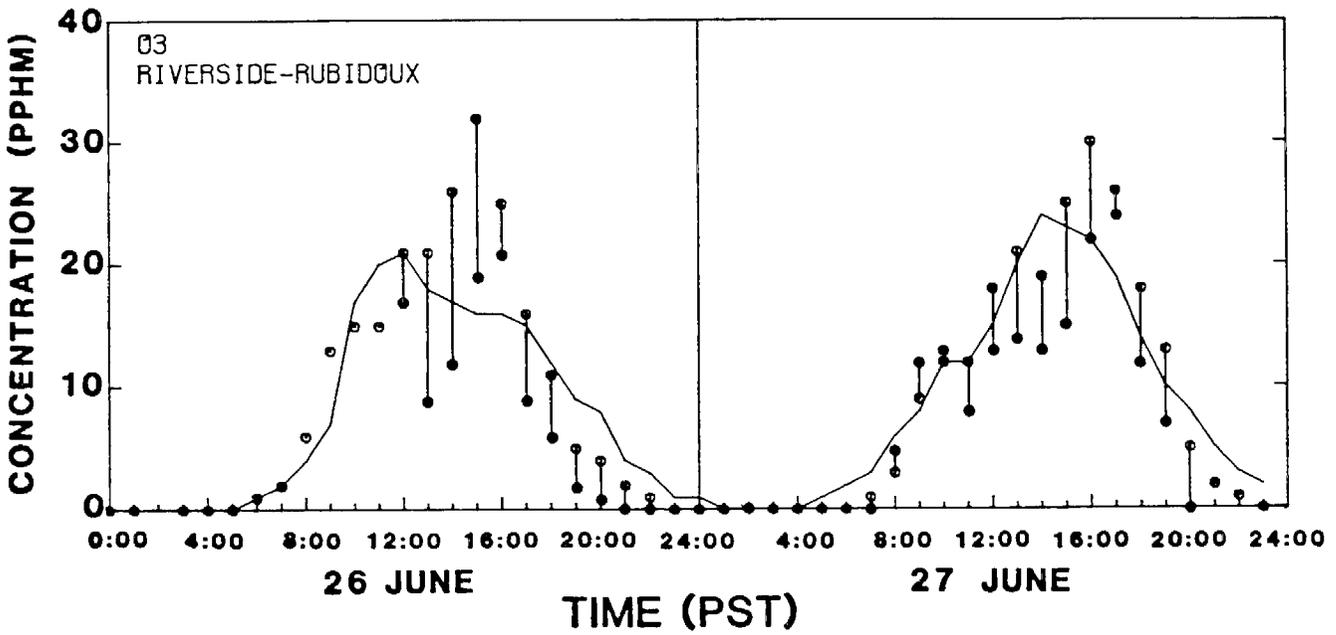
(a)



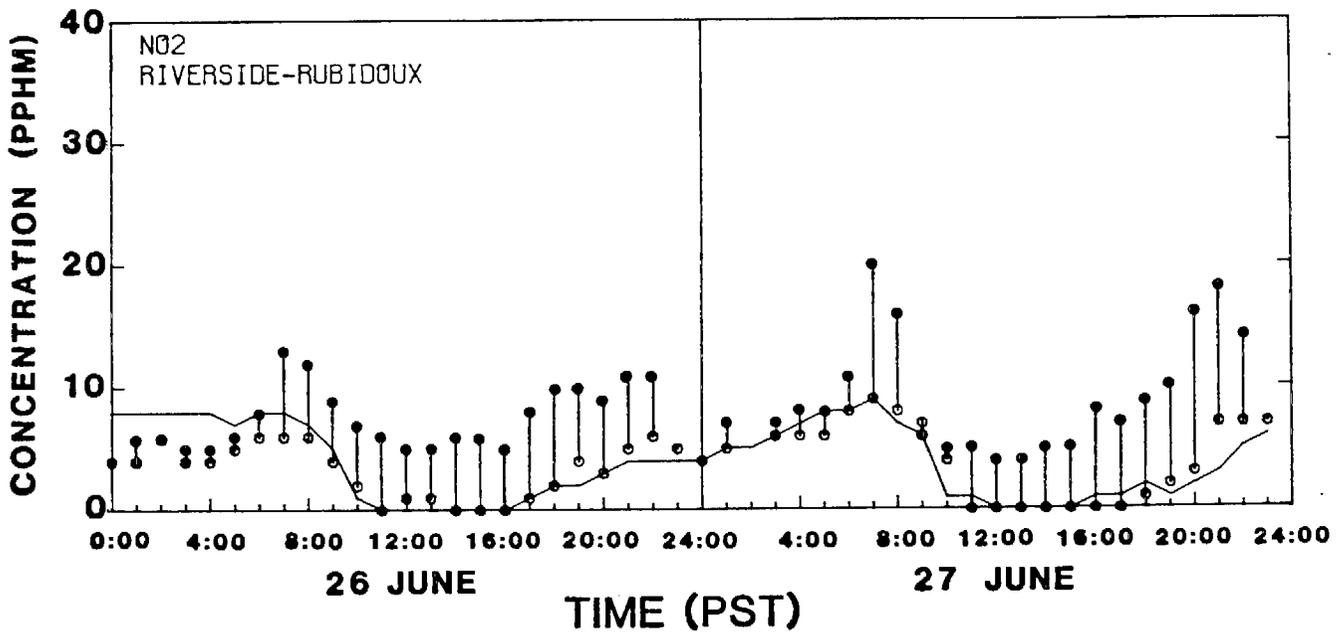
(b)

FIGURE 11.16

Predicted and Observed Concentrations of:  
 (a) Ozone and (b) Nitrogen Dioxide at Upland  
 (- predicted, o observed at CARB station,  
 ● observed at APCD monitoring site located 400 meters away).



(a)



(b)

FIGURE 11.17

Predicted and Observed Concentrations of:  
 (a) Ozone and Nitrogen Dioxide at Riverside  
 (- predicted, o observed at APCD station,  
 ● observed at ARB monitoring site located 1200 meters away).

predicted concentration which usually occurs between 1300 and 1400 PST. As air moves onshore and approaches the San Gabriel mountain range, bifurcation of the flow occurs. Some of the pollutants emitted in the western and downtown portions of the Basin are carried northward into the San Fernando Valley; other material is transported east to Azusa, Upland and Riverside. In most cases the model accurately reproduced both the magnitude and timing of the peak ozone concentration. Similar behavior was also noted for nitrogen dioxide except that the model tended to predict the peak values one to two hours earlier. The fact that the model satisfactorily described the observed concentration trends on the second day is particularly encouraging for control strategy calculations. The reason for this is that by running the model for a period longer than the characteristic ventilation of the airshed it is possible to minimize the influence of uncertainties in specifying the initial conditions. This capability is important for those situations where it is not possible to derive starting conditions from ambient monitoring data.

In summary, because the essential trends of the predictions and observations are in agreement and because the model components represent state-of-the-art knowledge of each aspect, we assume that the basic model framework is a valid representation of atmospheric concentration dynamics.

### 11.12 Statistical Analysis of Results

In many respects a statistical analysis of the deviations between predictions and observations is the heart of model performance evaluation. Although raw statistical comparison of observed and predicted values may not reveal the cause of discrepancies, it can tell much about the nature of the mismatch. Considerable attention has been given to statistical measures for comparing predicted and observed air pollutant concentrations. (Brier, 1975; Bowne, 1980; Fox, 1981; Bencala and Seinfeld, 1979 and Rao and Visaili, 1981). Fox (1981) in discussing the results of an American Meteorological Society workshop identified three basic classes of performance measures.

1. Analyses based on observed and predicted concentration field values paired for particular locations and times.
2. Examinations of the ability of the model to predict the peak concentrations.
3. Frequency distributions of the updated (in time) observed and predicted concentration values.

Bencala and Seinfeld (1979), for example, have discussed many of these measures and have developed a general computer program for evaluating them given a set of predicted and observed concentrations. In the present section this program has been applied to analyze the simulation of 26-27 June 1974. The results of these calculations are summarized in Table 11.11. While ideally an assessment of a model's performance, in reproducing observed concentration distributions, should be based on a comparison against recognized criteria no formal standards have as yet been established. The results reported below are offered in the

TABLE 11.11

Summary Statistics Determined Over All Times and Locations for 26-27 June 1974<sup>(a)</sup>

PERFORMANCE MEASURE	DEFINITION <sup>(b)</sup>	INTERPRETATION OF STATISTICAL TEST	RESULTS OF TEST		EVALUATION OF MODEL PERFORMANCE
			OZONE (O <sub>3</sub> )	NITROGEN DIOXIDE (NO <sub>2</sub> )	
Mean of Residuals	$u_i = \frac{1}{nm} \sum_{j=1}^n \sum_{k=1}^m w_i(x_j, t_k)$	A measure of the average bias in the predictions can be inferred from this test. The criterion indicates whether the model predominantly over-or-under-predicts the observed concentration.	0.0019 ppm [3%] <sup>(c)</sup>	0.0078 ppm [11%] <sup>(c)</sup>	While the model exhibits a slight tendency towards underprediction, the bias is of the order of typical monitoring instrument errors.
Root Mean Square Error (RMSE) Centered about the Mean	$v_i = \sqrt{\frac{1}{nm} \sum_{j=1}^n \sum_{k=1}^m [w_i(x_j, t_k) - u_i]^2}$	This test measures the average spread of the residuals and, more importantly, it is insensitive to any bias in the predictions.	0.0382 ppm	0.0348 ppm	These results provide a formal measure of the spread of the residual histograms presented in Figure 10.
Correlation Coefficient	$r_i = \frac{\frac{1}{nm} \sum_{j=1}^n \sum_{k=1}^m v_i(x_j, t_k) \gamma_i(x_j, t_k)}{\sqrt{\frac{1}{(nm)^2} \left( \sum_{j=1}^n \sum_{k=1}^m v_i^2 \right) \left( \sum_{j=1}^n \sum_{k=1}^m \gamma_i^2 \right)}}$ where $v_i(x_j, t_k) = c_i^p(x_j, t_k) - \bar{c}_i^p$ $\gamma_i(x_j, t_k) = c_i^o(x_j, t_k) - \bar{c}_i^o$ and $\bar{c}_i^o = \frac{1}{nm} \sum_{j=1}^n \sum_{k=1}^m c_i^o(x_j, t_k)$	The correlation coefficient measures the degree to which the magnitude of the predictions increase linearly with the magnitude of the observations. From a practical point of view it is important to note that the coefficient is insensitive to the extent of the increase. For example, if the predictions increase linearly at 1/10th of the rate of the observations then r will still be one.	0.89	0.67	For ozone (O <sub>3</sub> ) the predicted performance is excellent. In the case of nitrogen dioxide (NO <sub>2</sub> ) it is not possible to ascertain whether the low value of r is due to the model performance or interference from HONO <sub>2</sub> and PAN in the measurement of NO <sub>2</sub> (Adema, 1979; Higuchi et al., 1976).
Linear Least Squares Curve Fit	$c_i^p = b_i c_i^o + a_i$ where the slope $b_i$ is given by $b_i = \frac{\frac{1}{nm} \sum_{j=1}^n \sum_{k=1}^m v_i(x_j, t_k) \gamma_i(x_j, t_k)}{\frac{1}{nm} \sum_{j=1}^n \sum_{k=1}^m \gamma_i^2(x_j, t_k)}$ and intercept $a_i$ by $a_i = \bar{c}_i^o - b_i \bar{c}_i^o$	This performance measure can be used to assess the average increase in the predictions as the observations are increased. The slope parameter of the linear least squares curve fit is this measure. If the slope is nearly equal to one then the intercept is an indication of the bias.	slopes 0.851 intercepts 0.0115 ppm	0.709 0.0262 ppm	Both the slopes and intercepts for ozone (O <sub>3</sub> ) and nitrogen dioxide (NO <sub>2</sub> ) indicate that the model satisfactorily reproduces the observed concentration distributions.
Accuracy of Peak Prediction	$\max \frac{c_i^p(x_j, t_k)}{\max c_i^o(x_j, t_k)}$	Ratio of the maximum predicted peak concentration to the highest measured value.	$\frac{0.41}{0.51} = 0.80$	$\frac{0.31}{0.36} = 0.80$	For both ozone (O <sub>3</sub> ) and nitrogen dioxide (NO <sub>2</sub> ) the predicted highest concentrations are within 20% of the observations.
Timing of Peak Concentration Predictions	$\Delta t_i = t^o(x_j) - t^p(x_j)$	Difference in timing of predicted and observed peaks at the monitoring site with the highest observed concentration.	0 hrs <sup>(d)</sup>	-2 hrs <sup>(d)</sup>	As seen in Table 9 the predicted and observed ozone (O <sub>3</sub> ) concentration peaks were coincident at most monitoring sites. Differences of up to three hours were noted in the predicted times of the NO <sub>2</sub> peaks.
Error Bands	% of residuals over all j,k that satisfy $ w_i(x_j, t_k)  \leq \text{bound}$	This measure gives the percentage of predictions that fall within a particular concentration bound.	83.8% <sup>(e)</sup>	88.9% <sup>(e)</sup>	Most of the residuals were within the $\pm 0.05$ ppm concentration band.

## Footnotes:

- (a) In the statistical evaluation of model performance 1336 pairs of predictions and observations were used in the analysis of ozone (O<sub>3</sub>) and 973 for nitrogen dioxide (NO<sub>2</sub>).
- (b) The residual for species i at locations j=1,2,...,m and times k=1,2,...,m are defined as  $w_i(x_j, t_k) = c_i^o(x_j, t_k) - c_i^p(x_j, t_k)$  where  $c_i^o$  and  $c_i^p$  are respectively the observed and predicted concentrations of species i.
- (c) The values in brackets express the residuals as a percentage of the observed mean concentration. For ozone (O<sub>3</sub>) the observed and predicted means were 0.0661 and 0.0641 ppm and for nitrogen dioxide (NO<sub>2</sub>) 0.0709 and 0.0630 ppm respectively.
- (d) The peak observed value of ozone (O<sub>3</sub>) = 0.51 ppm occurred at Upland at 14:00 PST and the highest nitrogen dioxide (NO<sub>2</sub>) = 0.36 ppm at downtown Los Angeles at 10:00 PST.
- (e) Concentration bound set to  $\pm 0.05$  ppm.

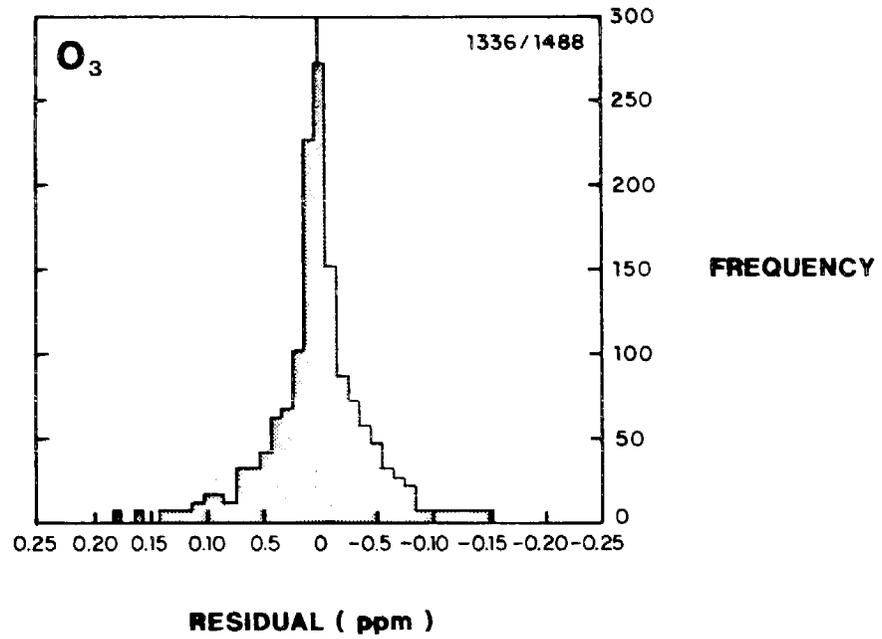
spirit of providing a reference level for performance evaluation of photochemical air pollution models.

### 11.13 Distribution of Residuals

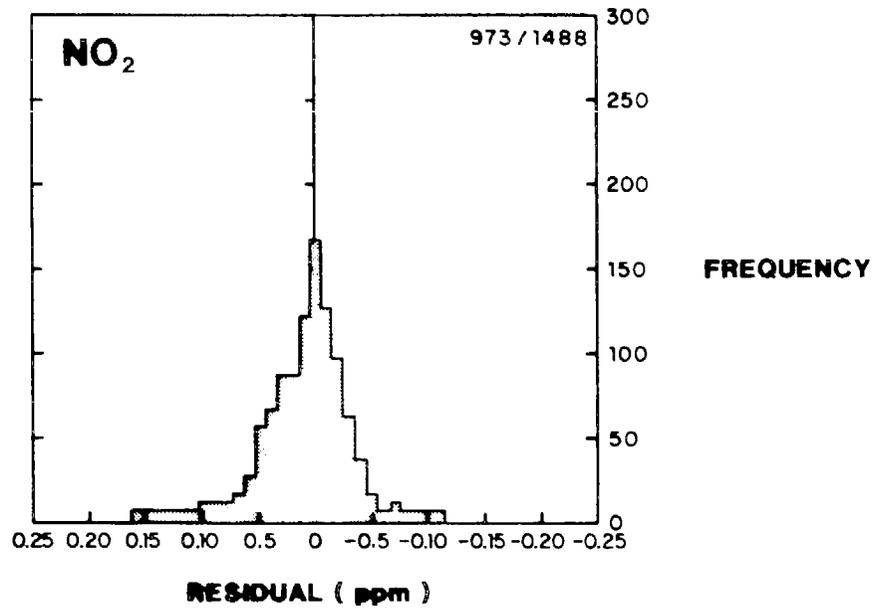
Figure 11.18 shows the frequency distributions of the residuals, i.e. observed minus predicted concentrations, for  $\text{NO}_2$  and  $\text{O}_3$  for all monitoring stations over the two day simulation. The distribution of residuals as a function of observed concentration is shown in Figure 11.19 and, as a function of time, in Figure 11.20. The mean residuals over all times and locations were 0.0078 ppm for  $\text{NO}_2$  and 0.0020 for  $\text{O}_3$  indicating a slight trend towards under-prediction. The standard deviation of the distributions shown in Figures 11.18-11.20 are within the error bounds associated with the routine air quality measurements. As noted by Fox (1981) analysis of paired data sets is one of the most stringent tests of a model. For pollutants that have a pronounced diurnal variation even a one hour difference in timing of the predicted maximum concentration can significantly change the results of some statistical tests. Figure 11.21, for example, shows the effect on a correlation plot of a one hour phase shift in the predicted concentration profile.

### 11.14 Predicted and Observed Concentration Maxima

An important criterion in evaluating an air pollution model is its ability to predict the observed concentration maxima. Table 11.12 shows a comparison of the magnitudes of the predicted and observed  $\text{O}_3$  maxima for 27 June at those stations where the observed maxima exceeded



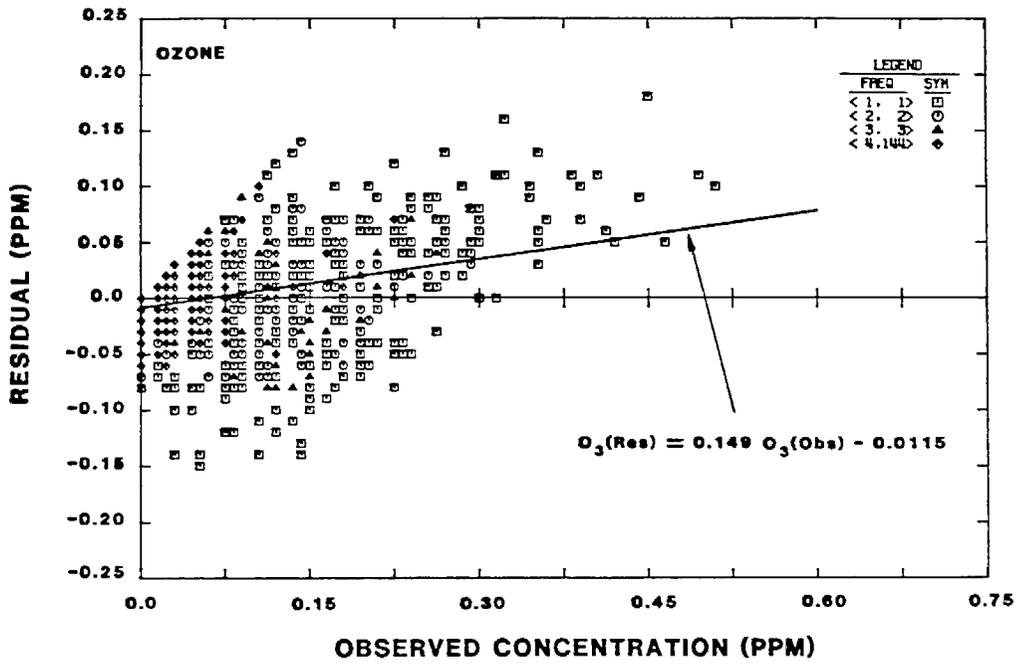
(a)



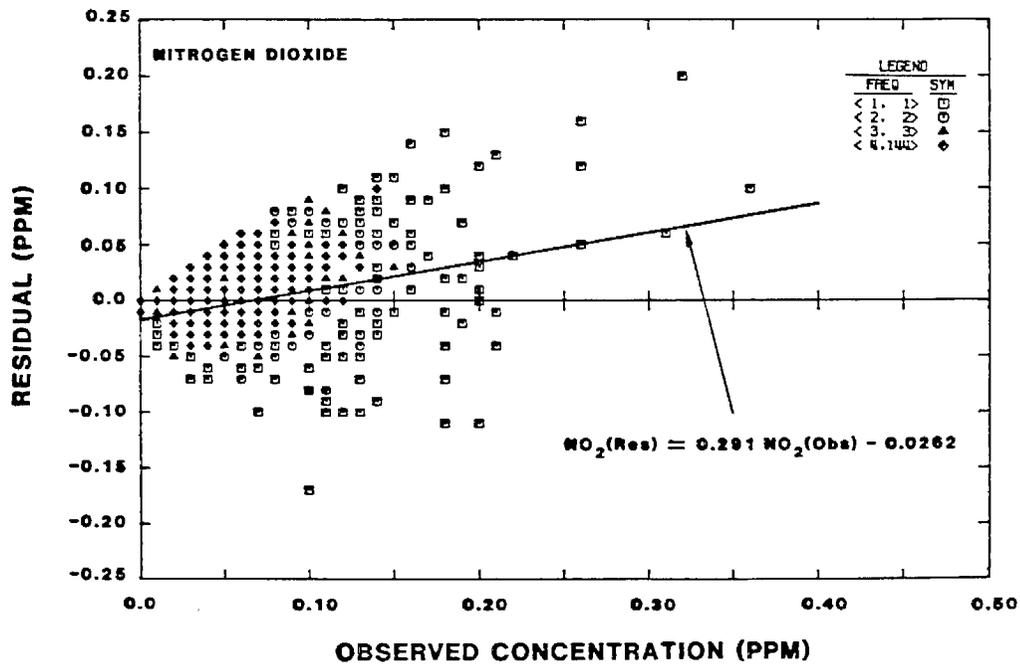
(b)

FIGURE 11.18

Histograms of Concentrations Residuals (Observed-Predicted) Determined Over All Times and Locations for the Two Day Period 26-27 June 1974:  
(a) Ozone (b) Nitrogen Dioxide



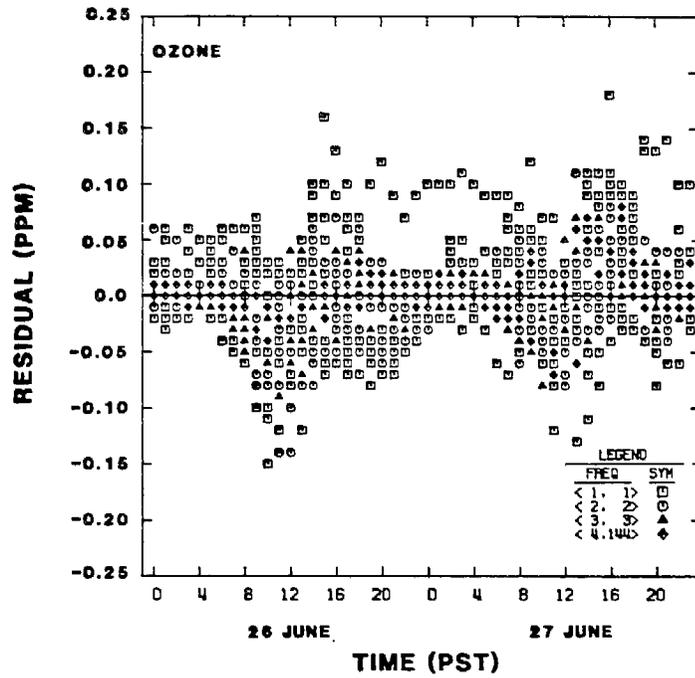
(a)



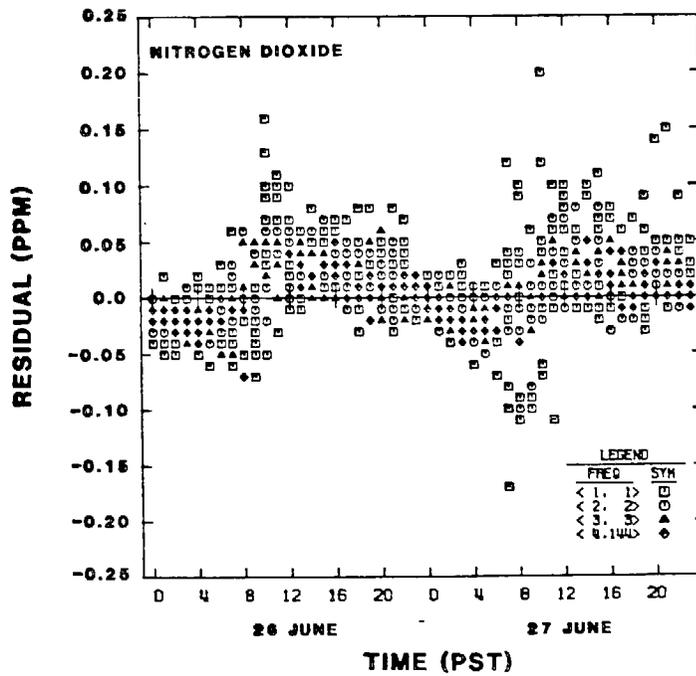
(b)

FIGURE 11.19

Distribution of Concentration Residuals (Observed-Predicted) as a Function of Observed Values Determined Over All Times and Locations for the Two Day Period 26-27 June 1974:  
 (a) ozone (b) nitrogen dioxide



(a)



(b)

FIGURE 11.20

Distribution of Concentration Residuals (Observed-Predicted) as a Function of Time Determined Over All Locations for the Two Day Period 26-27 June 1974: (a) Ozone (b) Nitrogen Dioxide

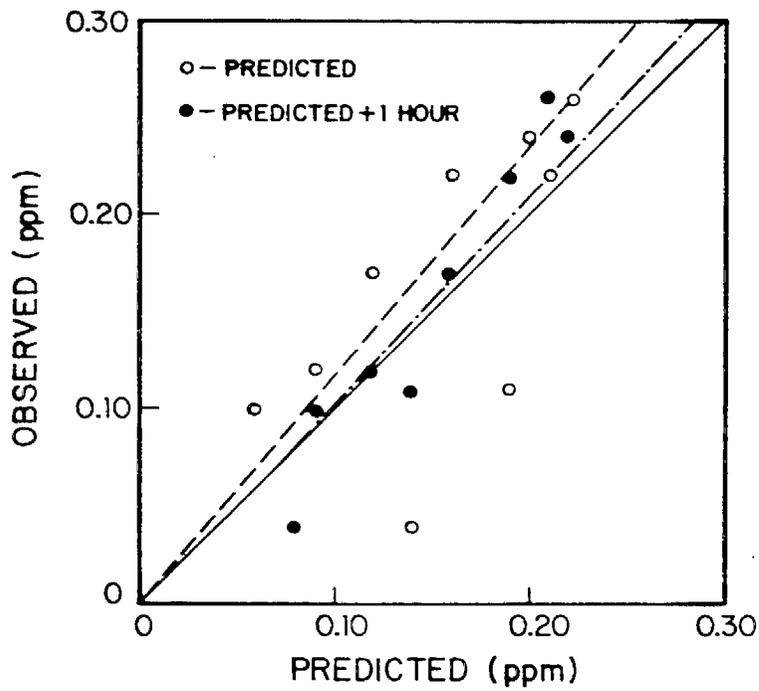
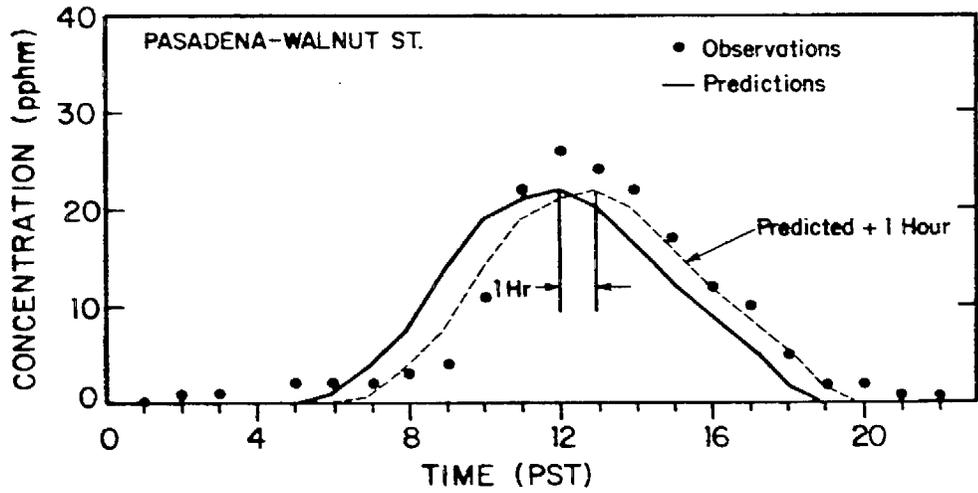


FIGURE 11.21

Effect on a Correlation Plot of a One Hour Phase Shift in the Predicted Concentration Time Profile. (26 June, 1974)

TABLE 11.12  
 Observed and Predicted Maximum 1-hr Ozone Concentrations at  
 SCAB Stations Where  $[O_3] > 0.20$  ppm and Timing of Ozone  
 Maxima, 27 June 1974

Station	$[O_3]$ , ppm		Time of maximum	
	Observed	Predicted	Observed	Predicted
Anaheim	0.23	0.21	1600	1600
La Habra	0.31	0.27	1500	1500
Los Alamitos	0.24	0.22	1700	1600
Norco-Prado Park	0.24	0.21	1600	1600
Riverside-Rubidoux	0.30	0.24	1500	1500
Riverside-Magnolia Avenue	0.24	0.24	1500	1500
San Bernardino	0.32	0.23	1500	1500
Chino	0.27	0.25	1400	1400
Upland-Civic Center	0.51	0.41	1600	1500
Upland-ARB	0.46	0.41	1500	1500
Fontana	0.49	0.38	1300	1400
Azusa	0.35	0.29	1200	1200
Burbank	0.30	0.30	1400	1300
Pomona	0.35	0.32	1100	1200
Whittier	0.38	0.30	1300	1200
Pasadena	0.31	0.31	1200	1200

0.20 ppm and a comparison of the predicted and observed hour of the  $O_3$  maximum at the same stations. The tendency toward under-prediction of  $O_3$  concentrations at high  $O_3$  levels is summarized in Figure 11.19, in which the residual  $O_3$  (observed minus predicted) concentrations are shown as a function of observed  $O_3$  concentration for all monitoring stations over the two days. This tendency toward underprediction at high  $O_3$  levels was also exhibited by the Systems Applications, Inc. model in simulations of the same two day period (Seigneur et al., 1981). The predicted times of occurrence of the  $O_3$  maxima agree exactly or are at most hour hour removed from those observed. Because the phasing of predicted  $O_3$  concentrations depends on virtually all the physical and chemical processes involved, the close agreement between observed and predicted temporal behavior suggests that these processes are accurately portrayed relative to their temporal dynamics.

Figures 11.13-11.17 show what might be termed "point comparisons." The observed values represent one-hour average concentrations measured at a fixed monitoring site. The predictions, on the other hand, represent averages over a computational grid volume 5 km by 5 km on a side and typically 10 to 20 m high. If a particular monitoring site is dominated by a local source, concentration measurements may not be representative of the grid-cell average concentration. In so-called grid models of air pollution there are, therefore, two inherent problems in comparing observed and predicted concentrations. On one hand, due to computational costs, there is effectively a minimum grid cell size that may be employed for a certain region. (There also exist

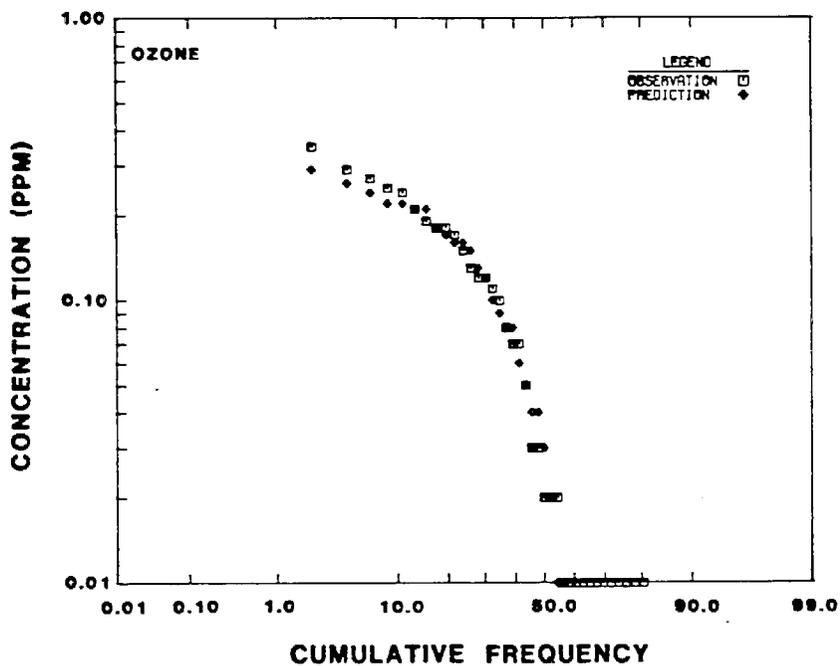
inherent limitations on the spatial and temporal resolution of the atmospheric diffusion equation (Lamb and Seinfeld, 1973).) On the other hand, the spatial representativeness of the measurements at a monitoring site is limited and may be influenced by local sources and flow patterns. An indication of the effects of subgrid scale concentration fluctuations can be seen in Figures 11.16 and 11.17.

#### 11.15 Frequency Distributions

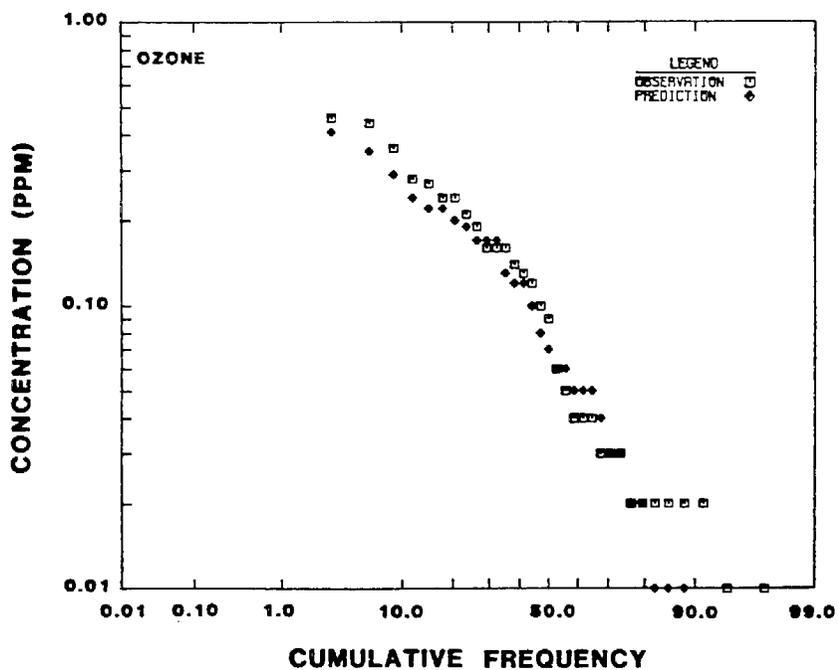
Figures 11.22a and 11.22b show the observed and predicted frequency distributions of hourly-averaged  $O_3$  concentrations at Azusa and Upland-ARB, respectively. Aside from the tendency toward under-prediction at the highest concentrations, the agreement is good at both stations. (Similar results, not shown, were obtained at other monitoring sites.)

#### 11.16 Observation Accuracy

Although we have indicated all observed concentrations by data points, suggesting exact values, the observed data have an associated level of accuracy that should be indicated by error bounds on each data point. Using the reported accuracy of the measuring instruments employed in 1974 as a function of concentration level (Higuchi et al., 1976; Higuchi, 1981), we replotted the observed and predicted  $O_3$  concentration at Pasadena including the  $\pm 2\sigma$  estimated error bounds on the data. These results, shown in Figure 11.23, again indicate that the model satisfactorily reproduces the ambient concentration dynamics. The model performance as indicated by the magnitude of the



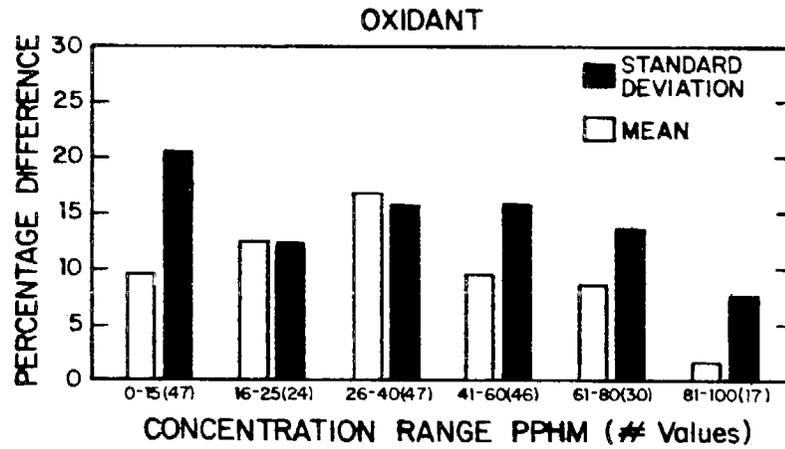
(a)



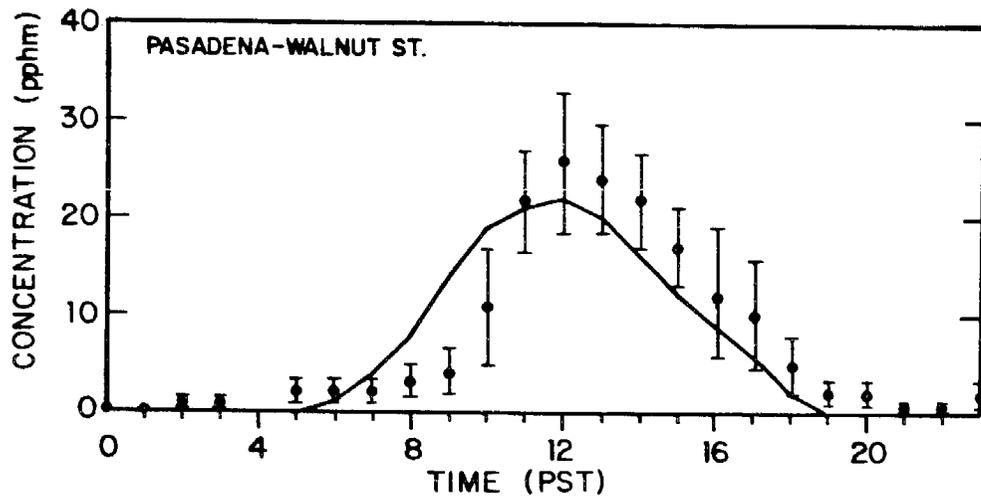
(b)

FIGURE 11.22

Frequency Distributions of Predicted and Observed Concentrations at (a) Azusa and (b) Upland



(a)



(b)

FIGURE 11.23

(a) Histogram of the Difference Between the Calibration Standards and Observed Concentrations for Oxidant Monitoring Instruments During the Period 1968-1975 (Source: Higuchi, 1981; Higuchi et al., 1976)

(b) Ozone Predictions at Pasadena Together with the  $\pm 2\sigma$  Calibration Error Bounds on the Measured Air Quality. (26 June, 1974).

concentration residuals compares quite well with the errors associated with the measurements.

#### 11.17 Conclusions

The major contribution of this research project has been the development of a mathematical model that can be used to describe urban-scale photochemical air pollution. Based on the species continuity equation the model incorporates the combined influences of advective transport, turbulent diffusion, chemical reaction, source emissions and surface removal processes. Satisfactory performance of the model has been demonstrated by comparing predicted and observed air quality over the South Coast Air Basin for the two-day period 26-27 June 1974. The calculated spatial and temporal trends of nitrogen dioxide ( $\text{NO}_2$ ) and ozone ( $\text{O}_3$ ) agree quite closely with routine monitoring measurements. These results and other tests indicate that the model can accurately reproduce the important features of photochemical air pollution over a major metropolitan region. While much of the testing has been performed using data available in the South Coast Air Basin, there is no reason why the model cannot be applied to evaluate air quality impacts of control strategies in other locations.

CHAPTER 12  
DIRECTION FOR FUTURE RESEARCH

12.1 Introduction

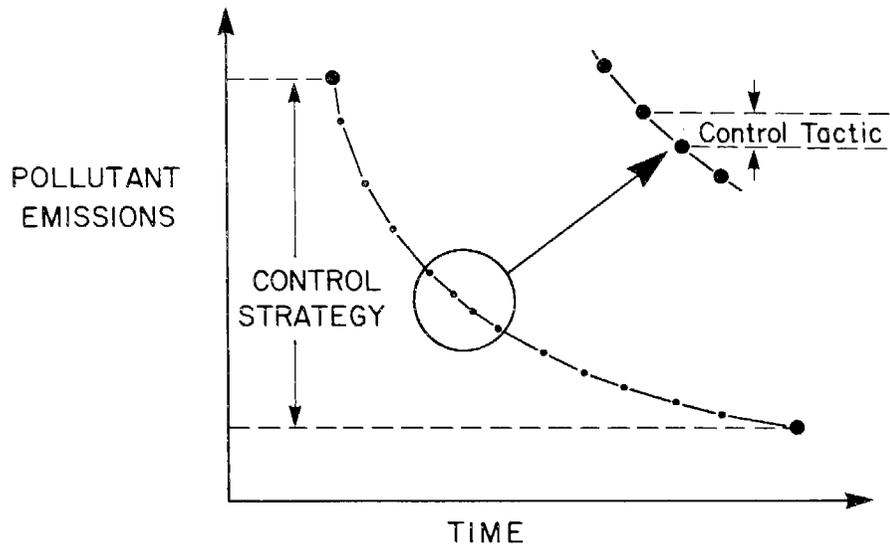
Inevitably in the course of any research project, topics for future investigation become apparent. The areas identified during this project can be broadly classified into three categories: applications of the modeling methodology, further basic research and additional experimental measurements. This chapter presents a discussion of each of these topics and develops some specific recommendations for further work. Even though there is some scope for additional study this should not be interpreted as a case for forestalling applications of the present modeling system. The verification results for both the individual components as well as the system as a whole indicate that the models can satisfactorily predict the ambient concentration dynamics.

12.2 Model Applications

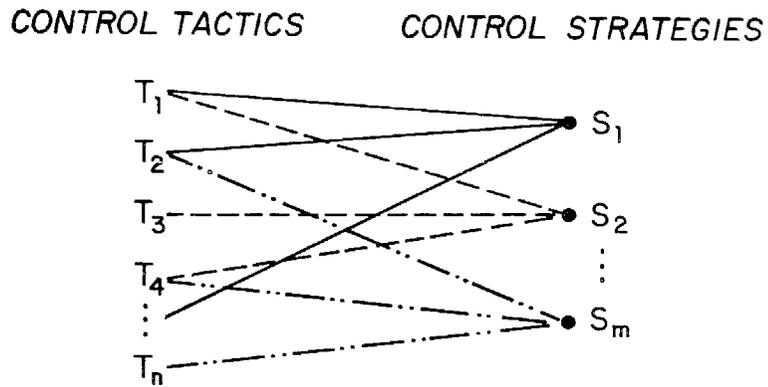
A major focus of this work has been the development of mathematical models that can predict the air quality impacts of changes in source emissions. Given this capability perhaps the most important question to be addressed is: how can this analysis methodology be best utilized in the design of control strategies that will achieve desired air quality objectives in a cost effective and equitable manner? There are three aspects of this question that need to be considered: the

control strategy design, its economic optimization and the relationship of the model predictions to the air quality standards.

Since the basic goal of most control programs is to achieve emissions reductions from many different sources it is important to distinguish between tactics applied to particular sources and the overall emission reduction strategy. An individual tactic  $T_i$ , is a control measure directed at a particular source or source class with the intent of reducing the amount, location or timing of emissions. Some typical control tactics might be the use of low excess air during combustion to reduce emissions of nitrogen oxides, vapor recovery during the handling of liquid hydrocarbons or catalytic reduction of vehicle exhaust gases. A control strategy  $S_j$ , on the other hand represents a composite set of tactics that, when applied to the region as a whole, produces a large reduction in emissions from many source classes. The distinction between these two aspects is illustrated in Figure 12.1 where it can easily be seen that a particular control strategy is composed of many individual tactics, each of which, are responsible for a small reduction in emissions. At present the most common utilization of air quality models is to simply test the air quality impact of different strategies. One area of research that has the potential for substantially reducing the cost of air pollution control is to identify solutions that are both feasible and optimal.



(a)



(b)

FIGURE 12.1

- (a) Emission Control Strategy Composed of Particular Tactics
- (b) Control Strategy Definition in Terms of Individual Tactics

The control strategy design problem can be compactly formulated as a mathematical programming problem

$$\text{select } \underline{S}(\underline{T}) \quad (12.1)$$

$$\text{that minimizes } \underline{C}[\underline{S}(\underline{T})] \quad (12.2)$$

$$\text{subject to } \underline{Q} [\underline{E}(\underline{x},t), \underline{r}(\underline{x},t), M(\underline{x},t), P] \leq \underline{Q}^s \quad (12.3)$$

This formulation is designed to select a control strategy  $\underline{S}$ , composed of tactics  $\underline{T} = (T_1, T_2, \dots)$ , that when applied to an emission pattern  $\underline{E}(\underline{x},t)$  minimizes the objective function  $\underline{C}$ , subject to air quality  $\underline{Q}$  at all receptor points  $\underline{r}(\underline{x},t)$  within the airshed domain remaining below the desired air quality goal  $\underline{Q}^s$ . In most applications the objective function  $\underline{C}$ , represents the total cost of control, however there is no reason why a number of different objectives cannot be addressed simultaneously. Both  $\underline{E} = (E_1, E_2, \dots, E_m)$  and  $\underline{Q} = (Q_1, Q_2, \dots, Q_p)$  have been defined as vector quantities to encompass cases where there are  $m$  emission species and  $p$  different pollutants. The problem is complicated by the fact that the air quality outcome  $\underline{Q}$  is a function not only of emissions but also of the meteorology  $M$ , and chemical reaction parameters,  $P$ . Other constraints, such as availability of clean fuels or technological limitations of different control techniques may also be incorporated into the formulation.

When there is a linear relation between emissions and air quality the system (12.1-12.3) can usually be stated as a set of linear equations and solved using standard linear or integer programming

techniques. Most of the applicable mathematical programming approaches are summarized in Franklin (1980), Shapiro (1979) and Wismer and Chattergy (1978). The inherently non-linear nature of oxidant formation does complicate the solution of the optimization problem. In fact most of the reported applications of photochemical models have been restricted to simply testing different emission patterns. Some procedures for estimating overall control requirements for oxidant abatement have been demonstrated using smog chamber data (Dimitriadis, 1977), aerometric data analysis (Trijonis, 1974; Bilger, 1978; Post, 1979) and mathematical box models that incorporate an explicit photochemical mechanism (Whitten and Hogo, 1978; Derwent and Hov, 1980). The Trijonis study and its extension by Kyan and Seinfeld (1974) provide the only economically optimized control strategy design procedures for photochemical smog demonstrated to date. Dynamic optimization techniques that minimize the cost of attaining emission control objectives over time also have been explored. Seinfeld and Kyan (1972) and Kyan and Seinfeld (1974) have addressed the problem of attaining and maintaining compliance with air quality standards over periods of successive years. The latter study employed dynamic programming together with the empirical photochemical air quality model of Trijonis (1974). A more detailed review of these studies is presented in Cass and McRae (1981). At present there are no studies that combine the use of both advanced air quality models and economic optimization.

While air quality models are an integral element of the control strategy design process there are other aspects that must be considered. Figure 12.2 presents in a highly simplified manner the steps that need to be undertaken if an economically optimized set of emission controls are to be identified. From an inspection of this diagram it is clear that many different types of data are required. What is not apparent, and frequently ignored in practice, is that the air quality model serves as a focus for much of the data used in control strategy analyses. From a practical point of view there is a critical need for developing formal procedures and quality control checks that can be used to collate the needed information at a consistent level of detail. For example, simply assembling emissions data without giving any consideration to the economics of the associated control technologies virtually precludes identifying least cost strategies.

Most of the above discussion has focused on the use of models to design control strategies that will achieve particular air quality goals. Currently the planning efforts of regulatory agencies are directed at satisfying statutory requirements mandated by the Clean Air Act. Most air quality standards are stated in the form of a particular air quality levels that are not to be exceeded, on an hourly basis, more than once per year. At present the resources required to use photochemical models are such that it is not feasible to model every day of the year. A critical area for future research is to determine if the current worst day design philosophy leads to strategies that will meet air quality objectives on all other days.

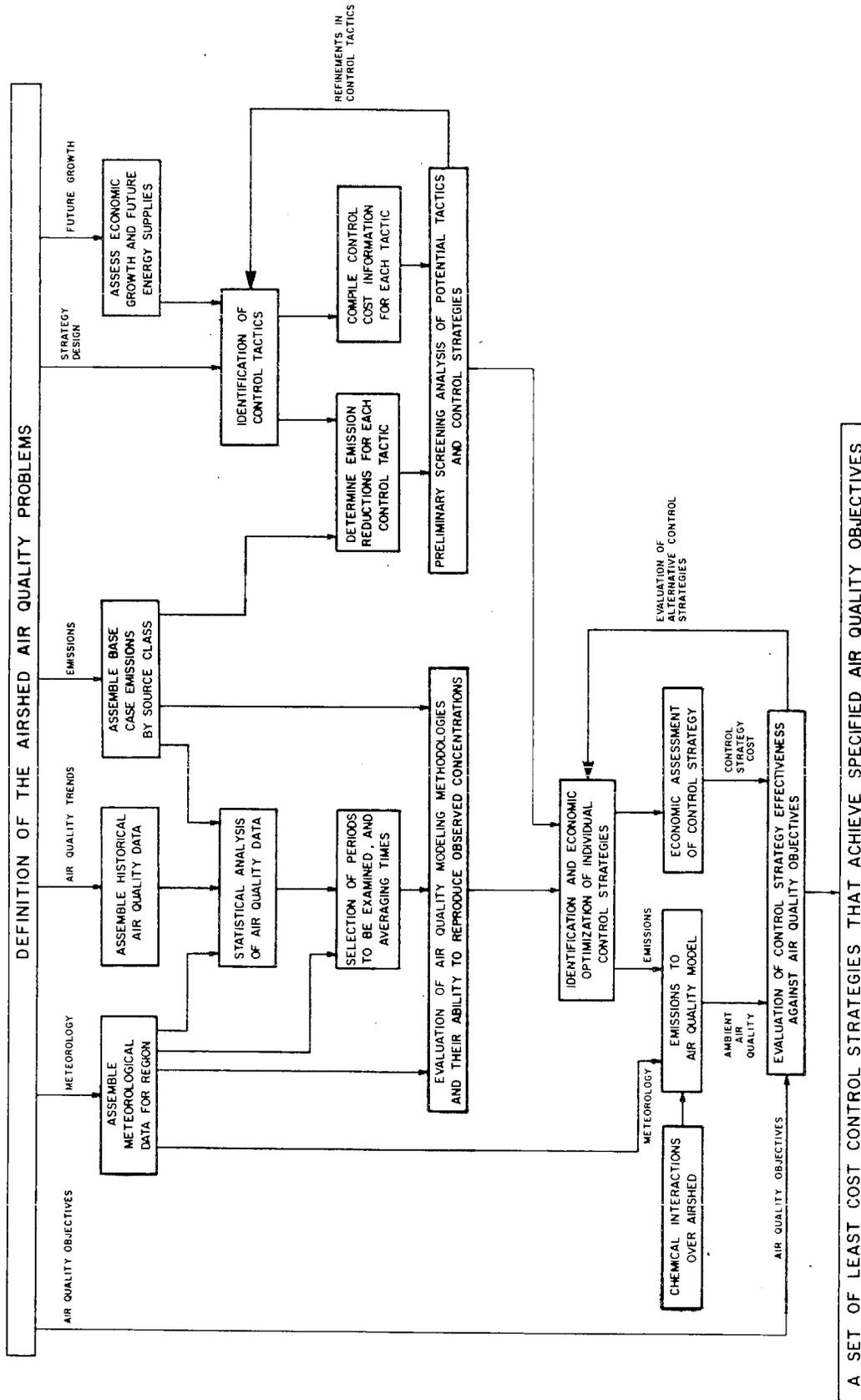


FIGURE 12.2

Detailed Elements of an Integrated Approach to Least Cost Control Strategy Design

### 12.3 Basic Research

During the course of this study many different research topics were identified. Since most of the potential refinements to the present modeling system have been discussed in previous chapters they will not be repeated here. (A summary of some of the more important issues is contained in Table 12.1.) Most of the current control programs are directed at reducing the concentration of those gas phase species for which there are ambient air quality standards. Two additional topics that offer considerable scope for future research are the incorporation of particulate formation processes into the model and a study of currently unregulated pollutants. Technically the most challenging is the implementation of the aerosol mechanics. The capability to predict the formation and growth of fine particulates will be an integral element of any strategy directed at improving the visibility in urban areas.

In addition to the species of regulatory interest the airshed model also predicts the concentration of many other pollutants that have known or anticipated effects on health and welfare. For example, gas phase nitric acid can react with ammonia to form particulate ammonium nitrate that in turn can have a major influence on visibility degradation. One area that deserves special attention is the feasibility of preferentially abating some of these pollutants as part of ongoing oxidant and particulate control programs.

TABLE 12.1

Summary of Areas and Questions for Additional Research

---

<u>Turbulence</u>	Chapters 2,4,5,7
Entrainment Process at Inversion Base	
Diffusive Transport Under Stable Conditions	
Cost Effective Closure Models	
<u>Objective Analysis Procedures</u>	3
Wind Field Generation in Remote Areas	
Applications of Remote Sensing	
A priori Generation of Mixing Heights	
<u>Surface Removal Processes</u>	6
Characterization of Deposition for Different Stabilities	
Surface Affinity Characterization	
<u>Point Source Treatment</u>	7
Dispersion Coefficients	
Procedures for Imbedding Plumes in Grid Model	
Plume Rise Calculations in Arbitrarily Stratified Environments	
<u>Chemistry</u>	8
More Detailed Lumping Mechanism for Aromatics	
Temperature Effects on Ozone Formation	
Reactions Involving Natural Hydrocarbon Emissions	
<u>Numerical Analysis</u>	9,10,11
Application of Higher Derivative Methods for Chemistry	
Formulation of Filtering Schemes into Advection Algorithms	
Theoretical Treatment of Boundary Conditions	

---

#### 12.4 Field and Experimental Measurements

In many areas further model development is hampered more by the paucity of measurements than by the understanding of the basic physics and chemistry. Data deficiencies occur in three areas: field measurements needed to verify a chemically resolved model, source test information required for construction of emissions inventories, and experimental determination of basic chemical data. These requirements are detailed in Tables 12.2 - 12.3. While not strictly a part of a measurement program one aspect that is often ignored is a thorough assessment of the accuracy of the basic data. This consideration is particularly relevant to the emissions information. Unless the emissions data have been prepared at a level consistent with the desired accuracy of the model predictions there is little point in using air quality models. Consistency checks need to be applied to individual sources, source classes, the region as a whole and should include fuel usage patterns, operating conditions, pollutant ratios, exhaust composition and control efficiencies. One useful approach is to compare the results from top-down and bottom-up estimating procedures. These methods can provide bounds on the accuracy of emissions inventories. A formal methodology using weighted sensitivity analysis techniques is described in Ditto et al. (1976)

TABLE 12.2

SUMMARY OF METEOROLOGICAL MEASUREMENTS NEEDED FOR MODEL EVALUATION

---

Wind Measurements

Vertical Shear Distributions  
Flow Patterns Close to Mountains (Upslope Flows)  
Magnitudes of Nocturnal Drainage Flows  
Quantitative Evaluation of Monitoring Site Exposure  
Characterization of the Effects of Surface Roughness

Mixing Height Distribution

Increased Spatial and Temporal Resolution of Mixing Height  
Effect Mixing Height Distributions Close to Mountains

Solar Radiation

Detailed Spatial and Temporal Measurements of uv Flux

---

TABLE 12.3

## SUMMARY OF NEEDED CHEMICAL MEASUREMENTS

---

Concentration Measurements - General Aspects

Quantitative Evaluation of Interference Effects  
Detailed Characterization of Monitoring Site Exposure  
Establishment of Bounds on Measurements due to Errors and Averaging  
Improved Resolution of Vertical Concentration Distributions  
Routine Measurements of Certain Non Criteria Pollutants

Hydrocarbon Measurements

Spatial and Temporal Variations of Hydrocarbon Reactivities  
Characterization of Aldehydes and Natural Hydrocarbons  
Need for Increased Species Resolution Beyond THC-RHC-CH<sub>4</sub>

Background Air Quality

Values Away From Urban Region  
Vertical Profiles of Ozone  
Hydrocarbon Concentration and Composition  
Concentration of NO, NO<sub>2</sub> and O<sub>3</sub>

Source Profiles and Emission Factors

Detailed Emissions Distributions From Mobile Sources  
Chemical Composition and Solvent Utilization by Industries  
Extent and Magnitude of Emissions from Gasoline Evaporation  
Industrial Fuel Usage Patterns  
Improved Characterization of Emissions from Area Sources

---

## 12.5 Conclusions

In this chapter many suggestions have been made for future refinements and the need for additional experimental measurements. Given the present state of model development, perhaps the greatest need is not for basic research, but rather for the application of these new tools to the design of cost-effective and equitable control strategies.

## CHAPTER 13

## SUMMARY AND CONCLUSIONS

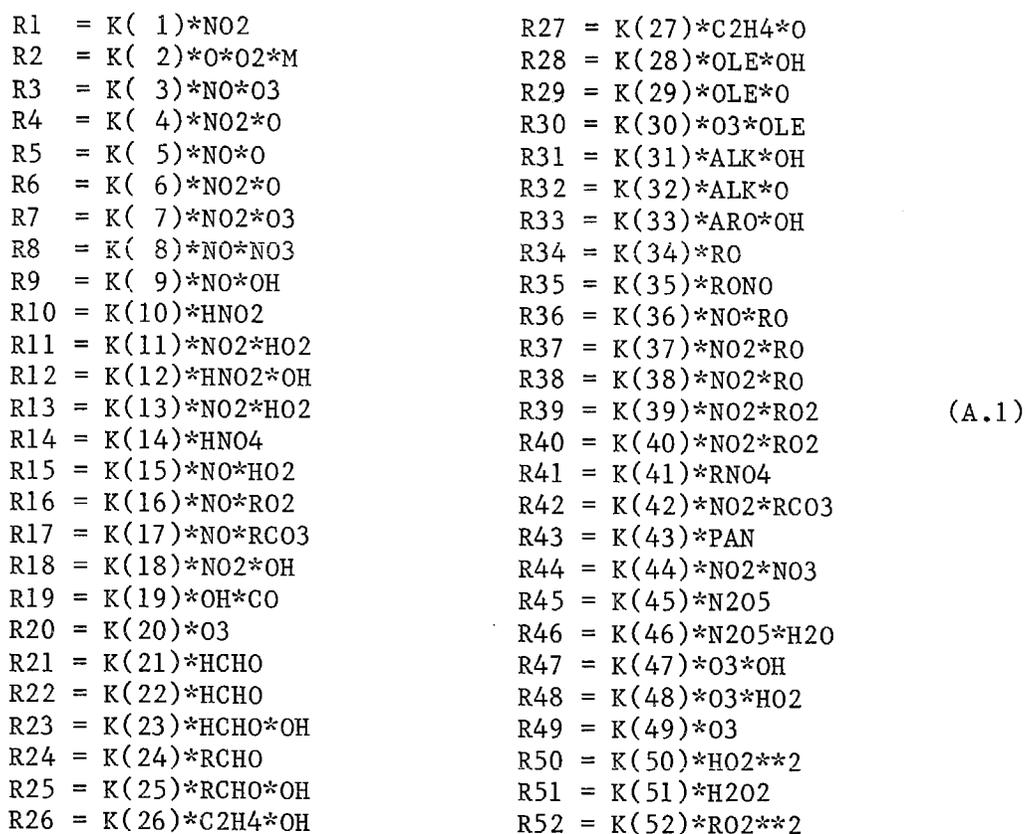
The major contribution of this work has been the formulation and computational implementation of a mathematical description of urban scale photochemical air pollution. Based on the species continuity equation, the modeling system incorporates the combined influences of advective transport, turbulent diffusion, chemical reactions, source emissions and surface removal processes. Given the potential for widespread utilization of these models careful attention has been given to delineating the assumptions underlying the valid applications of: three-dimensional, Lagrangian trajectory, vertically integrated and single cell air quality models.

While the mathematical formulation of the modeling system contains no regional or area specific information performance, evaluation studies were carried out using data measured in the South Coast Air Basin of Southern California. Detailed emissions and meteorological information were assembled for the period 26-28 June 1974. A comparison between calculated and observed air quality indicates that the models can satisfactorily describe urban scale atmospheric concentration dynamics. The results of these and other tests indicate that the models are now in a form that they can be used to predict the air quality impacts of alternative control measures.

## APPENDIX A

## KINETIC RATE EQUATIONS AND STEADY STATE APPROXIMATIONS

This appendix documents the differential and algebraic forms of the equations used to describe the kinetics of the chemical mechanism presented in Chapter 8. The notation has been chosen to simplify the implementation of the computational solution procedures. The forward reaction rates  $r_i$ ;  $i=1,2,\dots,m$  for the interactions between the  $c_i$ ;  $i=1,\dots,p$  species shown in Table 8.1 - 8.2 are given by



where  $K(i)$ ;  $i=1,\dots,m$  are the reaction rate constants.

Using the procedures presented in Chapter 11 it is possible to partition the concentration vector  $\underline{c}$  into two components ( $c_d|c_s$ ) where the species  $c_d$  are described by differential forms and  $c_s$  by algebraic equations. Given (A.1) the reaction set kinetics are of the form

$$\frac{d c_d}{dt} = F(c_d, c_s) \quad (\text{A.2})$$

The differential equations for the individual species are given by

$$F(\text{NO}) = +R1-R3+R4-R5-R8-R9+R10-R15-R16-R17+R35-R36 \quad (\text{A.3})$$

$$F(\text{NO}_2) = -R1+R3-R4+R5-R6-R7+2*R8-R11+R12-R13+R14+R15+R16 \\ +R17-R18-R37-R38-R39-R40+R41-R42+R43-R44+R45 \quad (\text{A.4})$$

$$F(\text{O}_3) = +R2-R3-R7-R20-R30-R47-R48-R49 \quad (\text{A.5})$$

$$F(\text{HCHO}) = -R21-R22-R23+A2*R30+B2*R34 \quad (\text{A.6})$$

$$F(\text{RCHO}) = -R24-R25+A1*R30+R33+A3*R34+R38+R40 \quad (\text{A.7})$$

$$F(\text{OLE}) = -R28-R29-R30 \quad (\text{A.8})$$

$$F(\text{ALK}) = -R31-R32 \quad (\text{A.9})$$

$$F(\text{ARO}) = -R33 \quad (\text{A.10})$$

$$F(\text{C}_2\text{H}_4) = -R26-R27 \quad (\text{A.11})$$

$$F(\text{CO}) = -R19+R21+R22+R23+R24 \quad (\text{A.12})$$

$$F(\text{H}_2\text{O}_2) = +R50-R51 \quad (\text{A.13})$$

$$F(\text{PAN}) = +R42-R43 \quad (\text{A.14})$$

$$F(\text{HNO}_2) = +R9-R10+R11-R12+R38 \quad (\text{A.15})$$

$$F(\text{RONO}) = -R35+R36 \quad (\text{A.16})$$

$$F(\text{RNO}_4) = +R39-R41 \quad (\text{A.17})$$

The coefficients A1-A6, B1-B3 are defined in Chapter 8.

Some species react sufficiently fast enough that their production and decay rates are approximately equal. Under these conditions it is possible to replace the differential equations by non-linear, implicit algebraic expressions of the general form

$$F(\underline{c}_d, \underline{c}_s) = 0 \quad (\text{A.18})$$

The equations which arise for each species are given by

$$F(O) = 0 = +R1 - R2 - R4 - R5 - R6 + R20 - R27 - R29 - R32 \quad (\text{A.19})$$

$$F(RO) = 0 = +R16 + A6 * R30 - R34 + R35 - R36 - R37 - R38 + 2 * R52 \quad (\text{A.20})$$

$$F(OH) = 0 = -R9 + R10 - R12 + R15 - R18 - R19 - R23 - R25 - R26 - R28 + A5 * R30 - R31 + R32 - R33 - R47 + R48 + 2 * R51 \quad (\text{A.21})$$

$$F(NO3) = 0 = +R6 + R7 - R8 - R44 + R45 \quad (\text{A.22})$$

$$F(RO2) = 0 = -R16 + R17 + R24 + R26 + R27 + R28 + R29 + A4 * R30 + R31 + R32 + R33 + (1 - B1) * M * R34 - R39 - R40 + R41 - 2 * R52 \quad (\text{A.23})$$

$$F(HO2) = 0 = -R11 - R13 + R14 - R15 + R19 + 2 * R21 + R23 + R24 + R27 + A3 * R30 + B1 * R34 + R47 - R48 - 2 * R50 \quad (\text{A.24})$$

$$F(RCO3) = 0 = -R17 + R25 + R29 - R42 + R43 \quad (\text{A.25})$$

$$F(N2O5) = 0 = +R44 - R45 - R46 \quad (\text{A.26})$$

$$F(HNO4) = 0 = +R13 - R14 \quad (\text{A.27})$$

From a computational point of view it is desirable to avoid situations which involve solutions of implicit non-linear systems. Under some conditions it is possible to replace (A.18) by the explicit form

$$\underline{c}_s = \underline{G}(\underline{c}_d) \quad (\text{A.28})$$

For the system (A.19 - A.27) a solution can be obtained from a series of successive eliminations.

Atomic oxygen can be determined directly from (A.19) as

$$0 = \frac{(K(1)*NO_2 + K(20)*O_3)}{(K(2)*O_2*M + K(4)*NO_2 + K(5)*NO + K(6)*NO_2 + K(27)*C_2H_4 + K(29)*OLE + K(32)*ALK} \quad (A.29)$$

NO<sub>3</sub> and N<sub>205</sub> can be found from a simultaneous solution of the system defined by (A.22) and (A.26) i.e.

$$Y_1(NO_3) + Y_2(N_{205}) = Y_3 \quad (A.30)$$

$$Y_4(NO_3) + Y_5(N_{205}) = 0 \quad (A.31)$$

where

$$Y_1 = -(K(8)*NO + K(44)*NO_2) \quad (A.32)$$

$$Y_2 = K(45) \quad (A.33)$$

$$Y_3 = -(K(6)*NO_2*O + K(7)*NO_2*O_3) \quad (A.34)$$

$$Y_4 = K(44)*NO_2 \quad (A.35)$$

$$Y_5 = -(K(45) + K(46)*H_2O) \quad (A.36)$$

Given these coefficients the solutions for NO<sub>3</sub> and N<sub>205</sub> are

$$NO_3 = \frac{Y_3*Y_5}{(Y_1*Y_5 - Y_2*Y_4)} \quad (A.37)$$

$$N_{205} = \frac{-Y_4*NO_3}{Y_5} \quad (A.38)$$

For the other species the algebraic expressions can be written as

$$0 = X_1 + X_2(OH) + X_3(RCO_3) \quad (A.39)$$

$$0 = X_4 + [X_5 + X_6(RO_2)](RO_2) + X_7(RO) \quad (A.40)$$

$$0 = X_8 + X_9(OH) + X_{10}(RO) + [X_{11} + X_{12}(HO_2)](HO_2) \quad (A.41)$$

$$0 = X_{13} + X_{14}(HO_2) + X_{15}(OH) \quad (A.42)$$

$$0 = X_{16} + X_{17}(RCO_3) + X_{18}(OH) + [X_{19} + X_{20}(RO_2)](RO_2) + X_{21}(RO) \quad (A.43)$$

The coefficients X1 - X21 in (A.39 - A.41) are given by

RCO3

$$X1 = K(29)*OLE*O+K(43)*PAN \quad (A.44)$$

$$X2 = K(25)*RCHO \quad (A.45)$$

$$X3 = -(K(17)*NO+K(42)*NO2) \quad (A.46)$$

RO

$$X4 = A6*K(30)*O3*OLE+K(35)*RONO \quad (A.47)$$

$$X5 = K(16)*NO \quad (A.48)$$

$$X6 = 2*K(52) \quad (A.49)$$

$$X7 = -(K(34)+K(36)*NO+K(37)*NO2+K(38)*NO2) \quad (A.50)$$

HO2

$$X8 = 2*K(21)*HCHO+K(24)*RCHO+K(27)*C2H4*O+ \\ A3*K(30)*O3*OLE \quad (A.51)$$

$$X9 = K(19)*CO+K(23)*HCHO+K(47)*O3 \quad (A.52)$$

$$X10 = B1*K(34) \quad (A.53)$$

$$X11 = -(K(11)*NO2+K(13)*NO2+K(15)*NO+K(48)*O3) + K(13)*NO2 \quad (A.54)$$

$$X12 = -2.0*K(50) \quad (A.55)$$

OH

$$X13 = K(10)*HNO2+A5*K(30)*O3*OLE+K(32)*ALK*O+2*K(51)*H2O2 \quad (A.56)$$

$$X14 = K(15)*NO+K(48)*O3 \quad (A.57)$$

$$X15 = -(K(9)*NO+K(12)*HNO2+K(18)*NO2+K(19)*CO+ \\ K(23)*HCHO+K(25)*RCHO+K(26)*C2H4+K(28)*OLE+ \\ K(31)*ALK+K(33)*ARO+K(47)*O3) \quad (A.58)$$

RO2

$$X16 = K(24)*RCHO+K(27)*C2H4*O+K(29)*OLE*O+ \\ A4*K(30)*O3*OLE+K(32)*ALK*O+K(41)*RNO4 \quad (A.59)$$

$$X17 = K(17)*NO \quad (A.60)$$

$$X18 = K(26)*C2H4+K(28)*OLE+K(31)*ALK+K(33)*ARO \quad (A.61)$$

$$X19 = -(K(16)*NO+K(39)*NO2+K(40)*NO2) \quad (A.62)$$

$$X20 = -2.0*K(52) \quad (A.63)$$

$$X21 = (1-B1)*M*K(34) \quad (A.64)$$

After considerable algebraic manipulation it is possible to develop a quadratic expression for H02 of the form

$$D1*H02**2 + D2*H02 + D3 = 0 \quad (A.65)$$

where the coefficients D1-D3 are given by

$$D3 = X8+GG*X10-X9*X13/X15 \quad (A.66)$$

$$D2 = X11+EE*X10*X14/X15-X9*X14/X15 \quad (A.67)$$

$$D1 = X12 \quad (A.68)$$

and the intermediate terms by

$$DD = 1.0/(X7*X19-X5*X21) \quad (A.69)$$

$$FF = DD*(X5*X16-X4*X19-X1*X5*X17/X3) \quad (A.70)$$

$$EE = DD*(X2*X5*X17/X3-X5*X18) \quad (A.71)$$

$$GG = FF + EE*X13/X15 \quad (A.72)$$

The solution of the quadratic is given by

$$H02 = (-D2-SQRT(D2*D2-4*D1*D3))/(2*D1) \quad (A.73)$$

Once H02 is available then the other steady state species are given by

$$OH = -(X13+X14*H02)/X15 \quad (A.74)$$

$$RCO3 = -(X1+X2*OH)/X3 \quad (A.75)$$

$$RO = -(X8+X9*OH+(X11+X12*H02)*H02)/X10 \quad (A.76)$$

$$R02 = -(X4+X7*R0)/X5 \quad (A.77)$$

$$\text{HNO}_4 = K(13) \cdot \text{NO}_2 \cdot \text{H}_2\text{O} / K(14) \quad (\text{A.78})$$

In some case there may be no  $\text{NO}_x$  present in the system, when this occurs the following reduced set of steady state expressions can be applied

$$\text{OH} = -X_{13}/X_{15} \quad (\text{A.79})$$

$$\text{RO}_2 = \text{SQRT}(-(X_{16} + X_{18} \cdot \text{OH})/X_{20}) \quad (\text{A.80})$$

$$\text{RO} = -(X_4 + X_6 \cdot \text{RO}_2 \cdot \text{RO}_2)/X_7 \quad (\text{A.81})$$

$$\text{H}_2\text{O} = \text{SQRT}(-(X_8 + X_9 \cdot \text{OH} + X_{10} \cdot \text{RO})/X_{12}) \quad (\text{A.82})$$

$$\text{NO}_3 = \text{N}_{205} = \text{RCO}_3 = \text{HNO}_4 = 0 \quad (\text{A.83})$$

Considerable care must be exercised during the computational implementation of the above expressions because various terms involve small differences between large quantities. The remaining species  $\{\text{O}_2, \text{H}_2\text{O}, \text{M}\}$  are treated as being constant during a time step and are supplied externally.

## APPENDIX B

A LINEAR FINITE ELEMENT SOLUTION OF THE  
CONSERVATIVE FORM OF THE ADVECTION EQUATIONB.1 Introduction

Finite element methods, as a class, are an increasingly popular approach for numerical solution of fluid flow problems. They are particularly attractive because of their high accuracy and, more importantly, the ease with which boundary conditions can be handled. This appendix is devoted to a detailed derivation of the finite element algorithm employed in Chapter 10 where, as part of the splitting sequence, it was necessary to solve the first order hyperbolic problem (B.1).

$$\frac{\partial u}{\partial t} + Lu = 0 \quad (\text{B.1})$$

Specifically in atmospheric flows (B.1) is associated with the scalar advection equation which is given by

$$\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} = 0 \quad (\text{B.2})$$

In (B.2)  $c(x,t)$  is the non-negative concentration field and  $u(x,t)$  the advective velocity. This appendix extends the recent work of Pepper et al. (1979) which presents a finite element model for the more restrictive nonconservative form of (B.2).

## B.2 Galerkin Formulation

A common approach to solve the hyperbolic problem (B.1) is to form the Galerkin equation using finite elements in space (Strang and Fix, 1973; Finlayson, 1972). With this technique approximations to the concentration and velocity fields  $C(x,t)$ ,  $U(x,t)$  are expressed in terms of time varying coefficients  $\alpha_i(t)$ ,  $\beta_j(t)$  and piecewise continuous basis function  $\phi_i(x)$ , i.e.

$$c(x,t) \approx C(x,t) = \sum_{i=1}^n \alpha_i(t) \phi_i(x) \quad (\text{B.3})$$

$$u(x,t) \approx U(x,t) = \sum_{i=1}^n \beta_i(t) \phi_i(x) \quad (\text{B.4})$$

where

$$\phi_i(x) = \begin{cases} \frac{x-x_{i-1}}{x_i-x_{i-1}} & ; \quad x_{i-1} \leq x \leq x_i \\ \frac{x_{i+1}-x}{x_{i+1}-x_i} & ; \quad x_i \leq x \leq x_{i+1} \\ 0 & ; \quad x < x_{i-1} \text{ or } x > x_{i+1} \end{cases} \quad (\text{B.5})$$

Equation (B.5) describes a set of linear basis function which are sometimes called Chapeau functions because of their similarity to hatlike shapes. The form of these functions is illustrated in Figure B.1. Other basis functions which vanish outside the interval  $[x_{i-1}, x_{i+1}]$  are described in Strang and Fix (1973), Connor and Brebbia (1977).

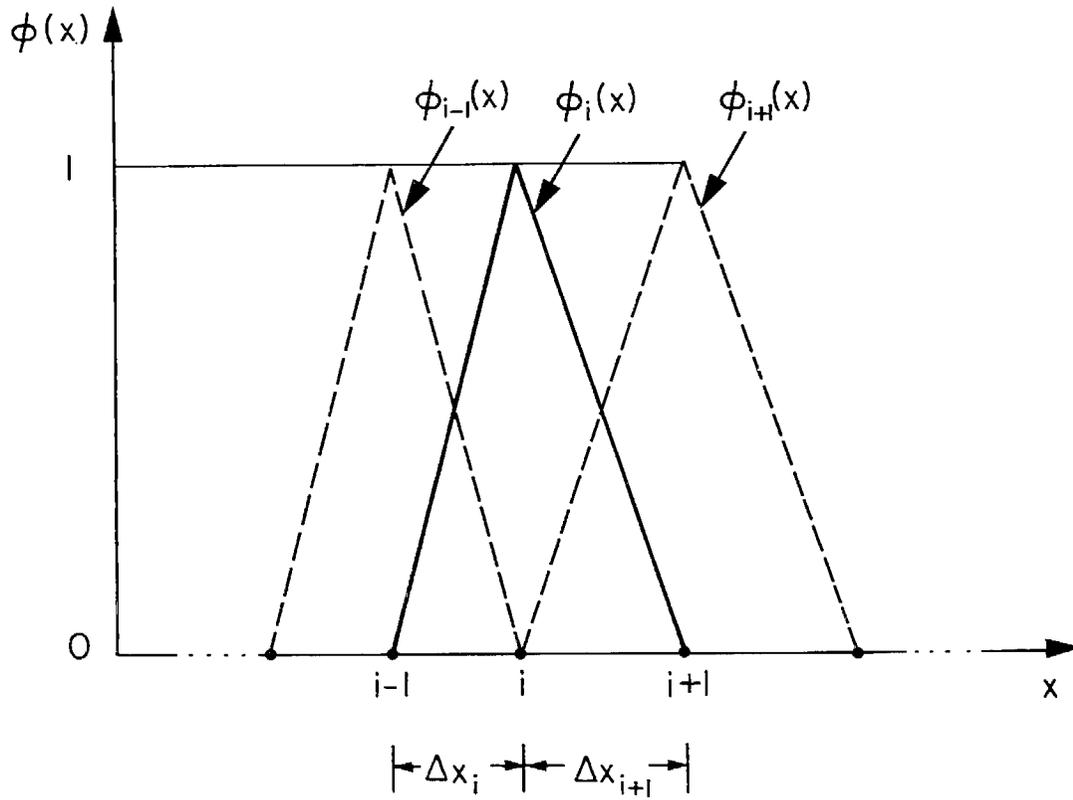


Figure B.1  
Linear Basis Functions for Galerkin  
Finite Element Model

Using the functions described by (B.3) and (B.4) the Galerkin method requires that for all  $\phi_i$

$$\langle \phi_i, \left\{ \frac{\partial \alpha_j \phi_j}{\partial t} + \frac{\partial}{\partial x} (\beta_k \phi_k \alpha_j \phi_j) \right\} \rangle = 0 \quad (\text{B.6})$$

Galerkin's method is a particular weighted residual scheme in which the weighting functions are the same as the trial functions (Finlayson, 1972). By expanding the inner product (B.6) the following set of ordinary differential equations in the dependent variable  $\alpha_j(t)$  can be derived

$$M_{ij} \frac{d \alpha_j(t)}{dt} + \beta_k(t) N_{ijk} \alpha_j(t) = 0 \quad (\text{B.7})$$

where

$$M_{ij} = \int \phi_i(x) \phi_j(x) dx \quad (\text{B.8})$$

$$N_{ijk} = \int \left[ \phi_i(x) \phi_j(x) \frac{\partial \phi_k(x)}{\partial x} + \phi_i(x) \phi_k(x) \frac{\partial \phi_j(x)}{\partial x} \right] dx \quad (\text{B.9})$$

Since  $\phi_i(x)$  vanishes outside the interval  $[x_{i-1}, x_{i+1}]$  there will be three integrals associated with  $M_{ij}$  and nine with  $N_{ijk}$  for a typical set of points  $i-1, i$  and  $i+1$ , i.e.

$$\begin{array}{lll}
M_{i,i-1} & M_{i,i} & M_{i,i+1} \\
N_{i,i-1,i-1} & N_{i,i-1,i} & N_{i,i-1,i+1} \\
N_{i,i,i-1} & N_{i,i,i} & N_{i,i,i+1} \\
N_{i,i+1,i-1} & N_{i,i+1} & N_{i,i+1,i+1}
\end{array}$$

The integrations are quite straightforward and to illustrate the process consider some typical terms, for example  $M_{i,i+1}$

$$M_{i,i+1} = \int_{x_{i-1}}^{x_{i+1}} \phi_i(x) \phi_{i+1}(x) dx \quad (\text{B.10})$$

$$= \int_{x_{i-1}}^{x_i} \phi_i \phi_{i+1} dx + \int_{x_i}^{x_{i+1}} \phi_i \phi_{i+1} dx \quad (\text{B.11})$$

Since  $\phi_{i+1}(x) = 0$  for  $x < x_i$  (B.11) can be written in the form

$$M_{i,i+1} = \int_{x_i}^{x_{i+1}} \left[ \frac{x-x_i}{x_{i+1}-x_i} \right] \left[ \frac{x_{i+1}-x}{x_{i+1}-x_i} \right] dx = \frac{x_{i+1} - x_i}{6} \quad (\text{B.12})$$

Similarly  $N_{i,i,i}$  is given by

$$N_{i,i,i} = \int_{x_{i-1}}^{x_{i+1}} 2\phi_i^2(x) \frac{\partial \phi_i(x)}{\partial x} dx = 0 \quad (\text{B.13})$$

After all the terms have been evaluated the governing set of ordinary differential equations is given by

$$\begin{aligned} \frac{d}{dt} \left[ (x_{i+1} - x_i) \alpha_{i+1} + 2(x_{i+1} - x_{i-1}) \alpha_i + (x_i - x_{i-1}) \alpha_{i-1} \right] \\ + (2\beta_{i+1} + \beta_i) \alpha_{i+1} + (\beta_{i+1} - \beta_{i-1}) \alpha_i - (2\beta_{i-1} + \beta_i) \alpha_{i-1} = 0 \quad (\text{B.14}) \end{aligned}$$

Various simplifications are possible; consider for example the case of constant grid spacing in which  $\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$ . For this situation (B.14) reduces to

$$\begin{aligned} \frac{d}{dt} \left[ \alpha_{i+1} + 4\alpha_i + \alpha_{i-1} \right] + \frac{1}{\Delta x} \left[ (2\beta_{i+1} + \beta_i) \alpha_{i+1} + (\beta_{i+1} - \beta_{i-1}) \alpha_i \right. \\ \left. - (2\beta_{i-1} + \beta_i) \alpha_{i-1} \right] = 0 \quad (\text{B.15}) \end{aligned}$$

If the velocity  $u(x,t)$  is uniform, then (B.15) simplifies still further to

$$\frac{d}{dt} \left[ \alpha_{i+1} + 4\alpha_i + \alpha_{i-1} \right] + \frac{3u}{\Delta x} \left[ \alpha_{i+1} - \alpha_{i-1} \right] = 0 \quad (\text{B.16})$$

Time integration of the difference - differential equations can be accomplished by standard methods. For example, the classic Crank-Nicholson  $O(\Delta t^2)$  scheme when applied to (B.15) gives

$$\begin{aligned} \frac{1}{\Delta t} \left[ (\alpha_{i+1}^{k+1} - \alpha_{i+1}^k) + 4(\alpha_i^{k+1} - \alpha_i^k) + (\alpha_{i-1}^{k+1} - \alpha_{i-1}^k) \right] = \\ \frac{1}{2\Delta x} \left[ (\beta_i + 2\beta_{i+1}) (\alpha_{i+1}^{k+1} + \alpha_{i+1}^k) + (\beta_{i+1} - \beta_{i-1}) (\alpha_i^{k+1} + \alpha_i^k) - (\beta_i + 2\beta_{i-1}) \right. \\ \left. (\alpha_{i-1}^{k+1} + \alpha_{i-1}^k) \right] \quad (\text{B.17}) \end{aligned}$$

This system of tridiagonal equations can be readily solved using the Thomas algorithm (Roache, 1976). A discussion of the stability and convergence of the finite element approximation is contained in Chapter 10 and for this reason will not be repeated here.

## APPENDIX C

GRAPHICAL DISPLAY OF OBSERVED AND PREDICTED AIR QUALITY  
FOR THE TWO-DAY PERIOD 26-27 JUNE 1974

This appendix presents the calculated and observed levels of ozone ( $O_3$ ) and nitrogen dioxide ( $NO_2$ ) at monitoring sites within the South Coast Air Basin. The spatial distribution of measurement stations is shown in Figure C.1. Within the computational region defined by Figure C.2 each station can be located by using the coordinates presented in Table C.1. The station names, codes and locations correspond to those used by local air pollution agencies in June 1974.

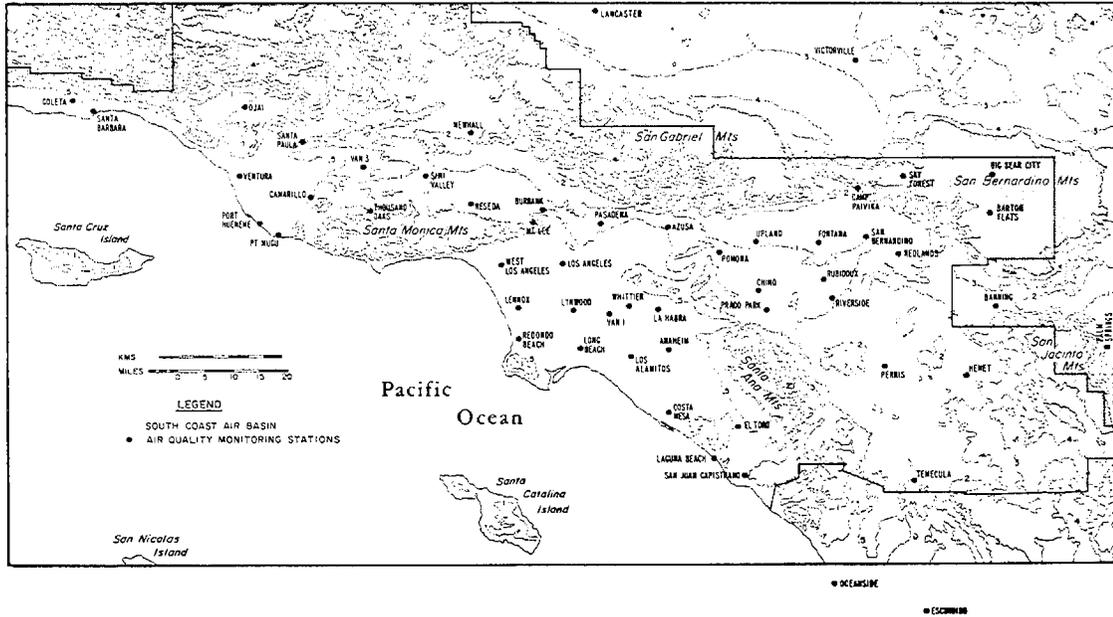
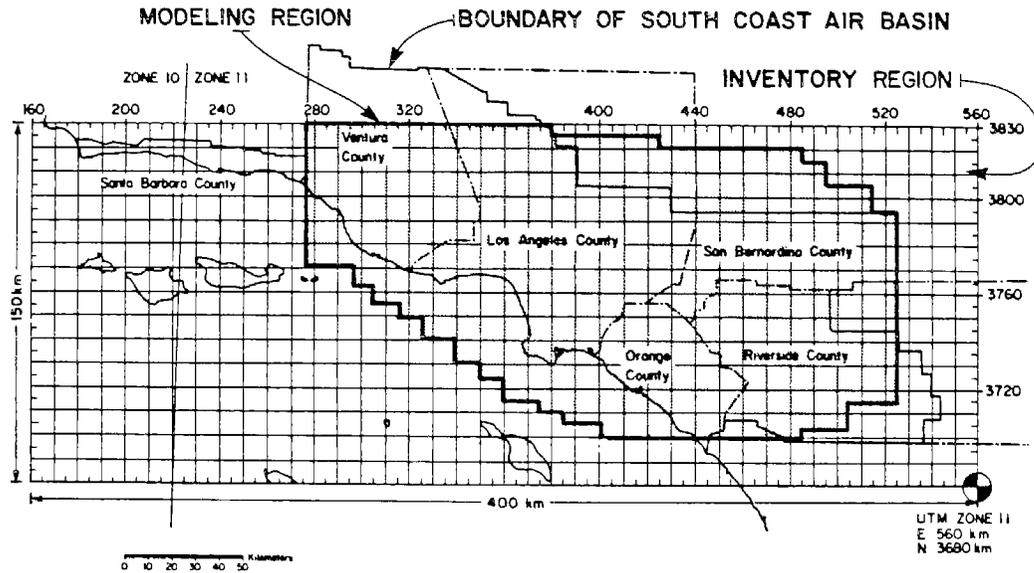
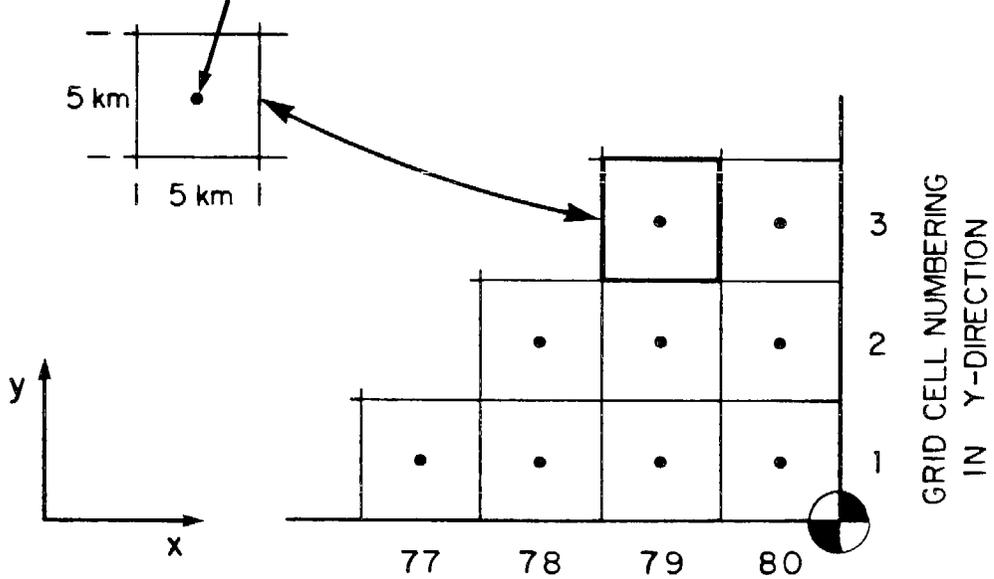


FIGURE C.1  
Location of Air Quality Monitoring Sites  
within the South Coast Air Basin



COMPUTATIONAL GRID POINT



ORIGIN:  
 E 560 km  
 N 3680 km  
 UTM, ZONE 11

FIGURE C.2

Definition of the Origin of the Computational Grid System

TABLE C.1

Air Quality Monitoring Sites Used in Statistical  
Analysis of Model Results for 26-27 June 1974

STATION <sup>(a)</sup> CODE	MONITORING STATION	GRID COORDINATES (x,y)	
30176	Anaheim	51.0	12.5
30177	La Habra	50.4	14.8
30190	Los Alamitos-Orangewood Ave	48.8	12.1
33140	Norco-Prado Park	56.8	14.7
33144	Riverside-Rubidoux	60.1	16.5
33146	Riverside-Magnolia Ave	60.4	15.3
36151	San Bernardino	62.6	18.8
36173	Chino-Riverside Ave	56.3	15.8
36174	Upland-Civic Center	56.1	18.7
36175	Upland ARB	56.5	18.8
36176	Fontana-Foothill Blvd	59.8	18.5
36191	Camp Paivika-USFS	62.5	21.9
56408	Camarillo-Palm	30.6	21.6
56409	Point Mugu	28.7	19.6
56412	Port Hueneme	27.6	20.1
56413	Simi Valley	37.2	22.6
56414	Ventura-Telegraph Rd	26.6	22.8
56415	Thousand Oaks-Windsor Dr	34.0	20.7
70001	Los Angeles-Downtown	45.0	17.4
70060	Azusa	51.4	19.6
70069	Burbank	43.9	20.6
70071	West Los Angeles	41.5	17.5
70072	Long Beach	46.0	12.6
70075	Pomona	54.0	18.0
70076	Lennox	42.6	15.0
70078	Redondo Beach	42.4	13.2
70080	Whittier	48.7	15.0
70083	Pasadena-Walnut St	47.2	19.7
70084	Lynwood	45.6	14.8
70406	Mt Lee Dr-Mobile Van	43.3	19.5
70585	Vanl-105 Frwy (Prop)	47.6	14.6

Notes:

(a) California Air Resources Board Code Number

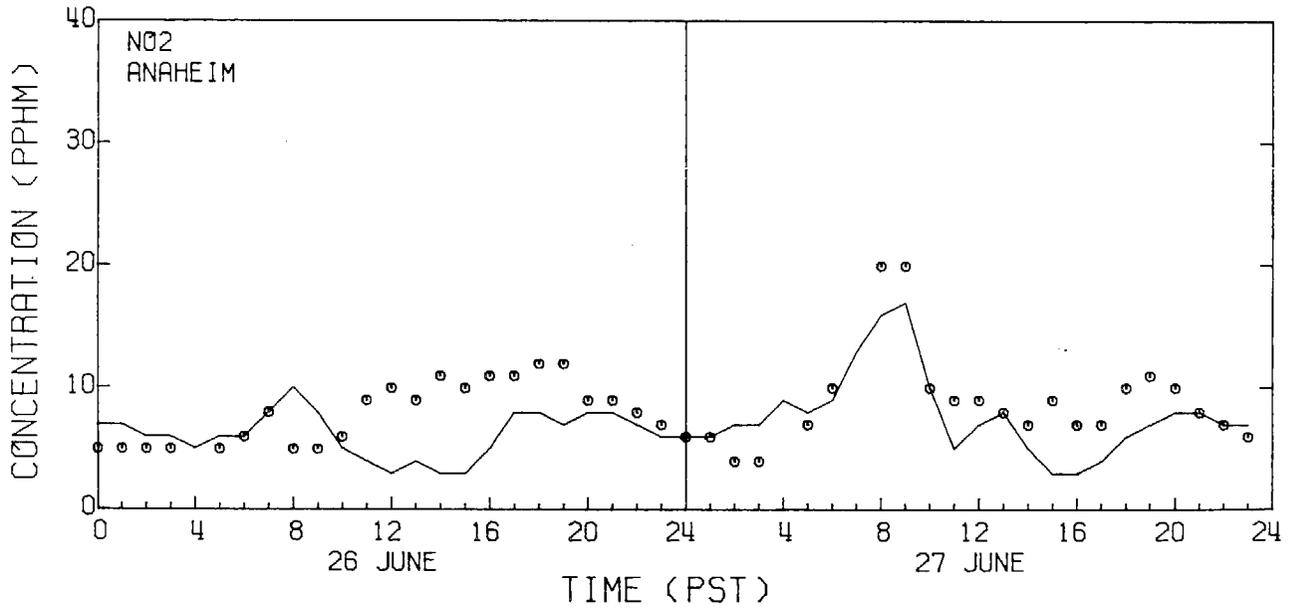
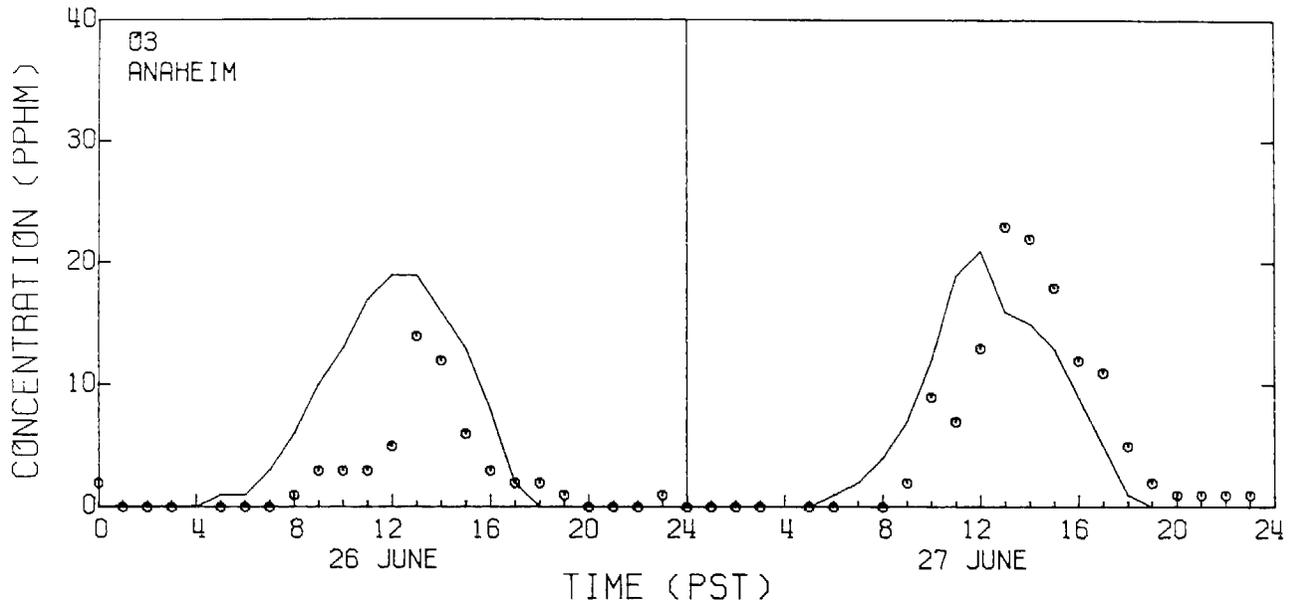


FIGURE C.4  
Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Anaheim

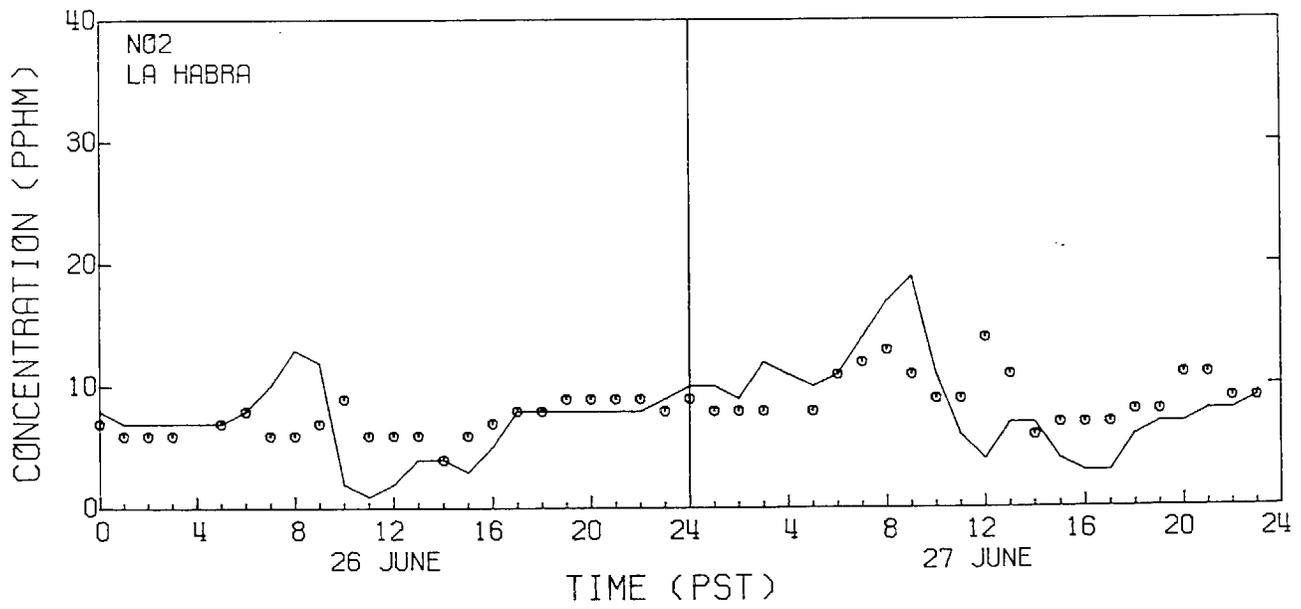
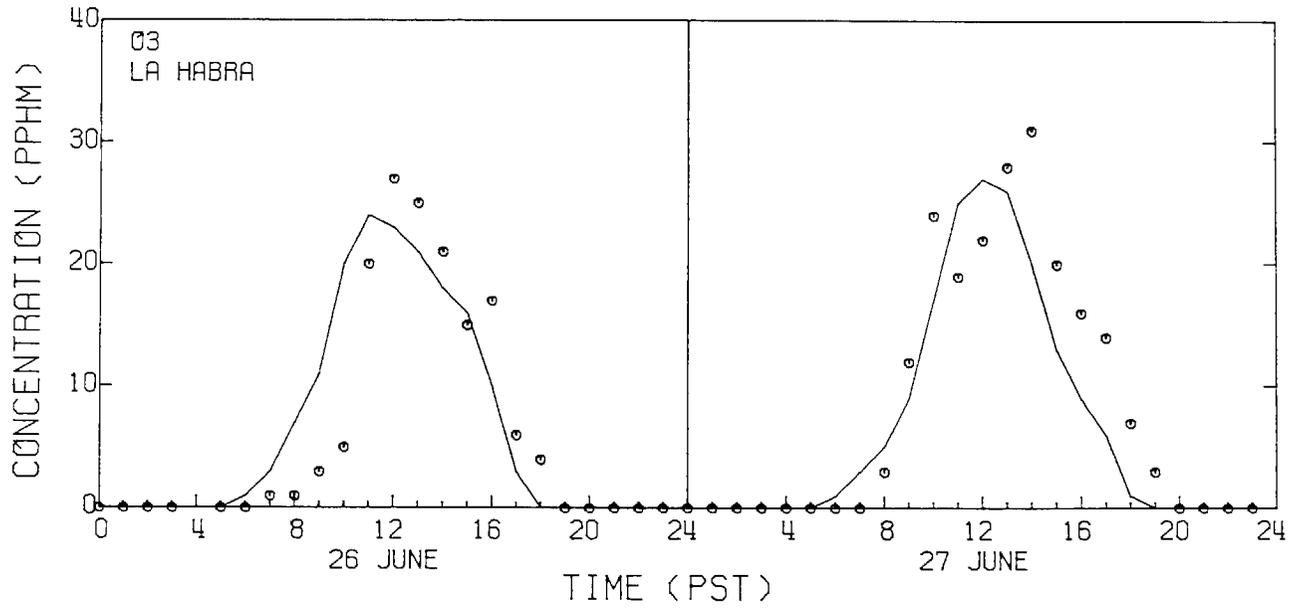


FIGURE C.5

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at La Habra

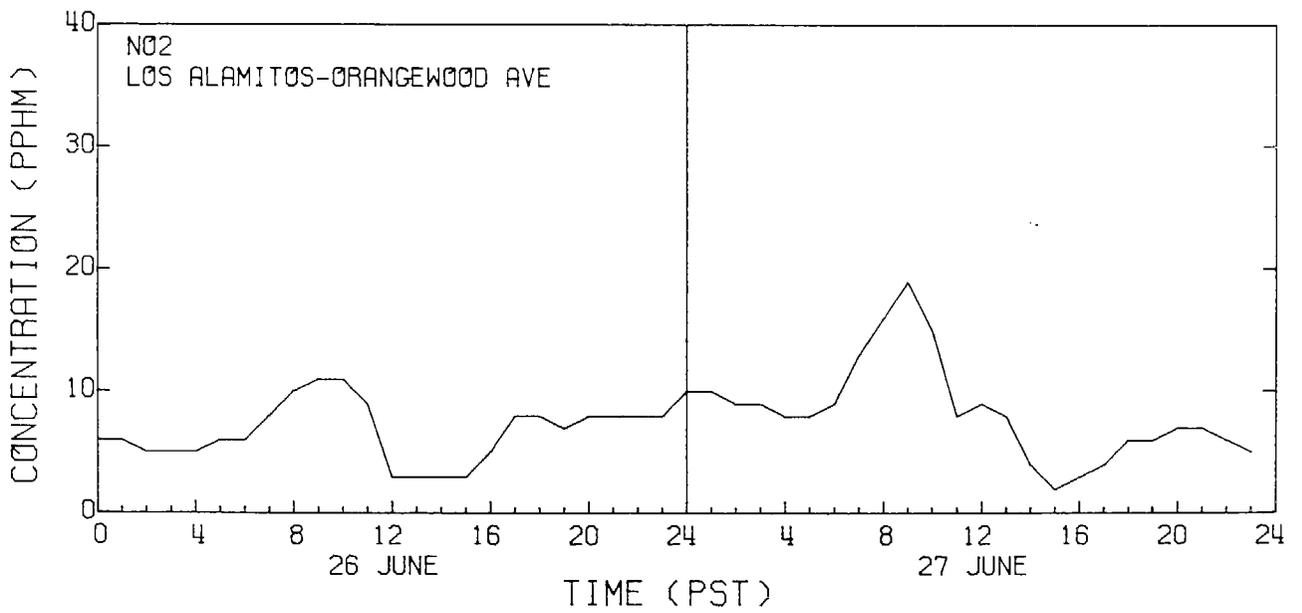
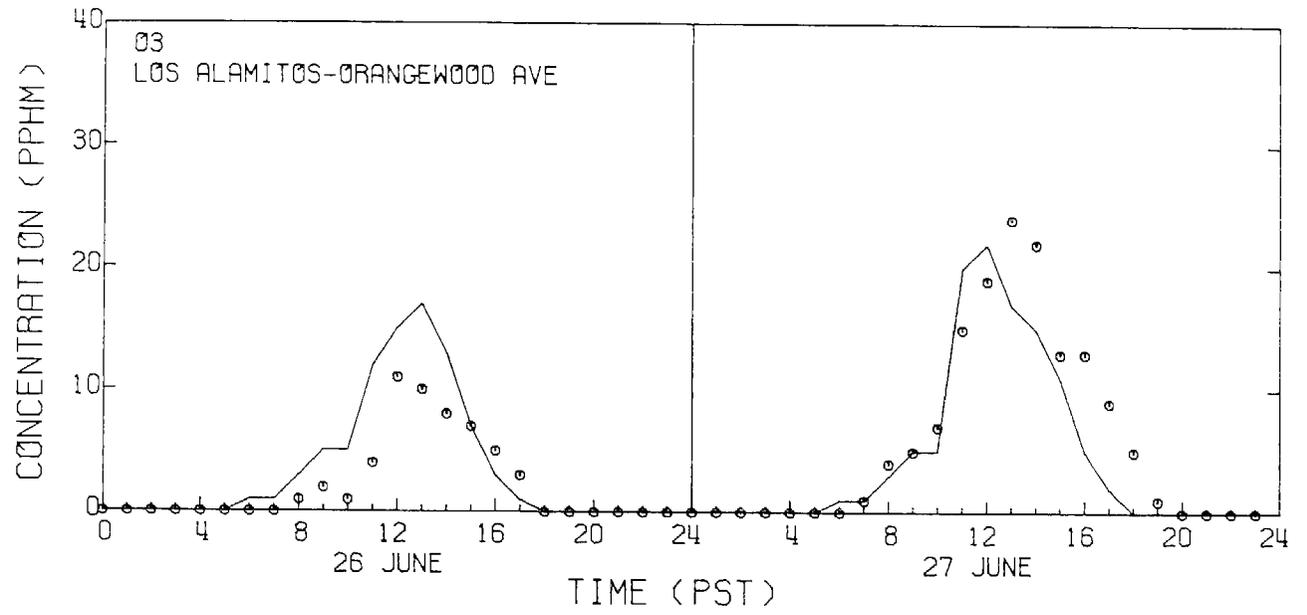


FIGURE C.6

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Los Alamitos-Orangewood Avenue

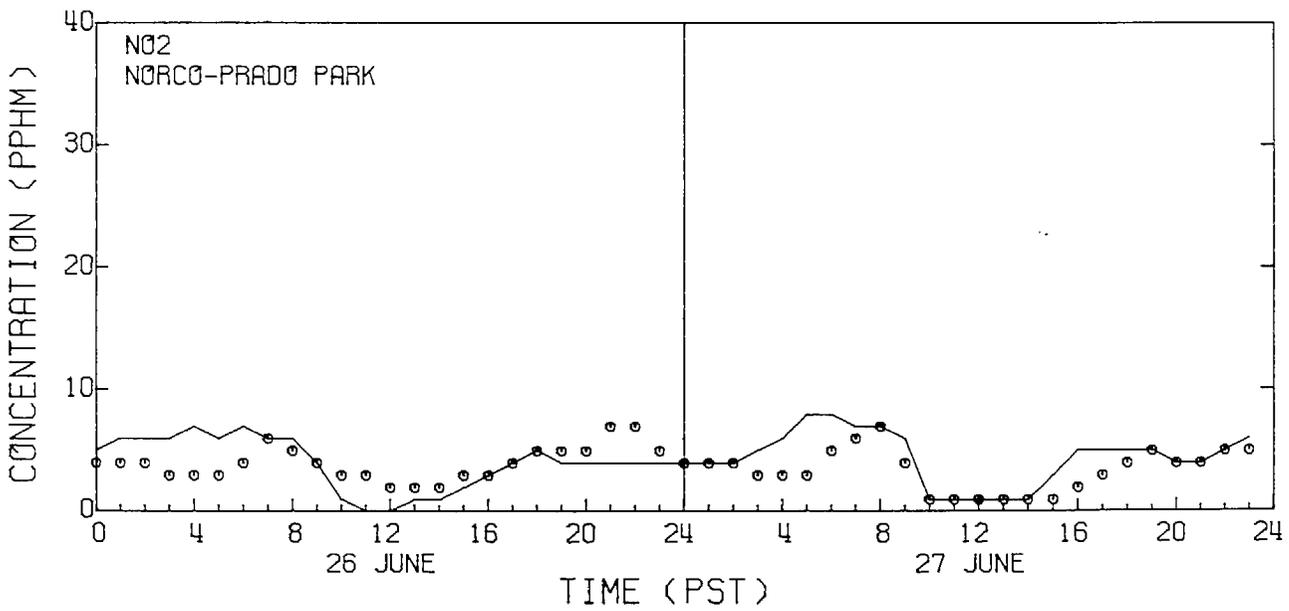
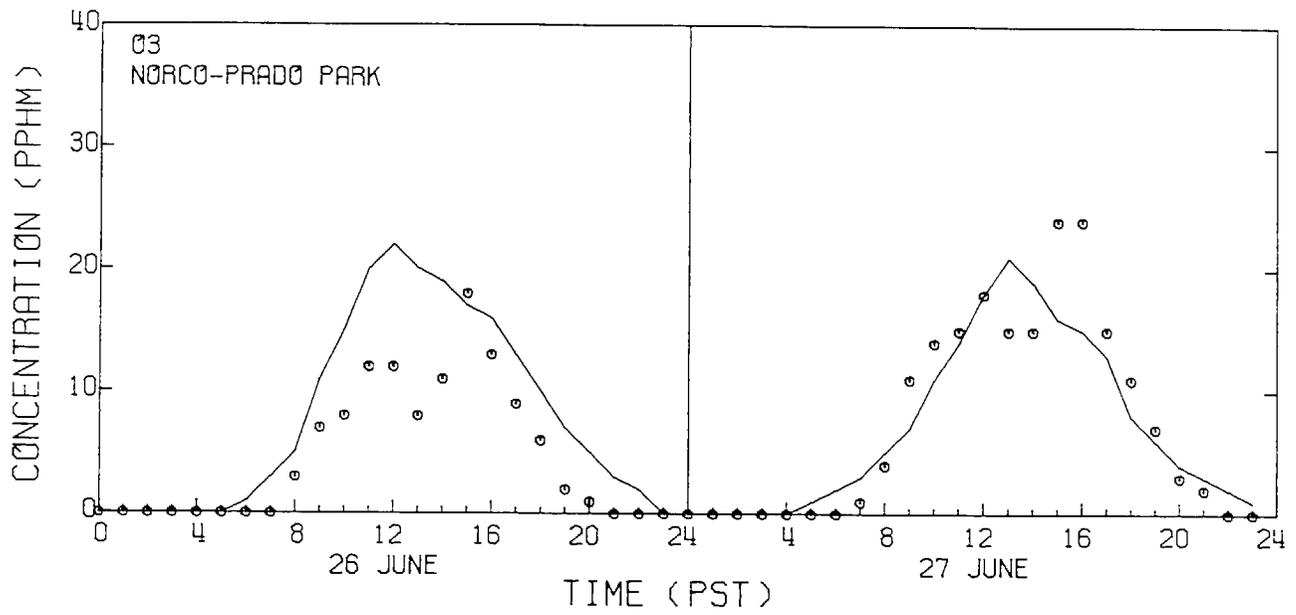


FIGURE C.7

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Norco-Prado Park

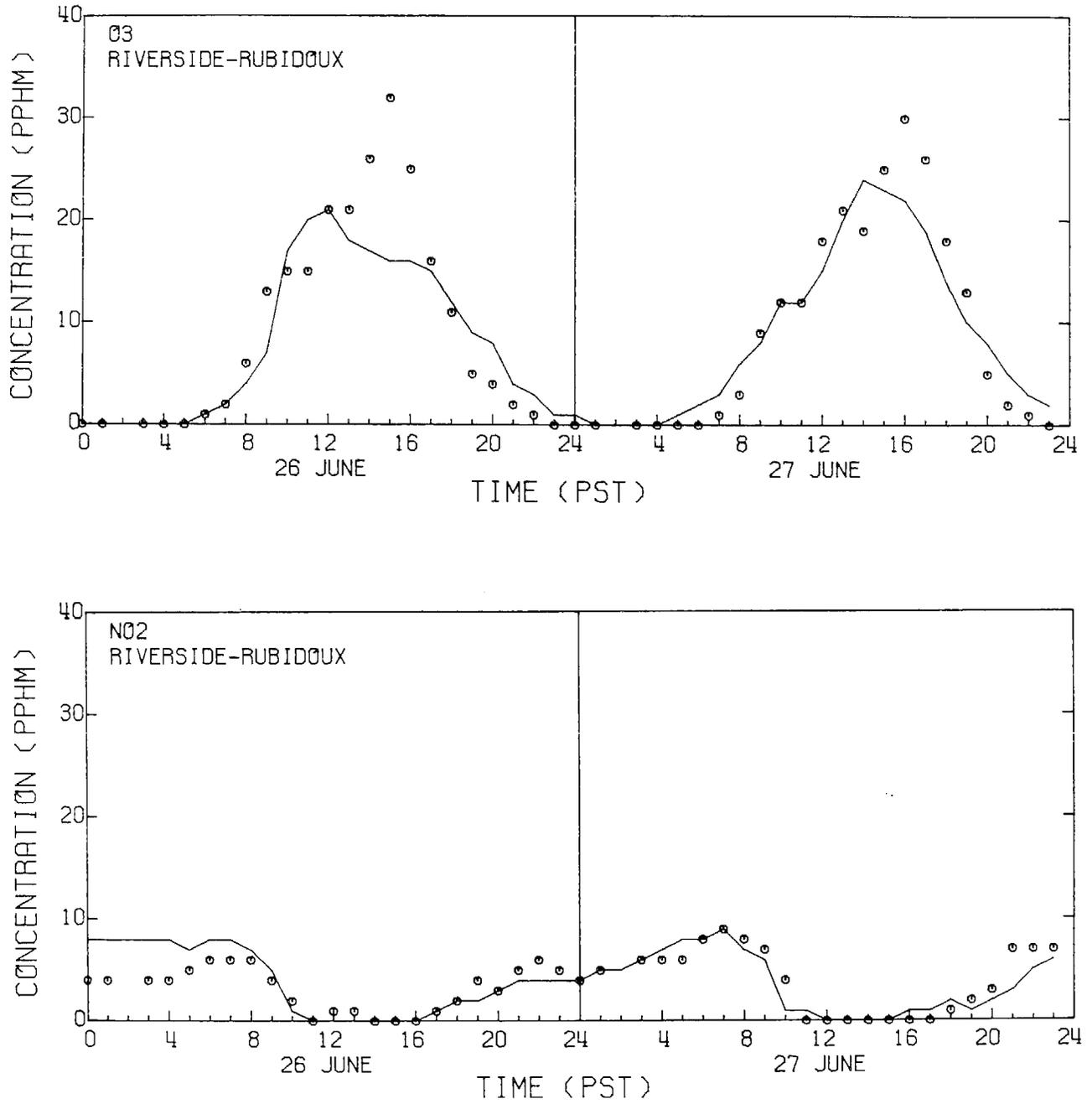


FIGURE C.8

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Riverside-Rubidoux

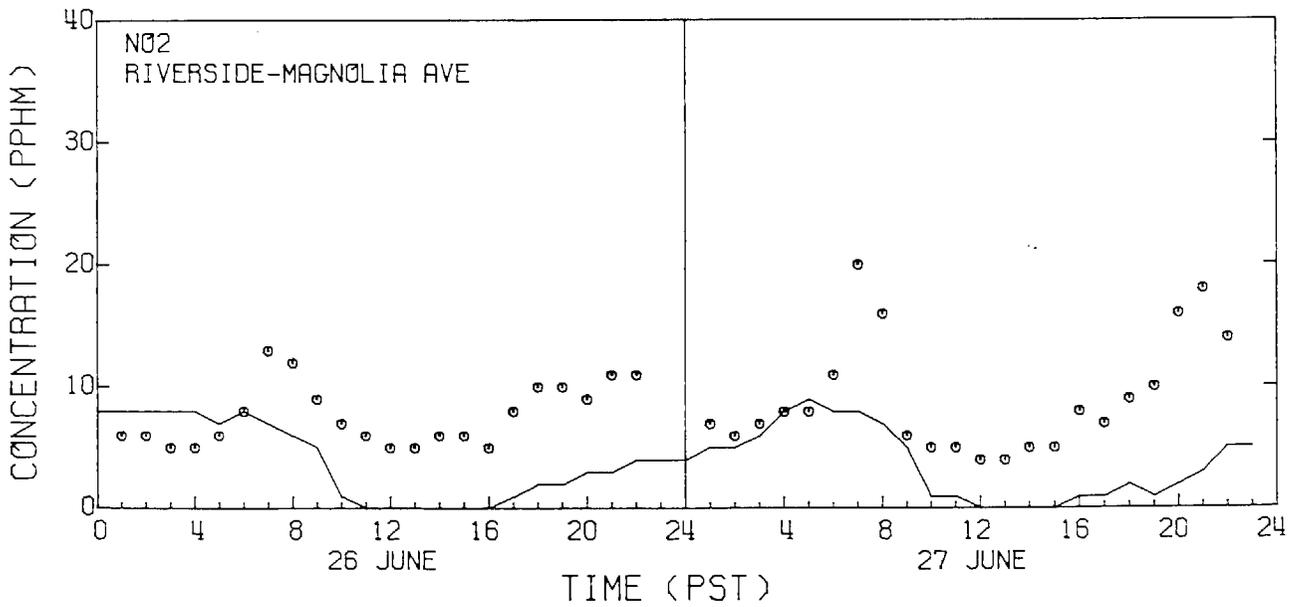
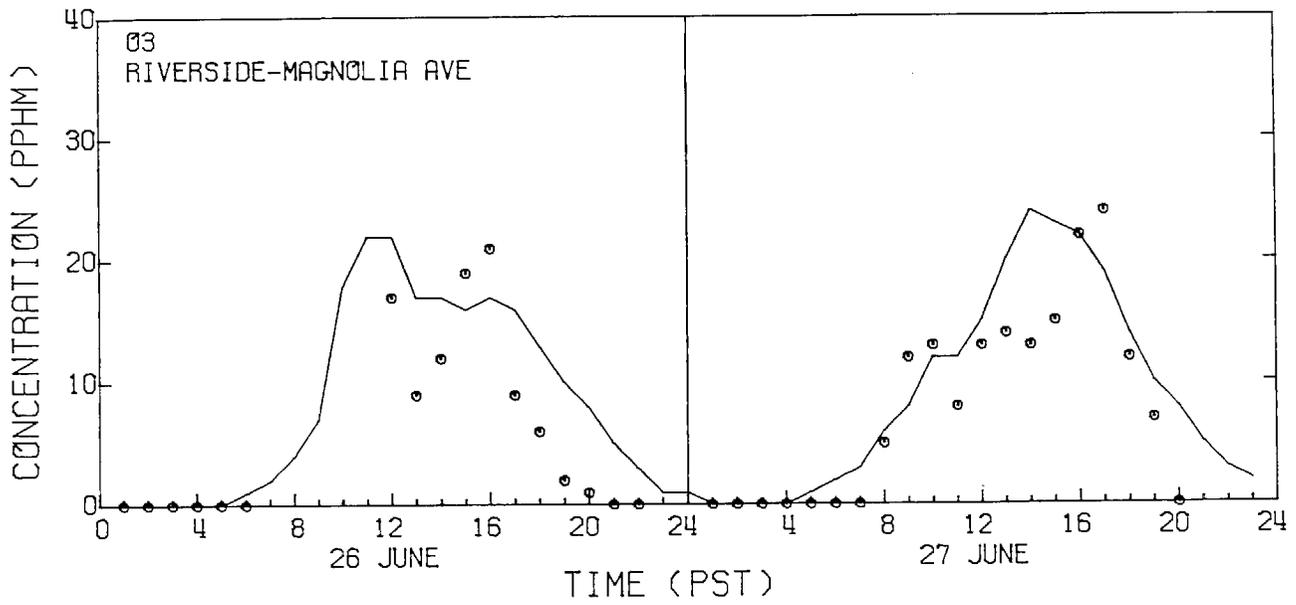


FIGURE C.9

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Riverside-Magnolia Avenue

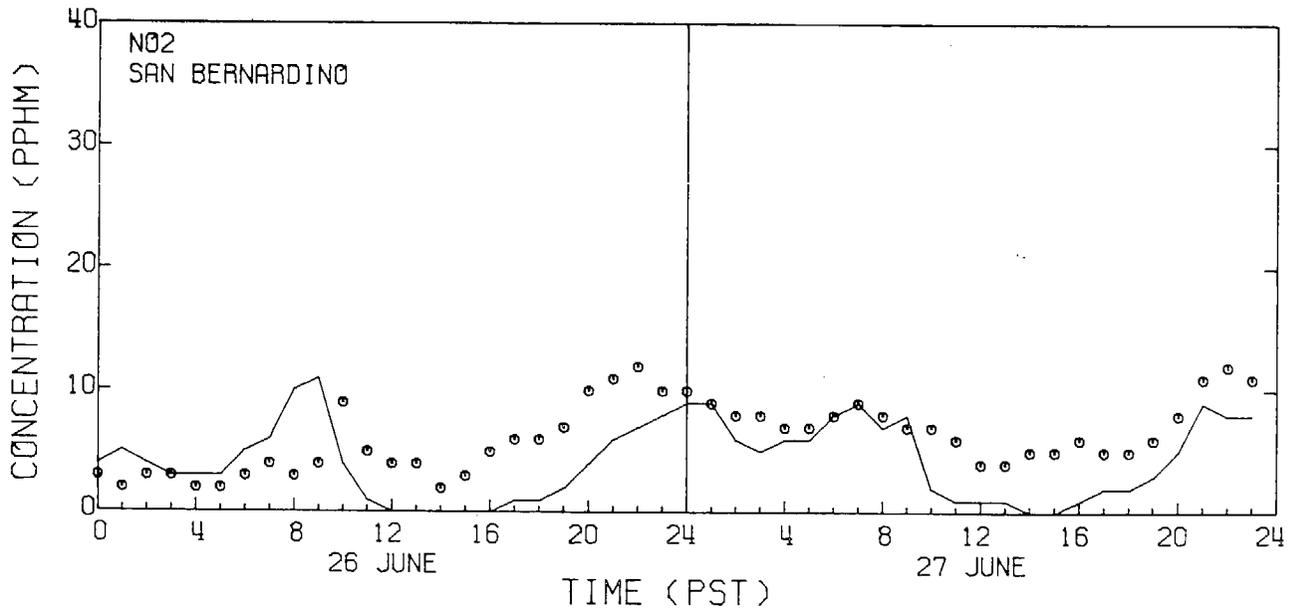
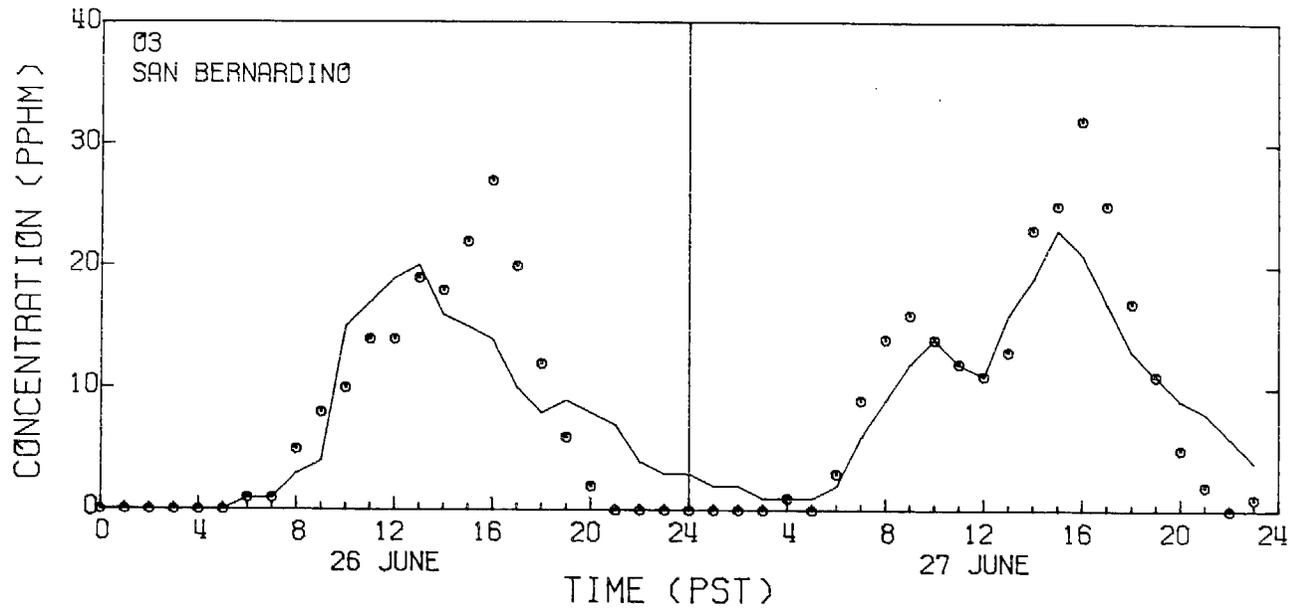


FIGURE C.10

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at San Bernardino

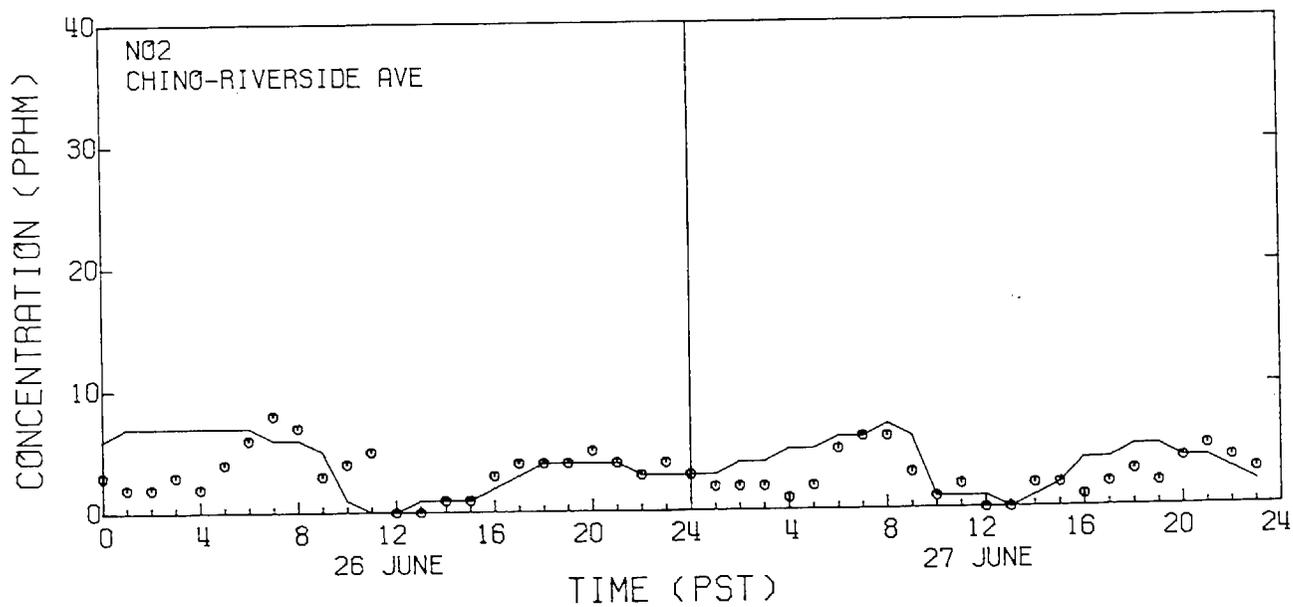
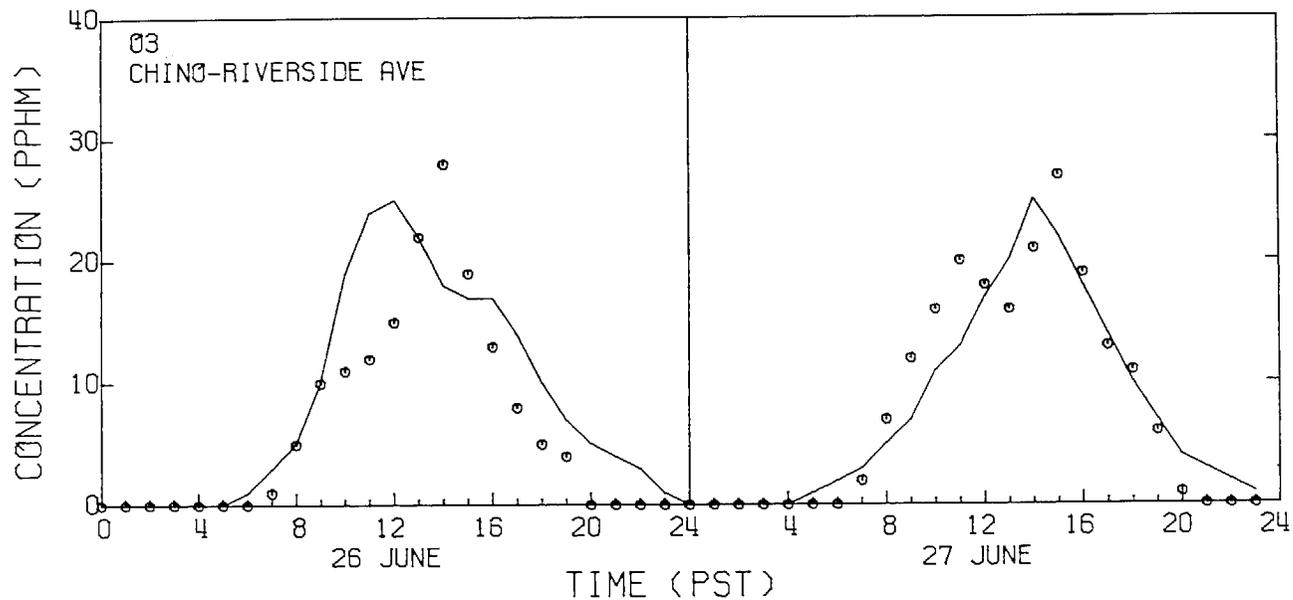


FIGURE C.11

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Chino-Riverside Avenue

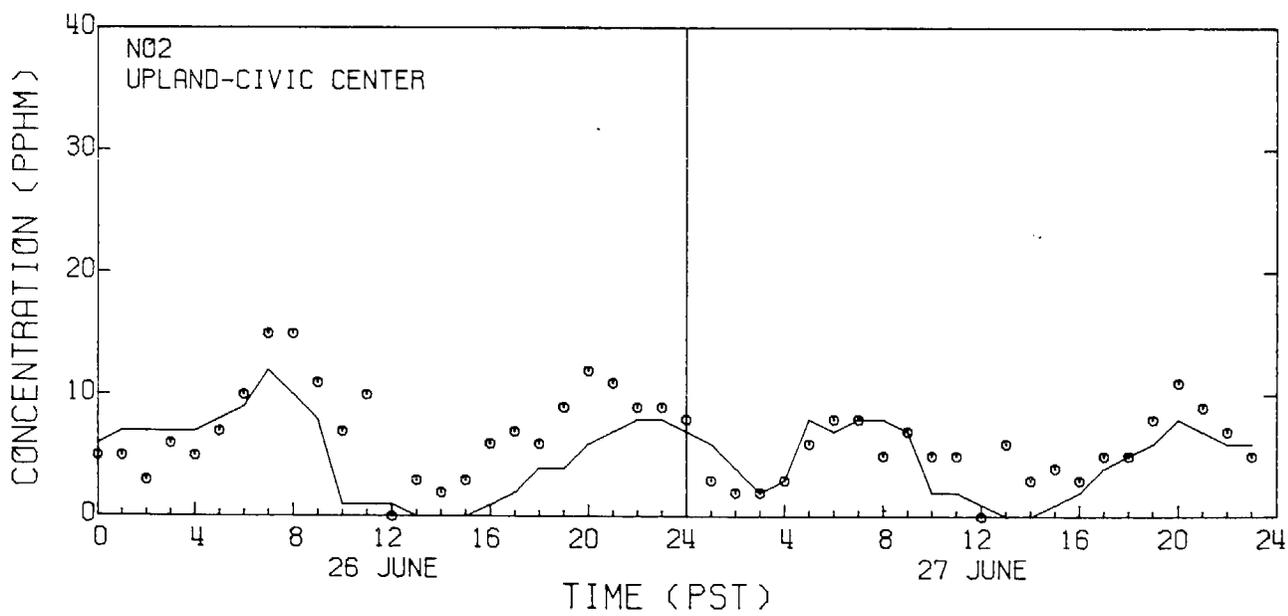
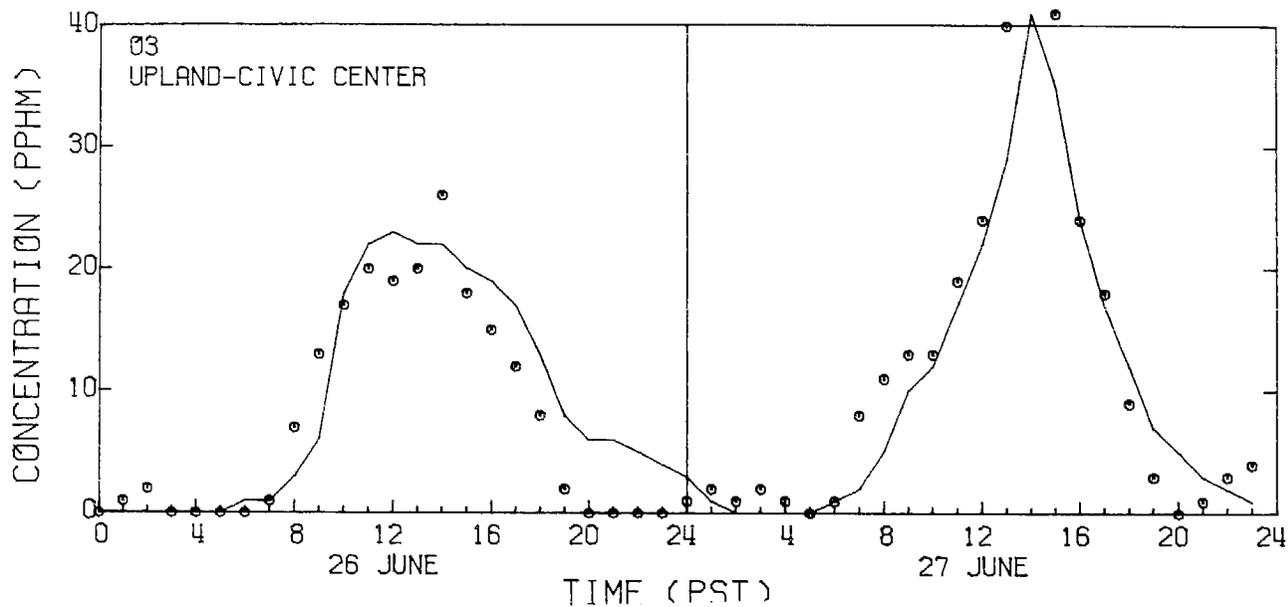


FIGURE C.12

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Upland-Civic Center

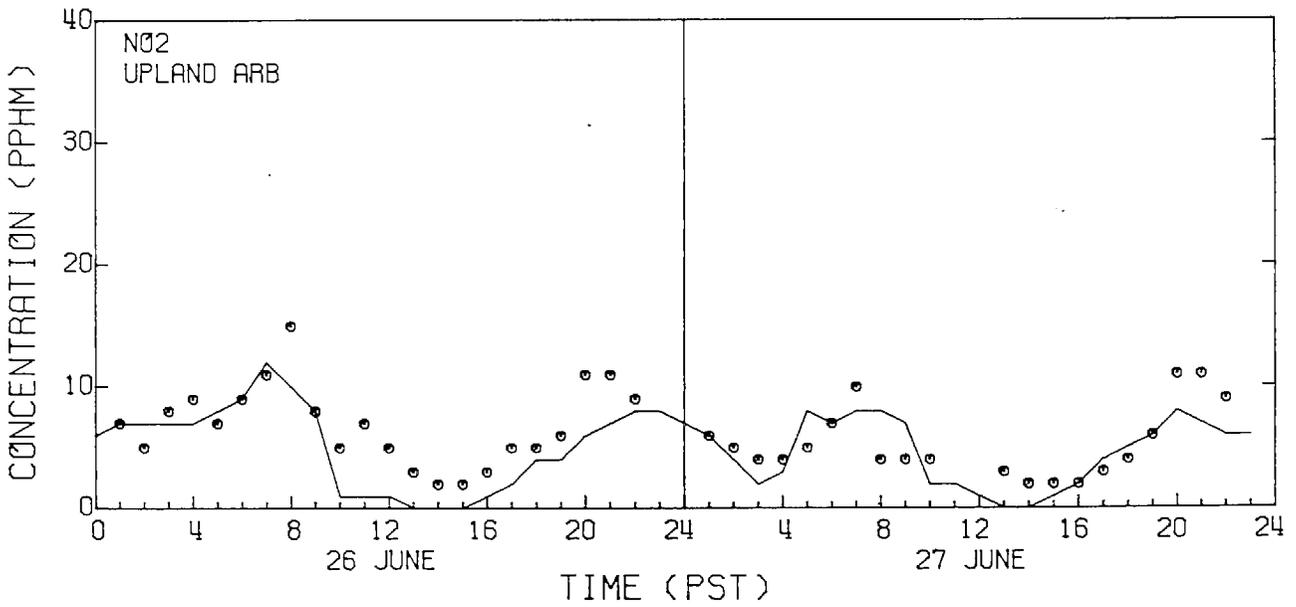
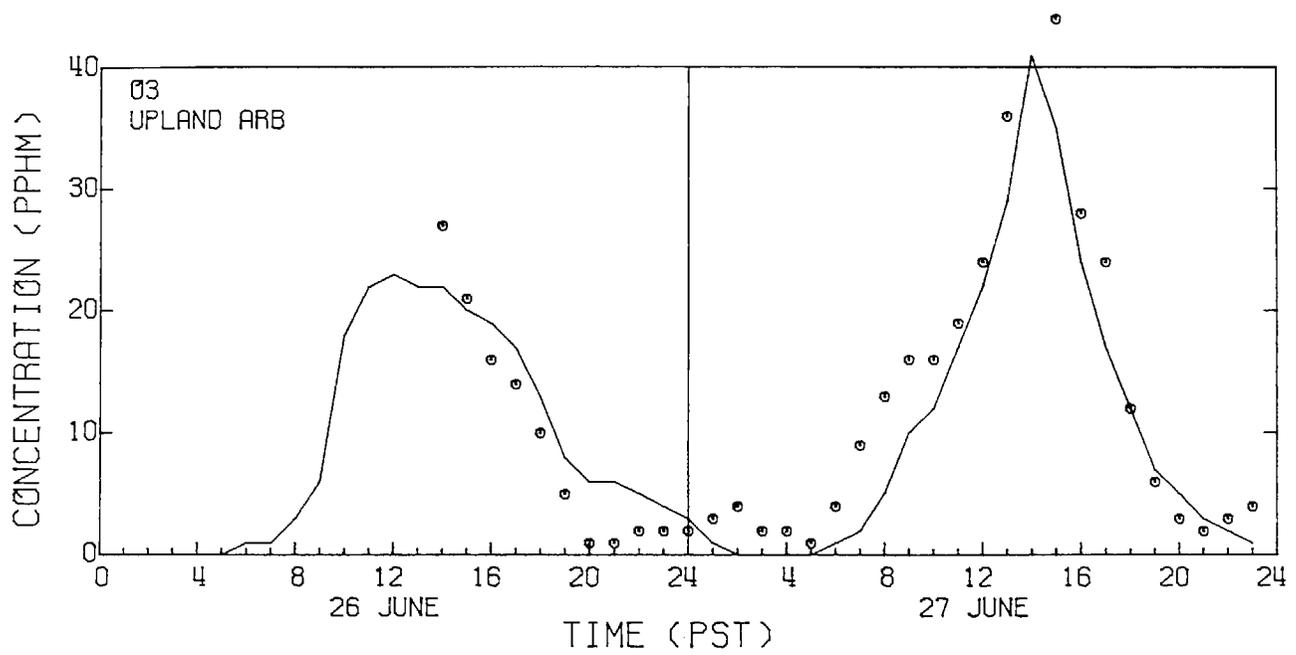


FIGURE C.13

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Upland ARB

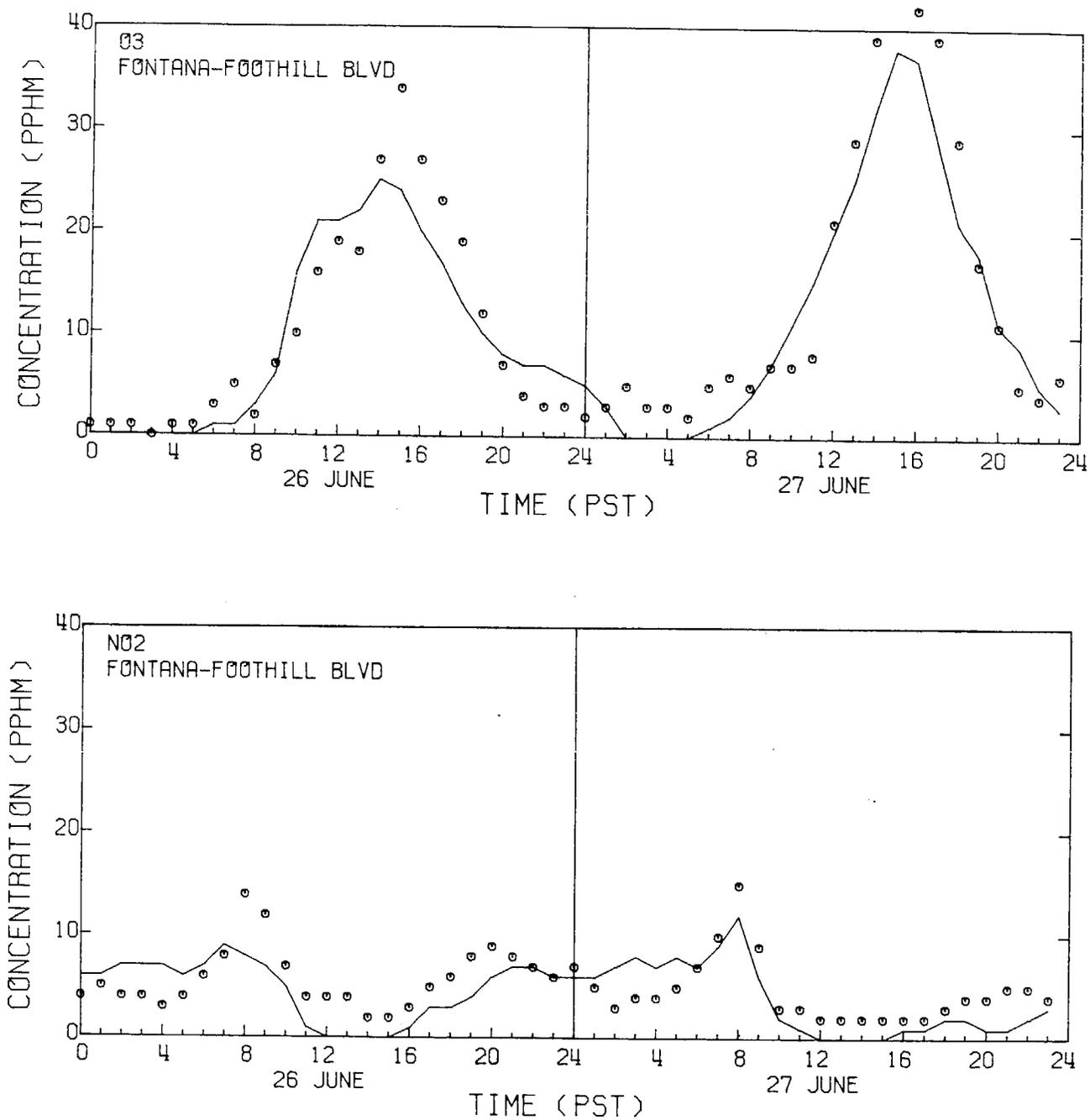


FIGURE C.14

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Fontana-Foothill Blvd

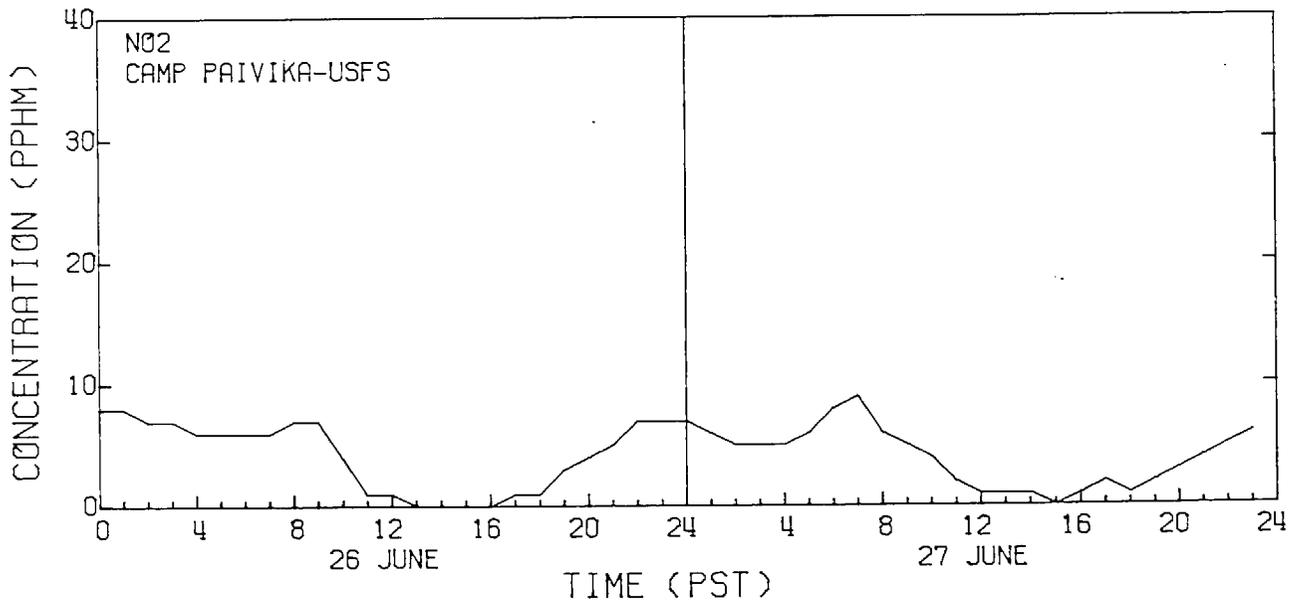
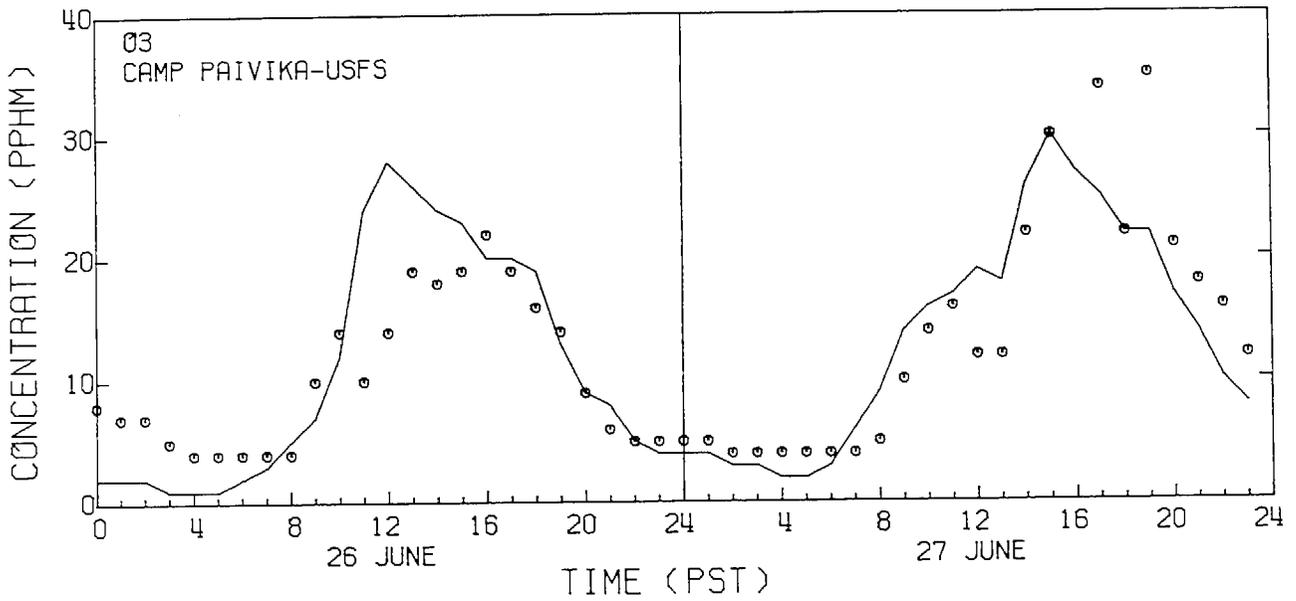


FIGURE C.15

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Camp Paivika-USFS

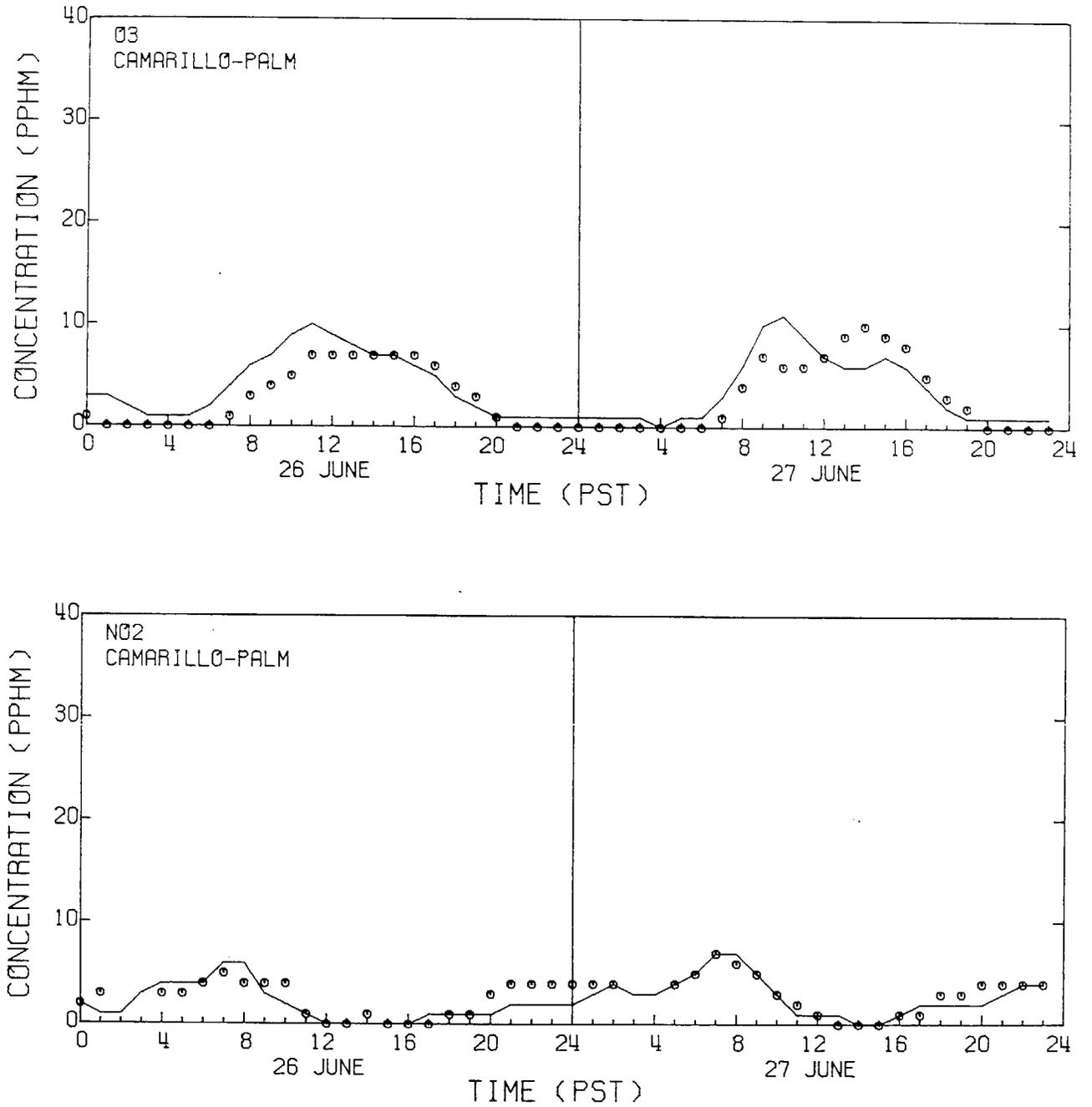


FIGURE C.16  
Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Camarillo-Palm

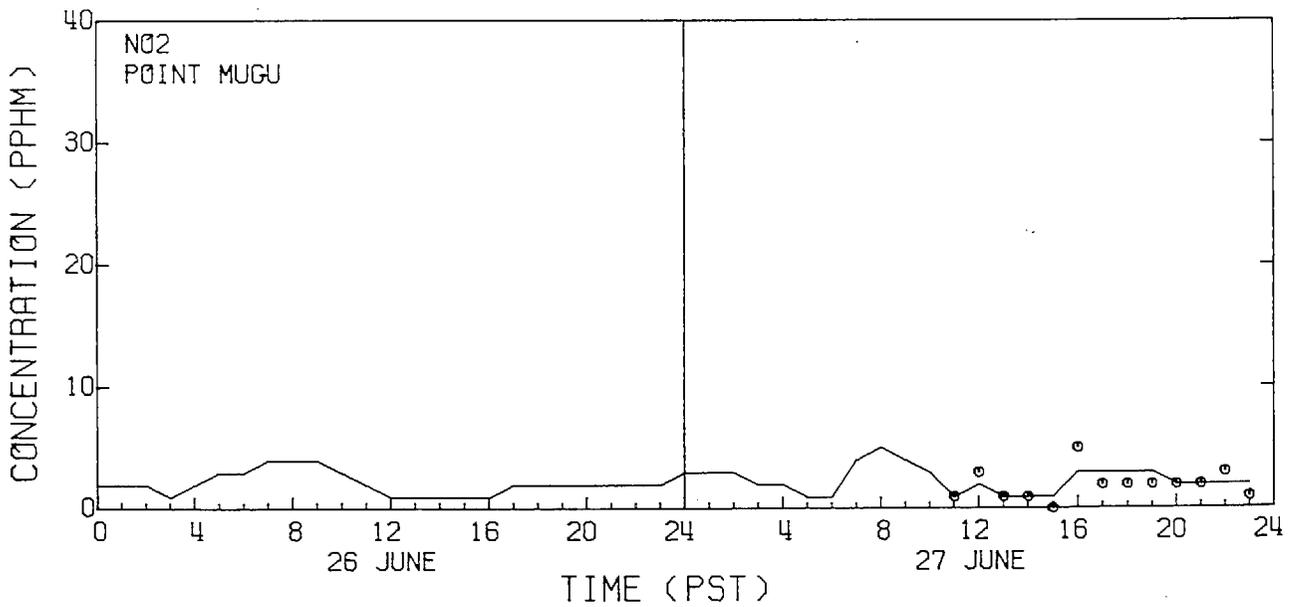
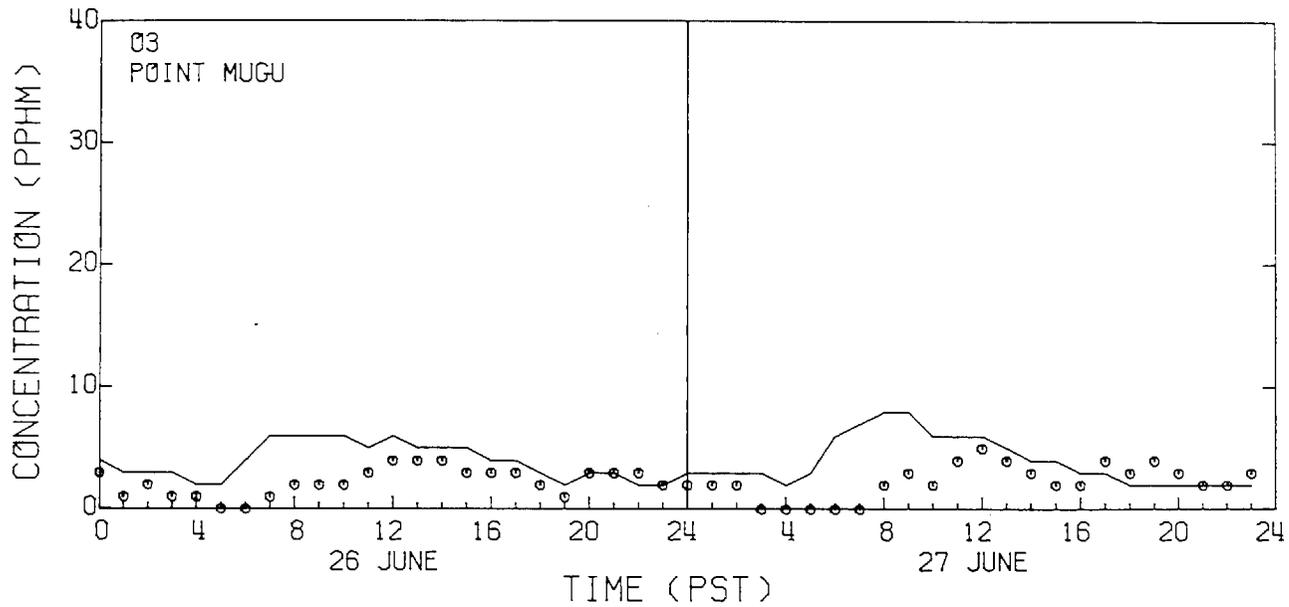


FIGURE C.17

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Point Mugu

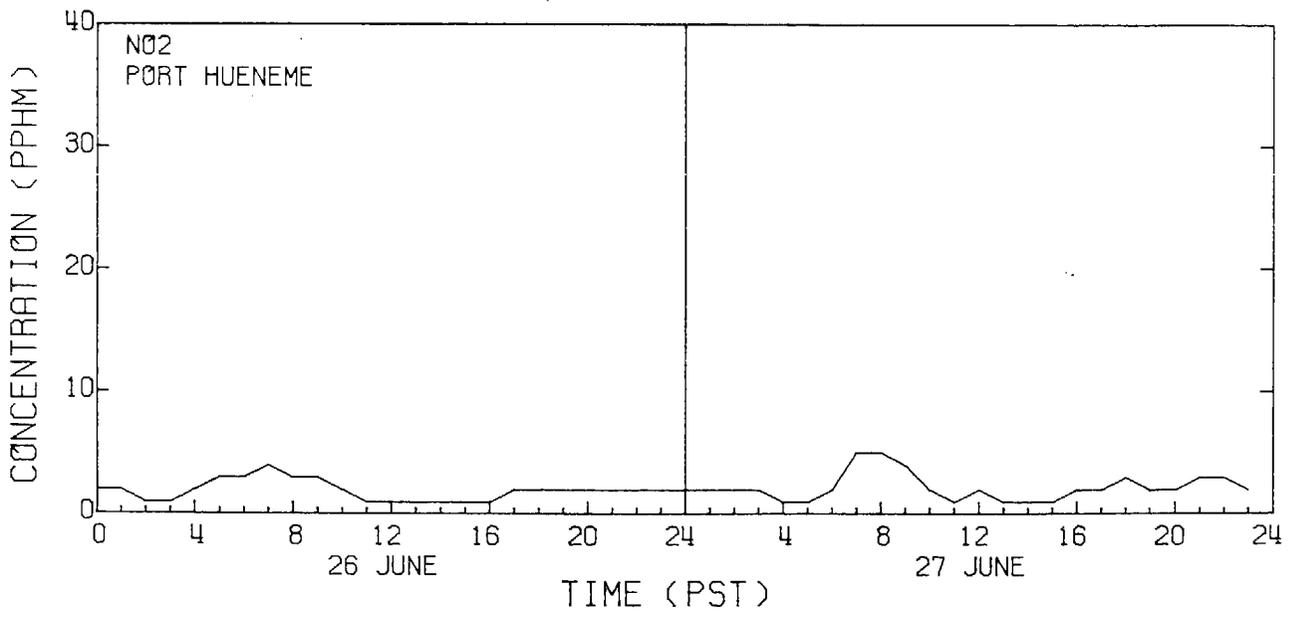
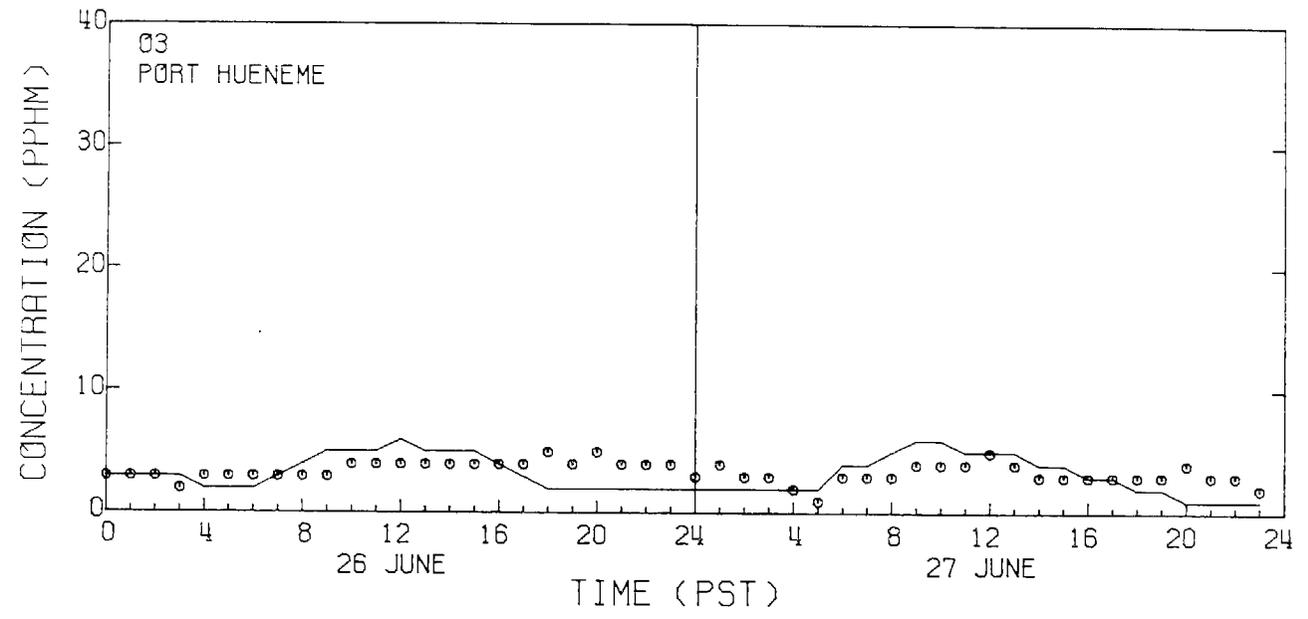


FIGURE C.18

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Port Hueneme

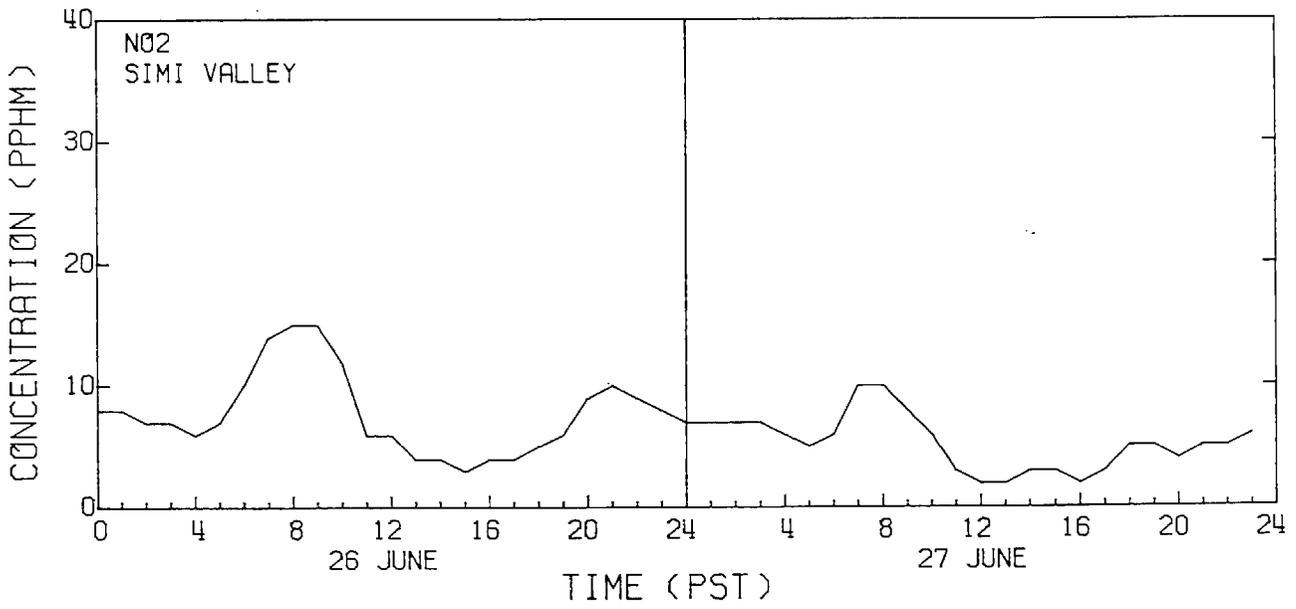
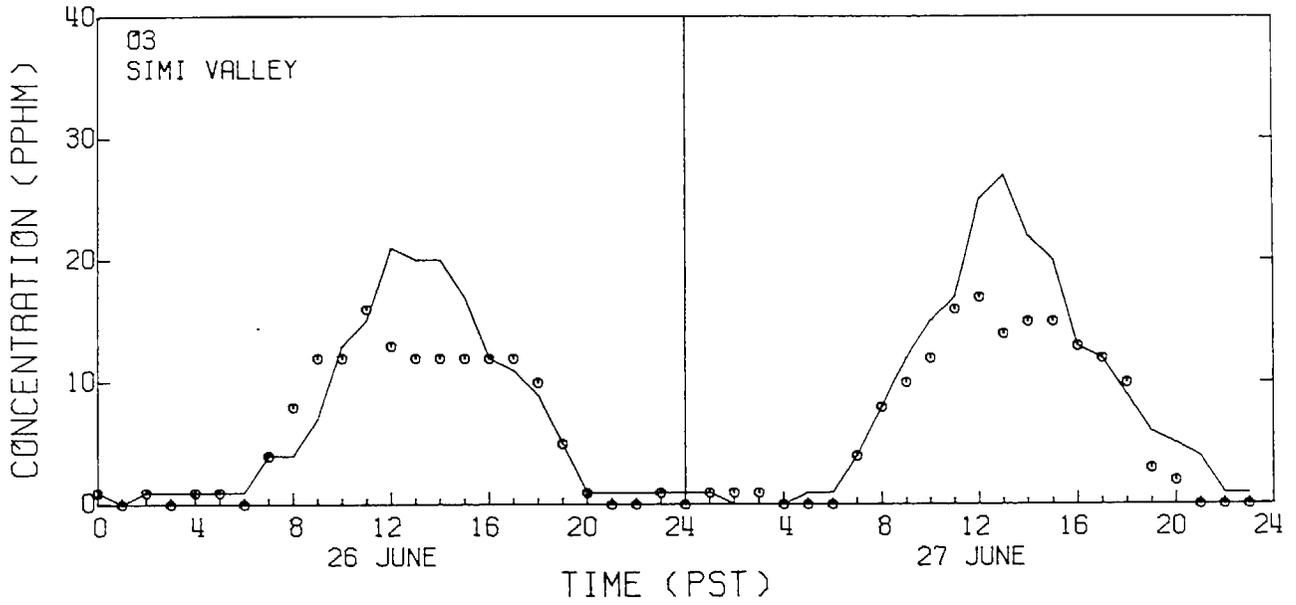


FIGURE C.19  
 Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
 Air Quality at Simi Valley

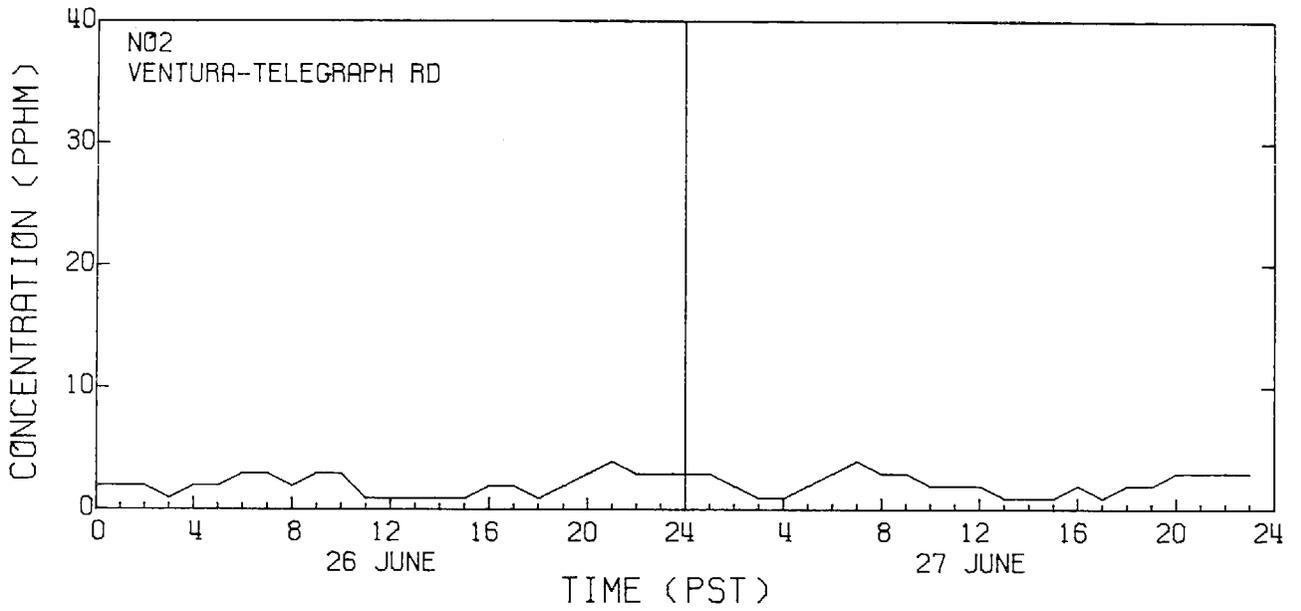
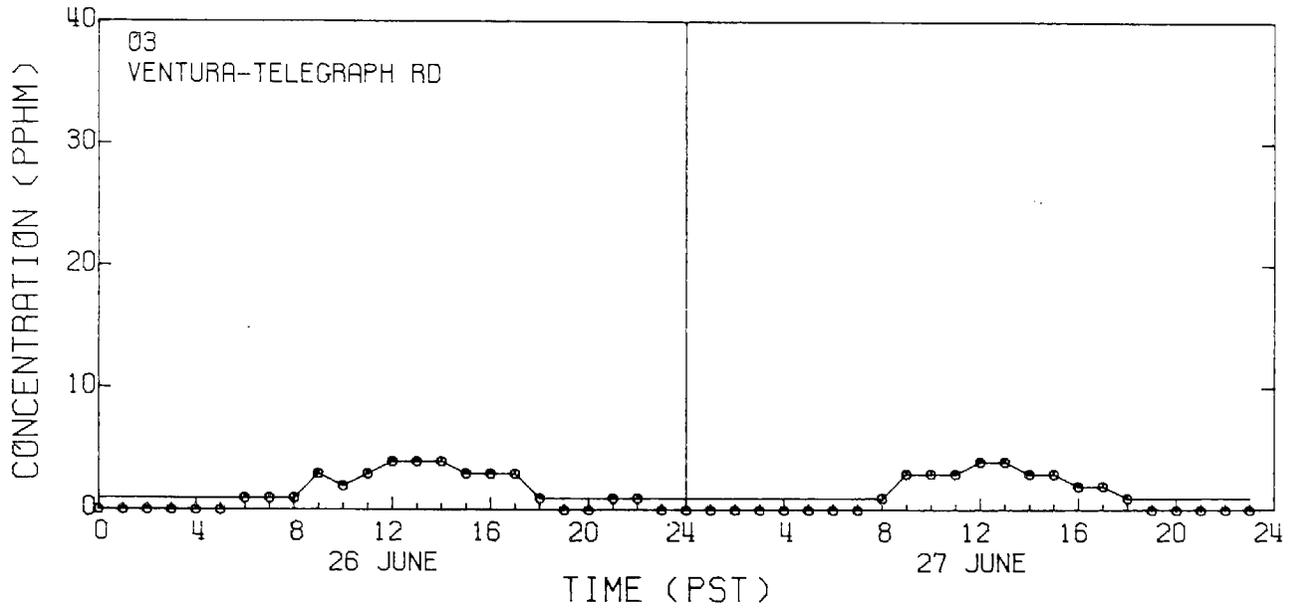


FIGURE C.20

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Ventura-Telegraph Rd

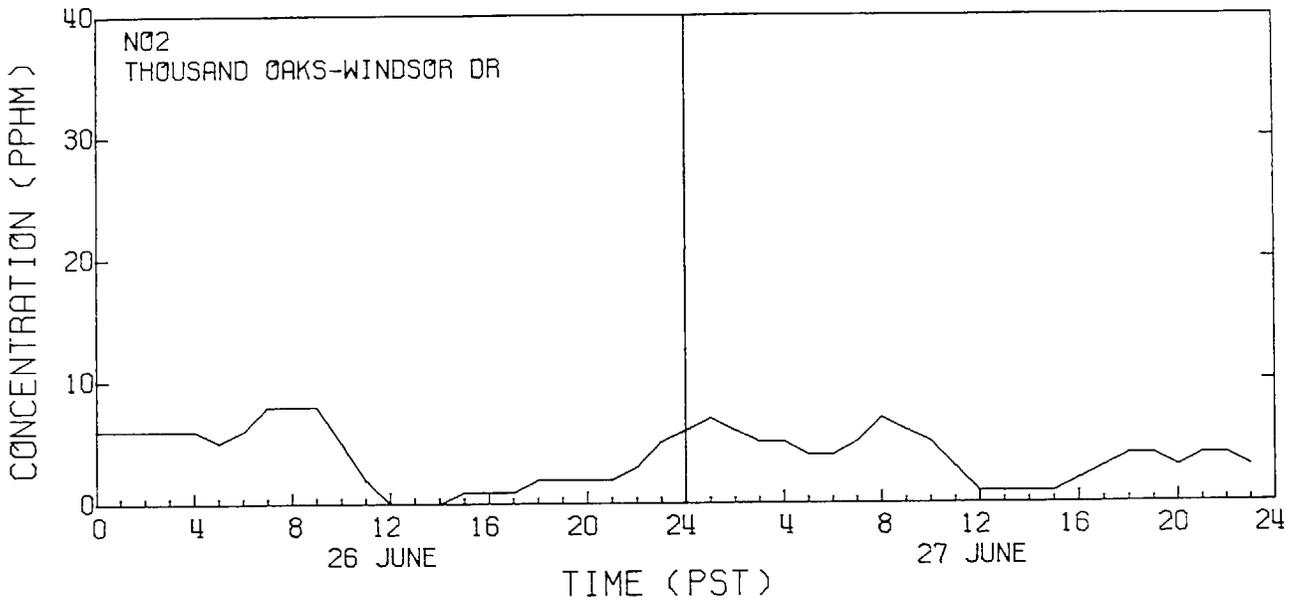
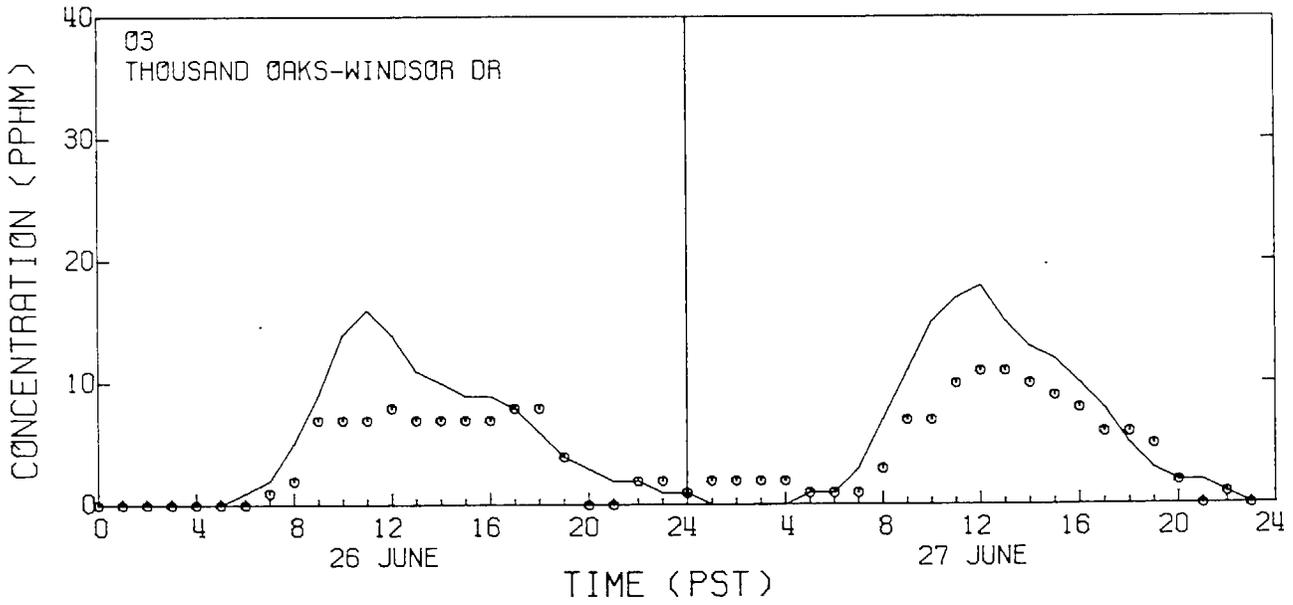


FIGURE C.21

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Thousand Oaks-Windsor Dr

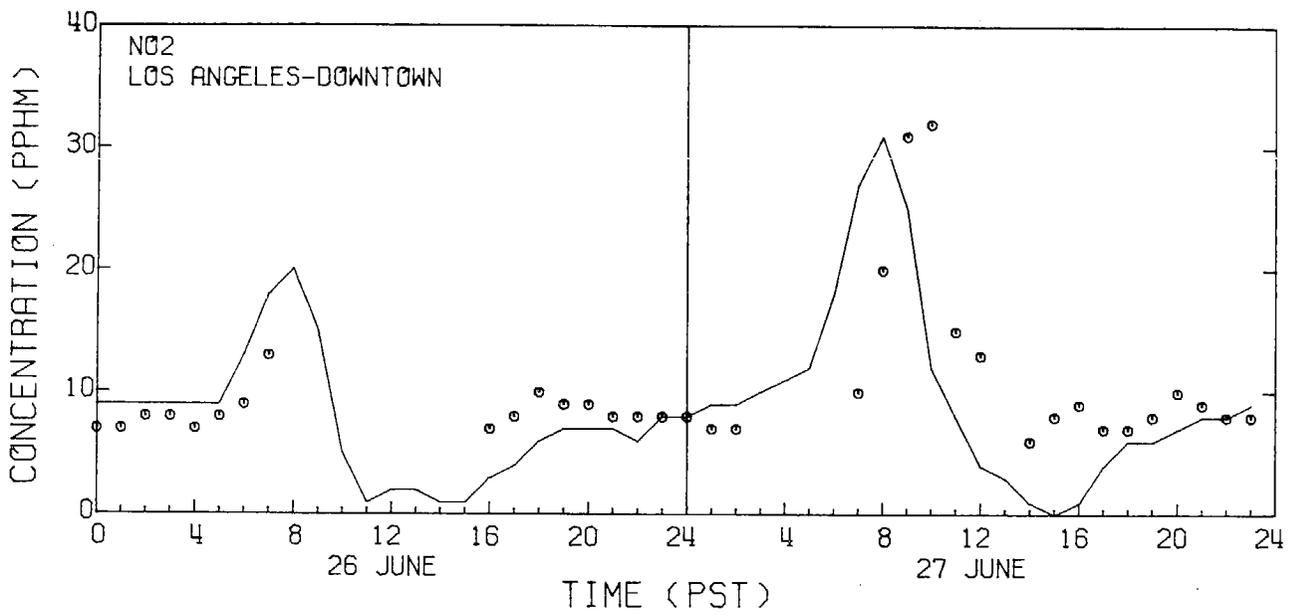
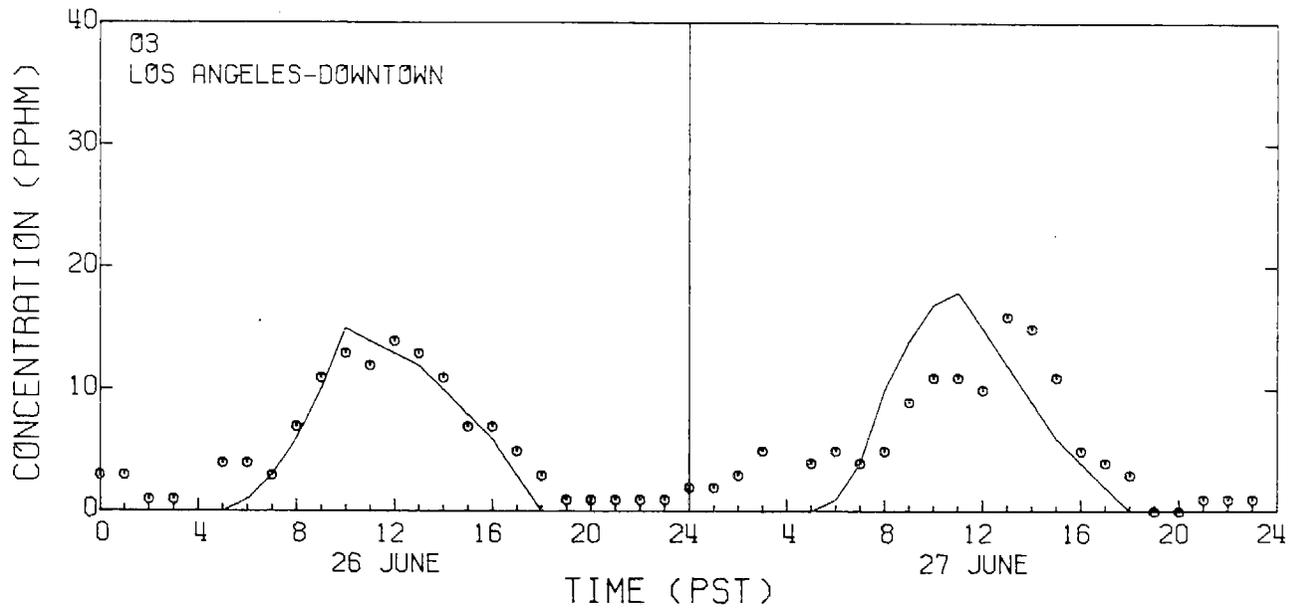


FIGURE C.22

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Los Angeles-Downtown

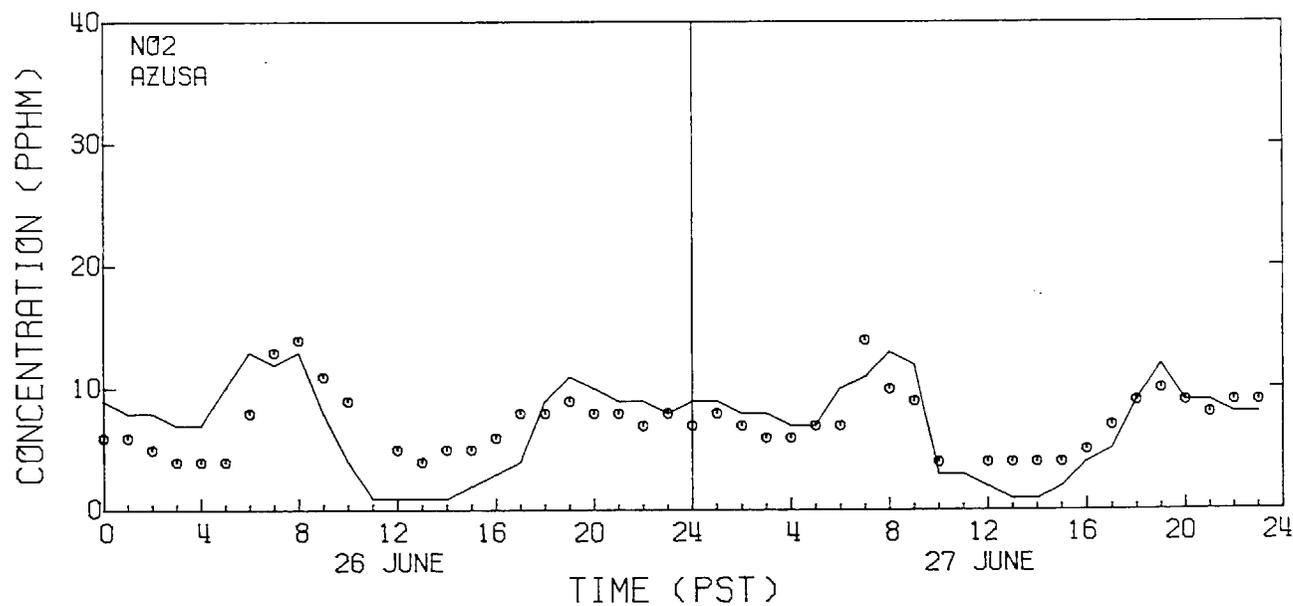
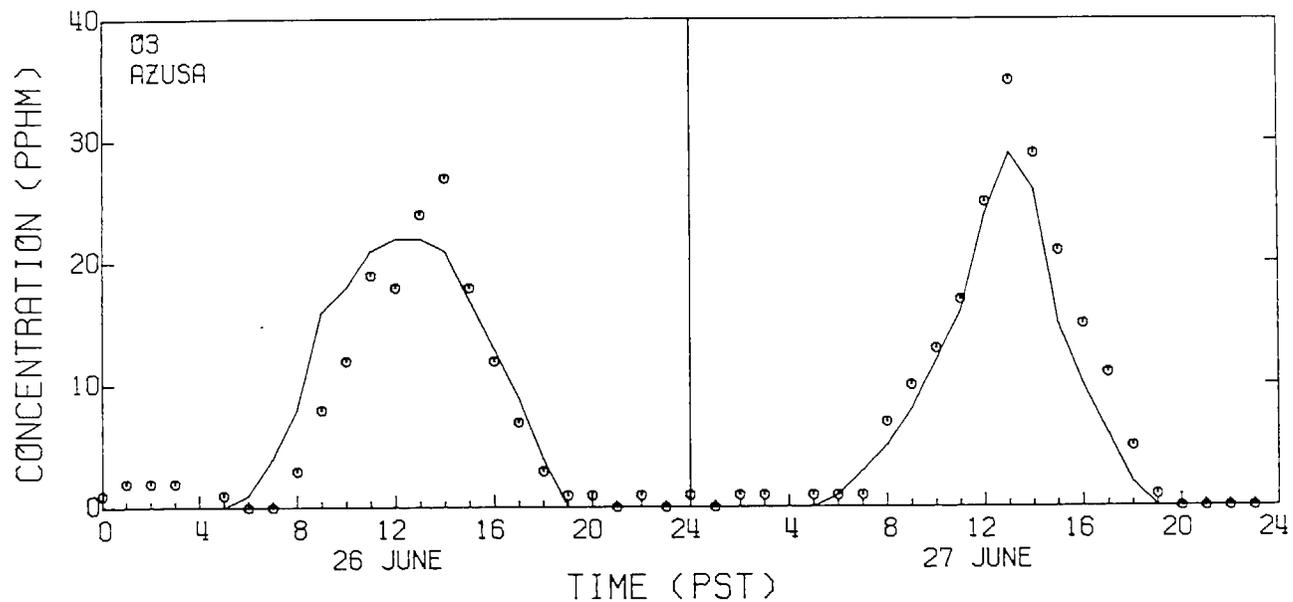


FIGURE C.23

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Azusa

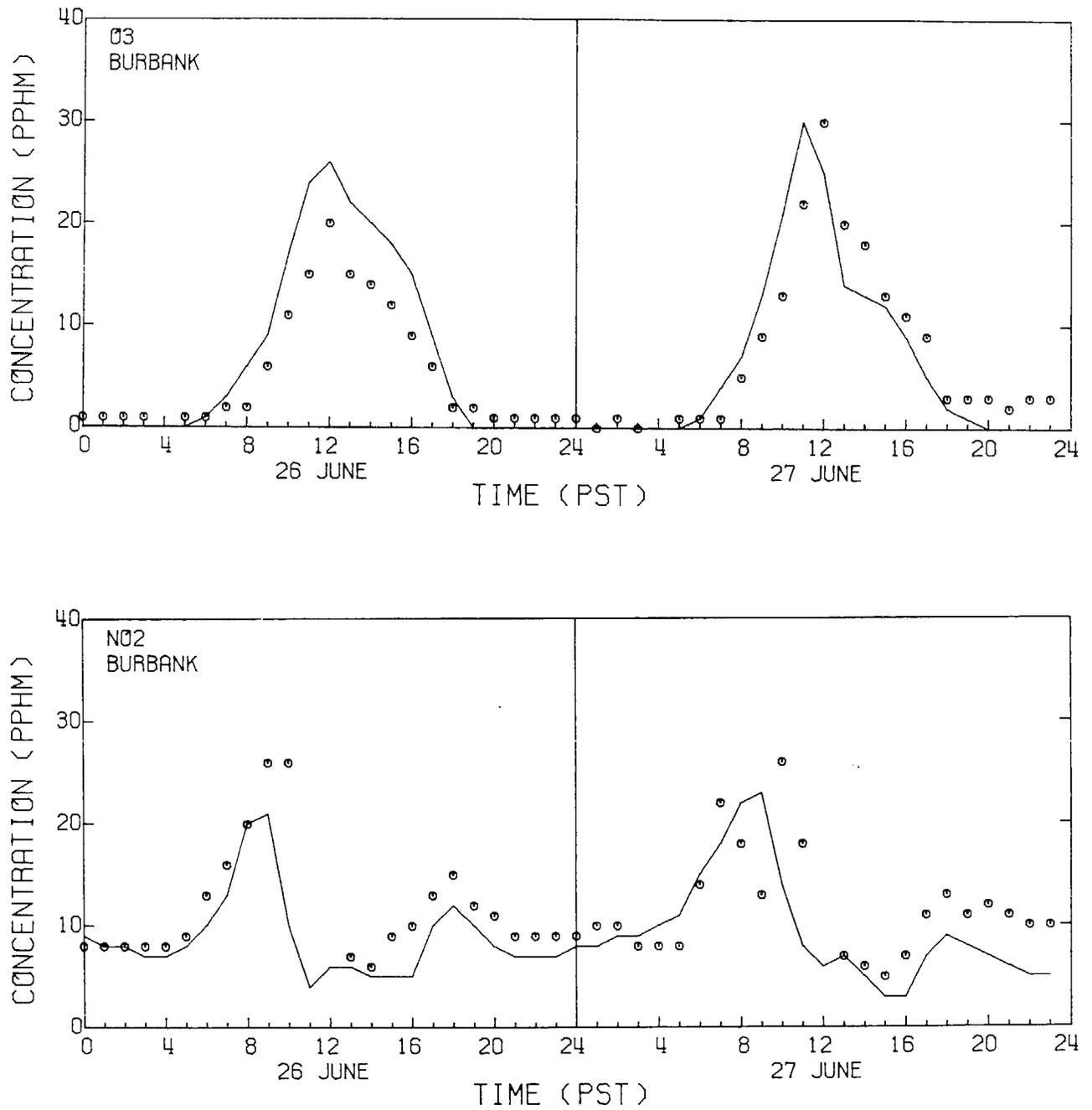


FIGURE C.24

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Burbank

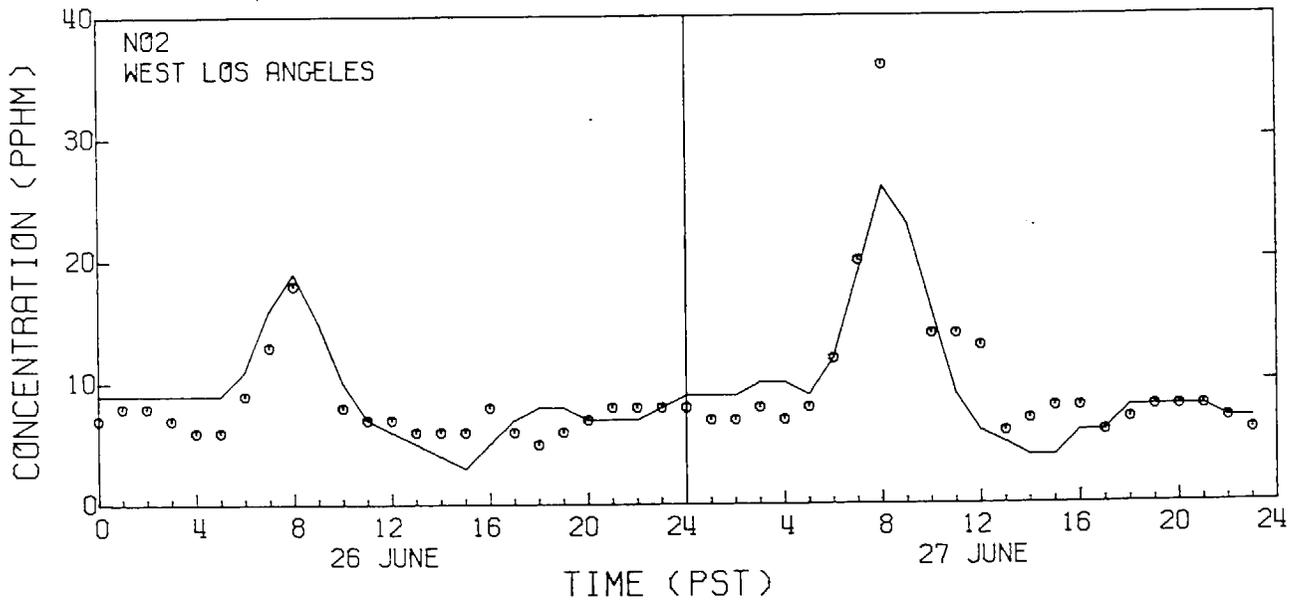
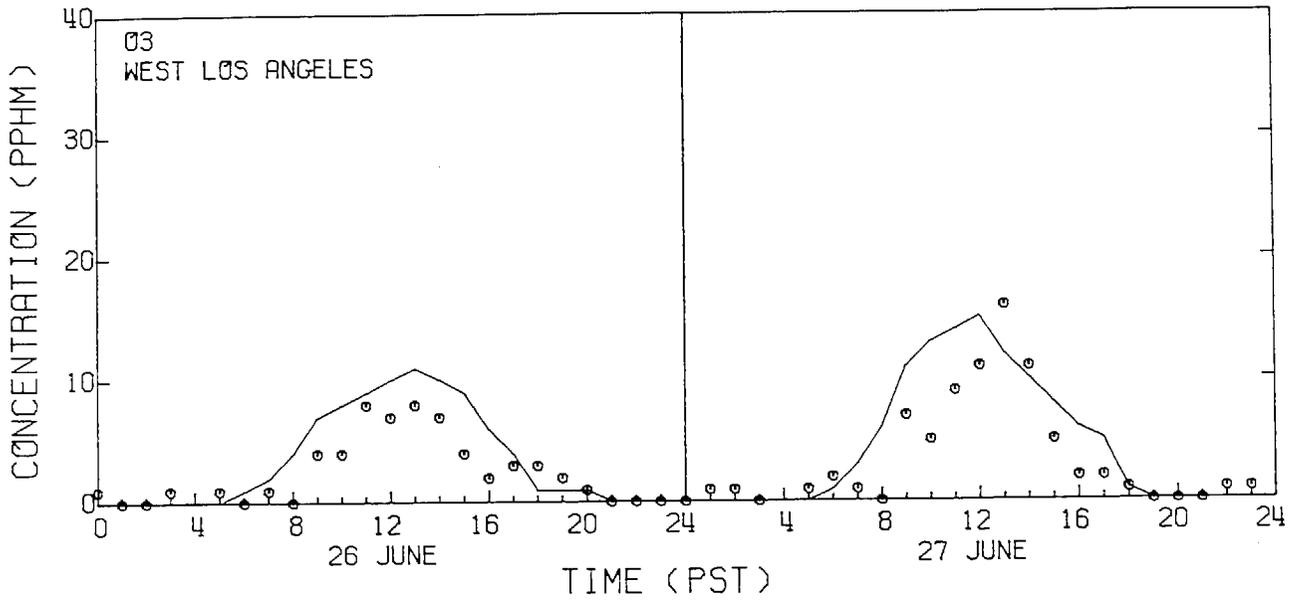


FIGURE C.25

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at West Los Angeles

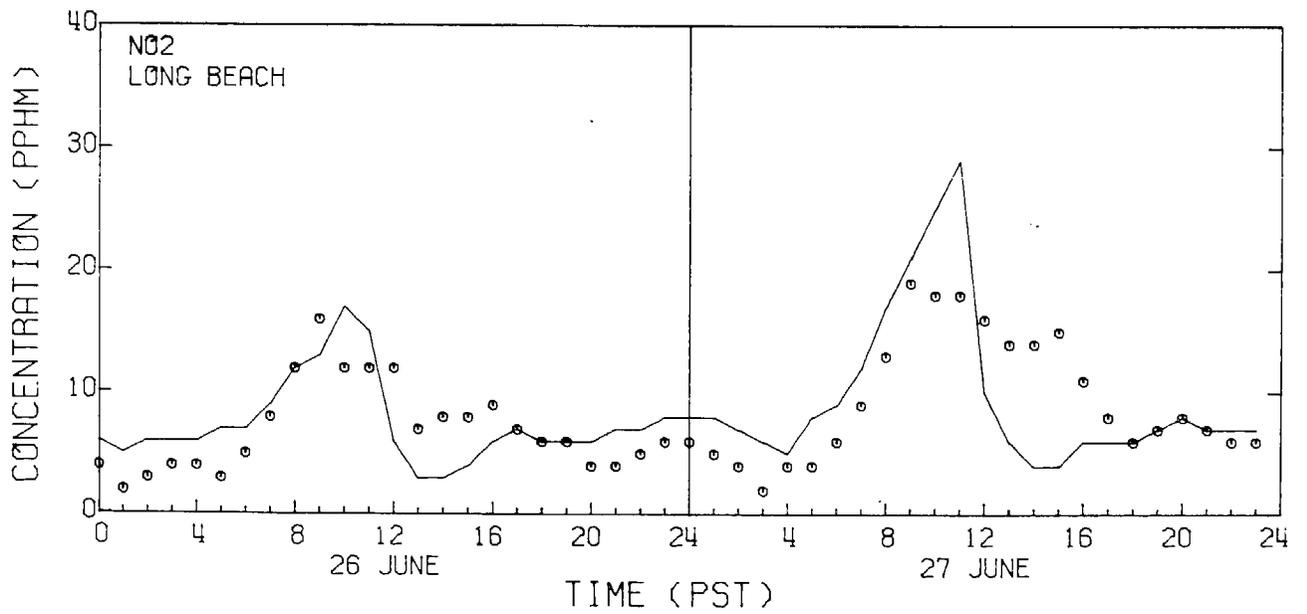
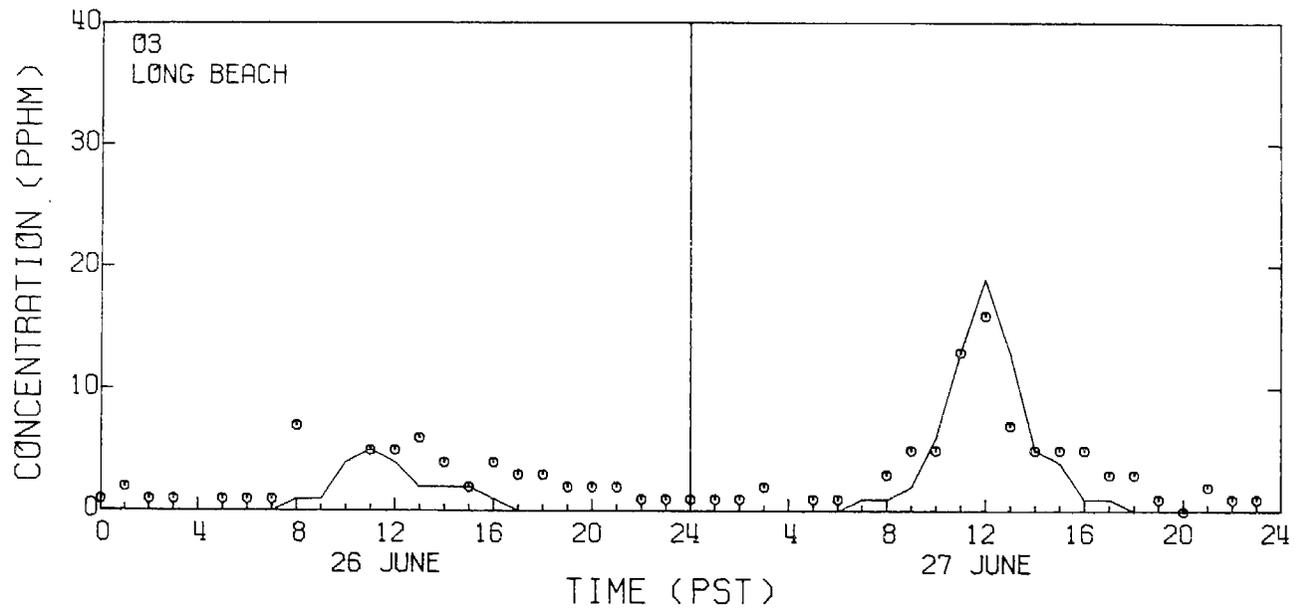


FIGURE C.26

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Long Beach

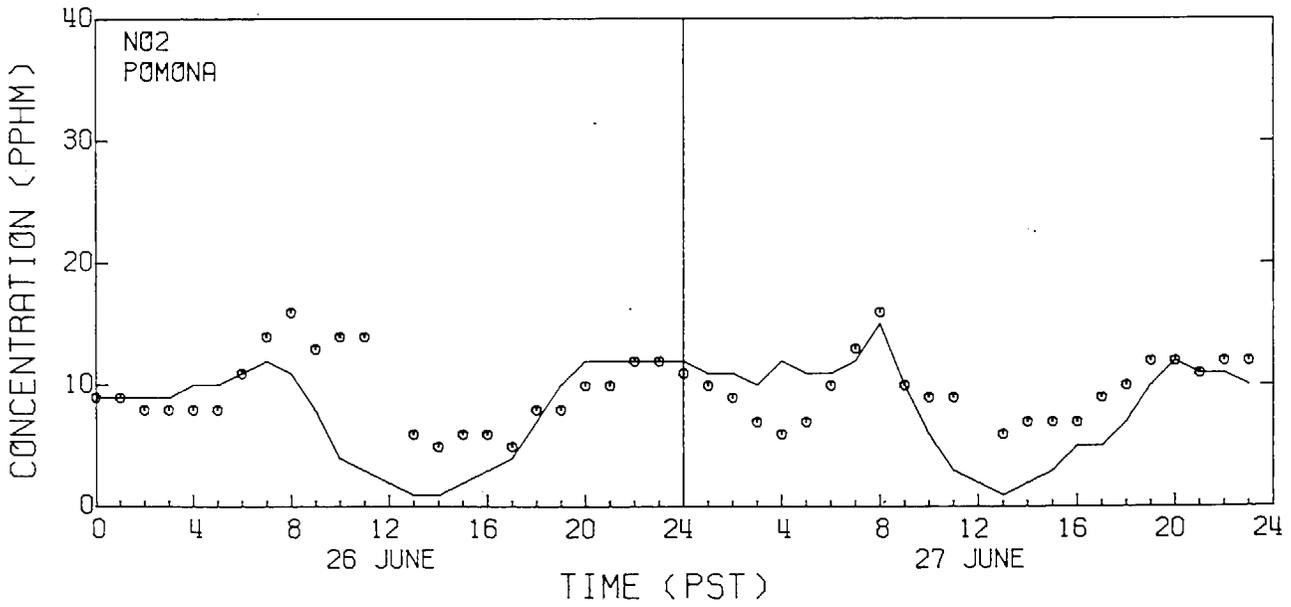
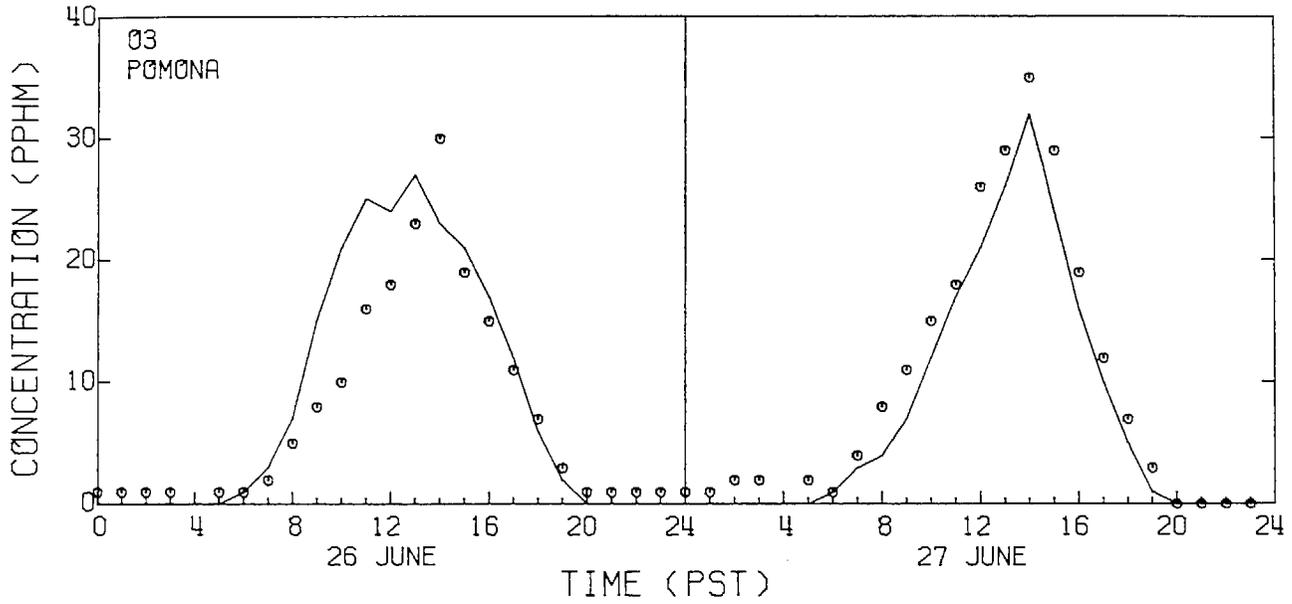


FIGURE C.27

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Pomona

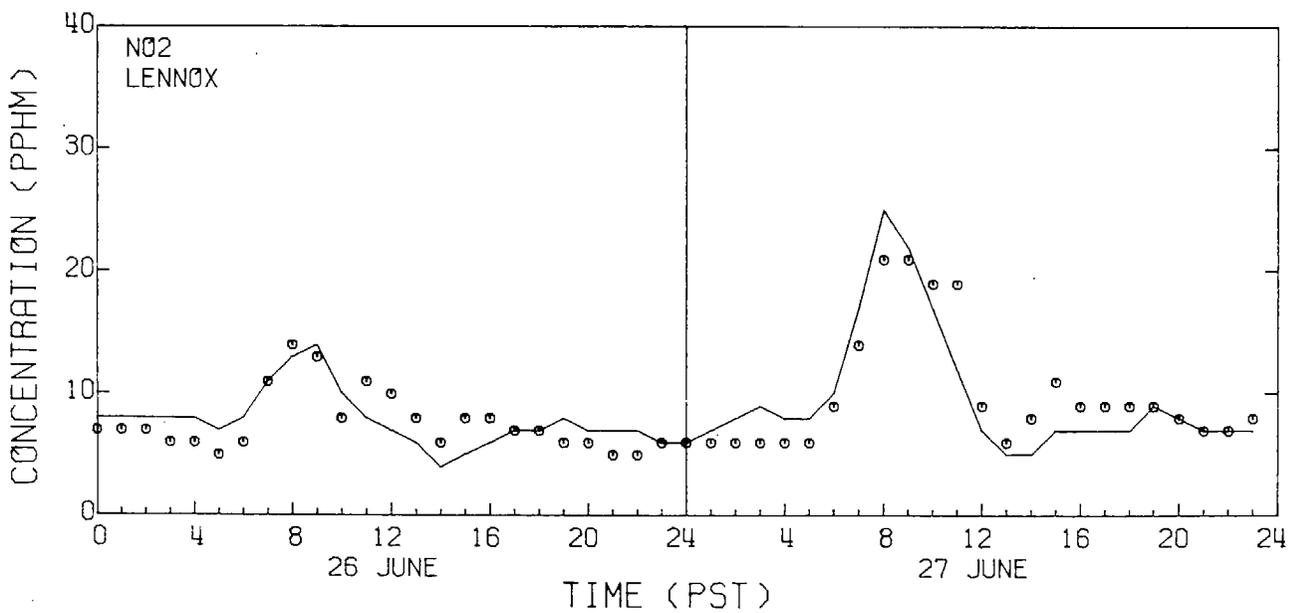
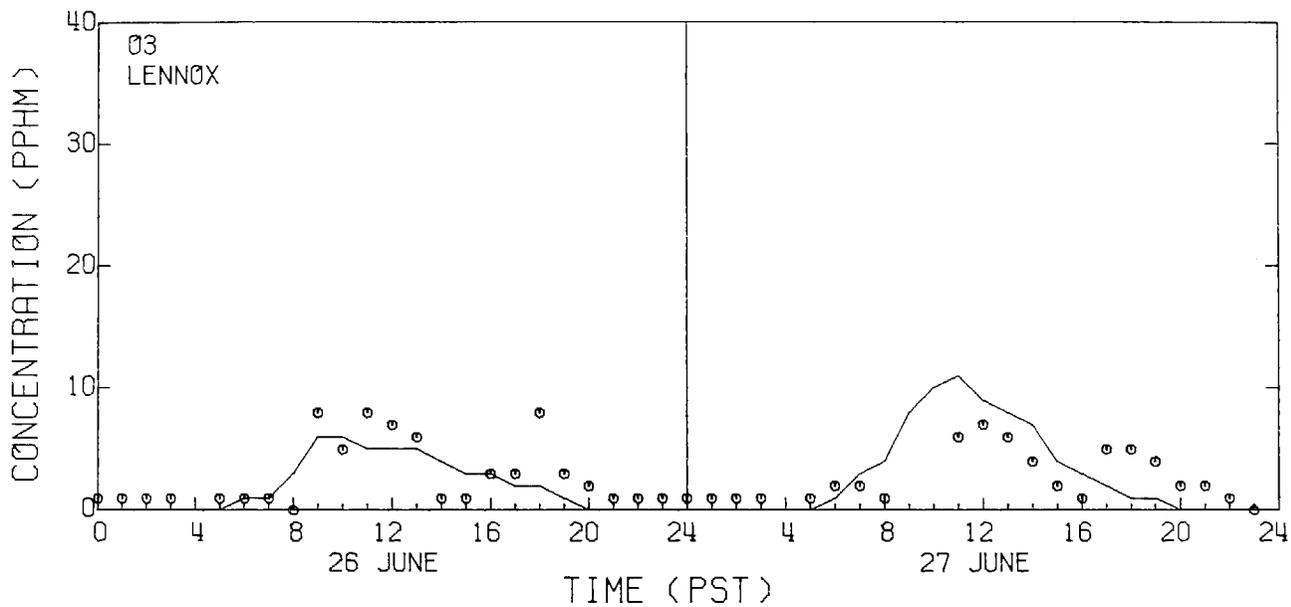
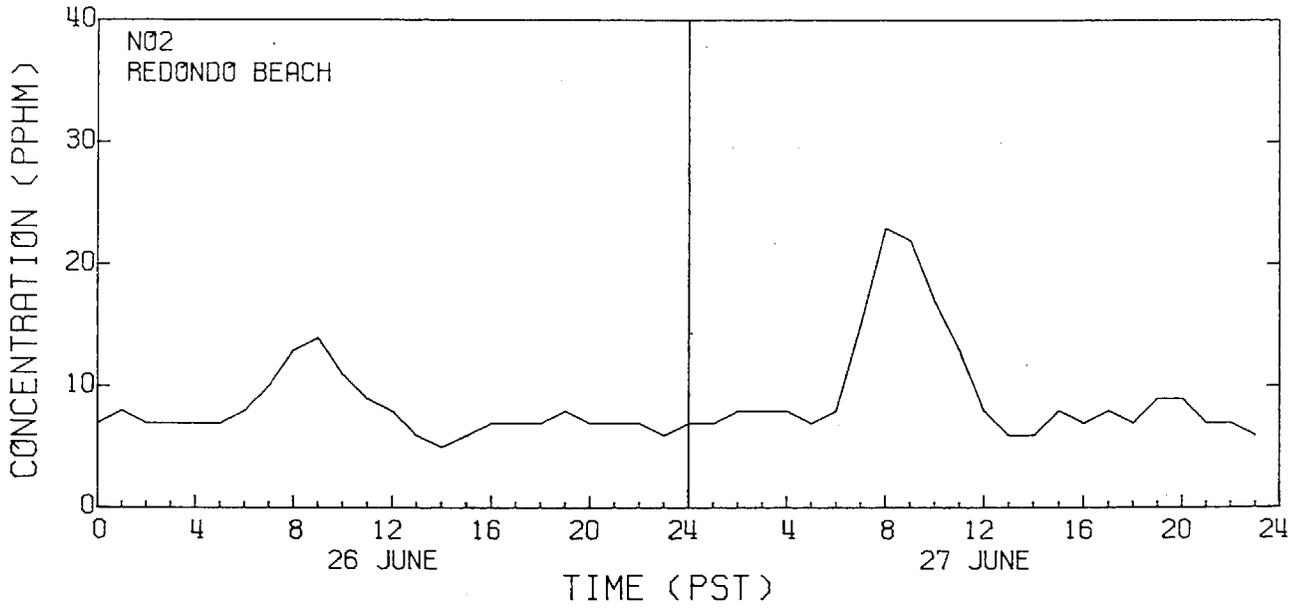
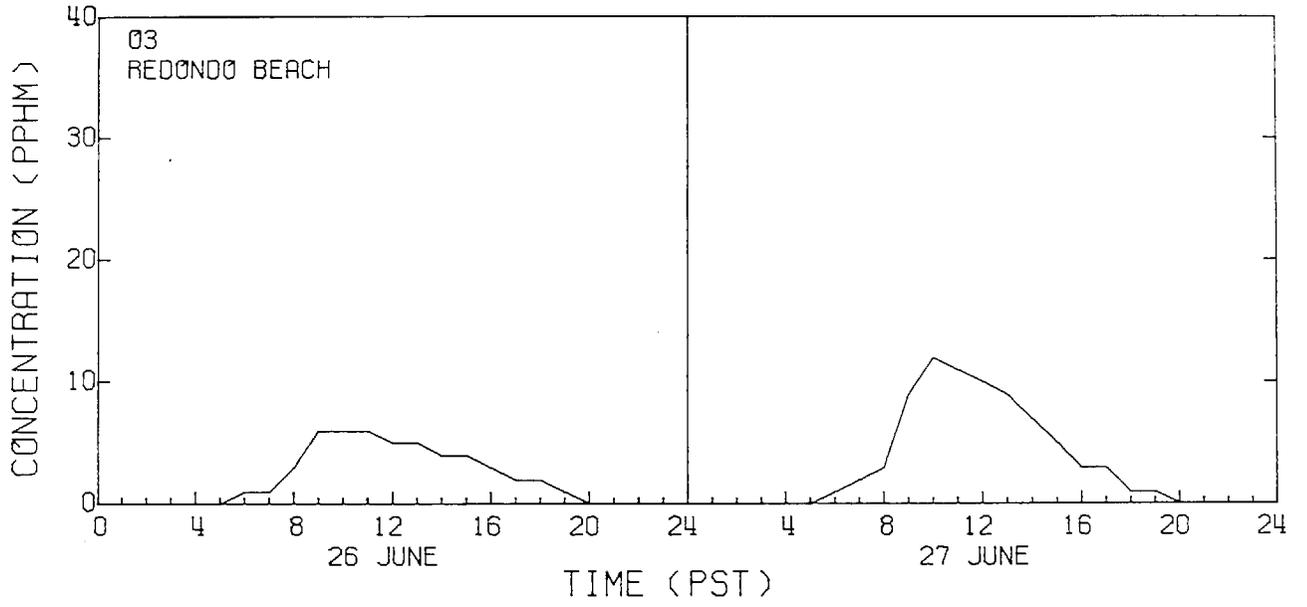
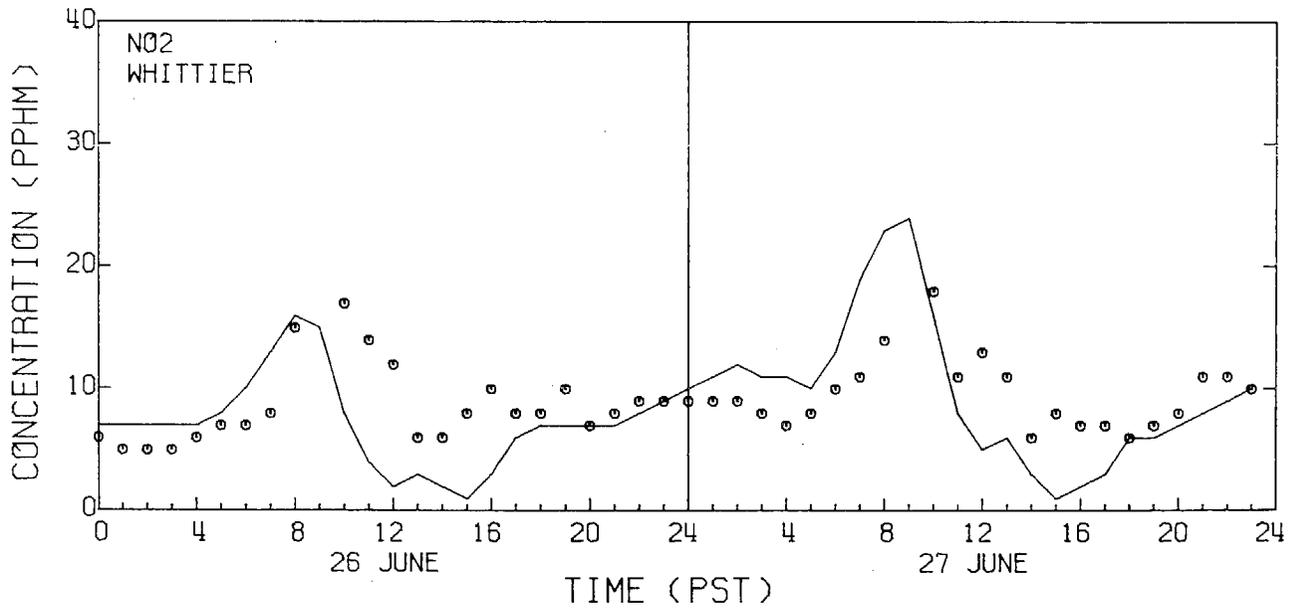
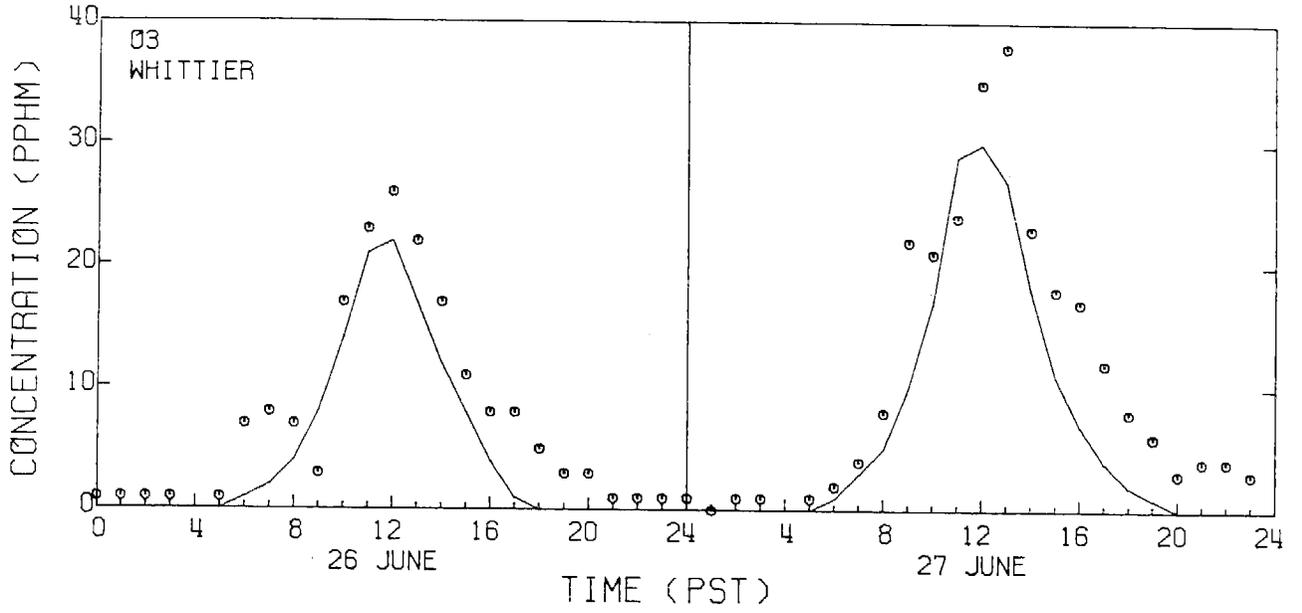


FIGURE C.28

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Lennox





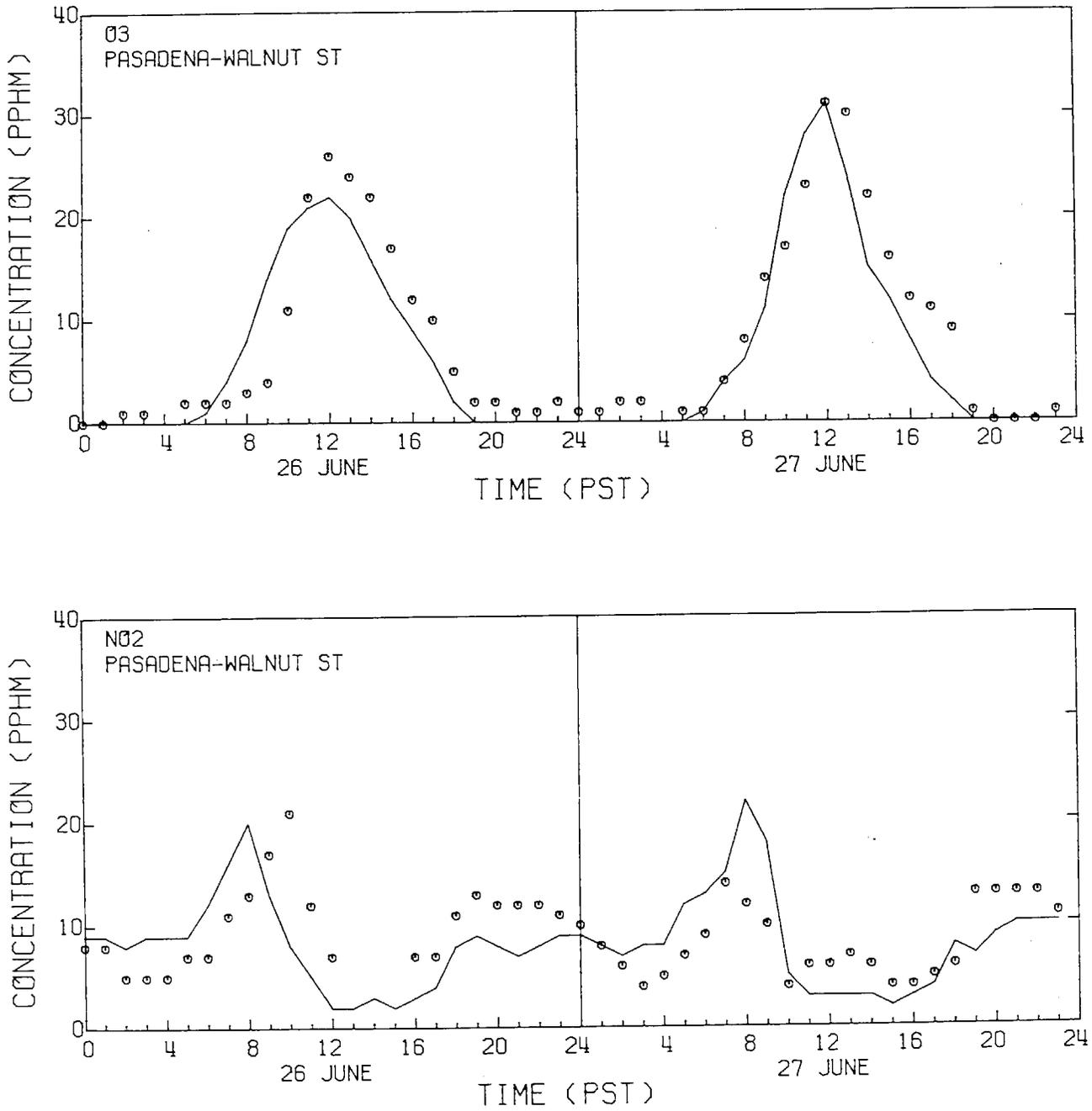


FIGURE C.31  
Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Pasadena-Walnut St

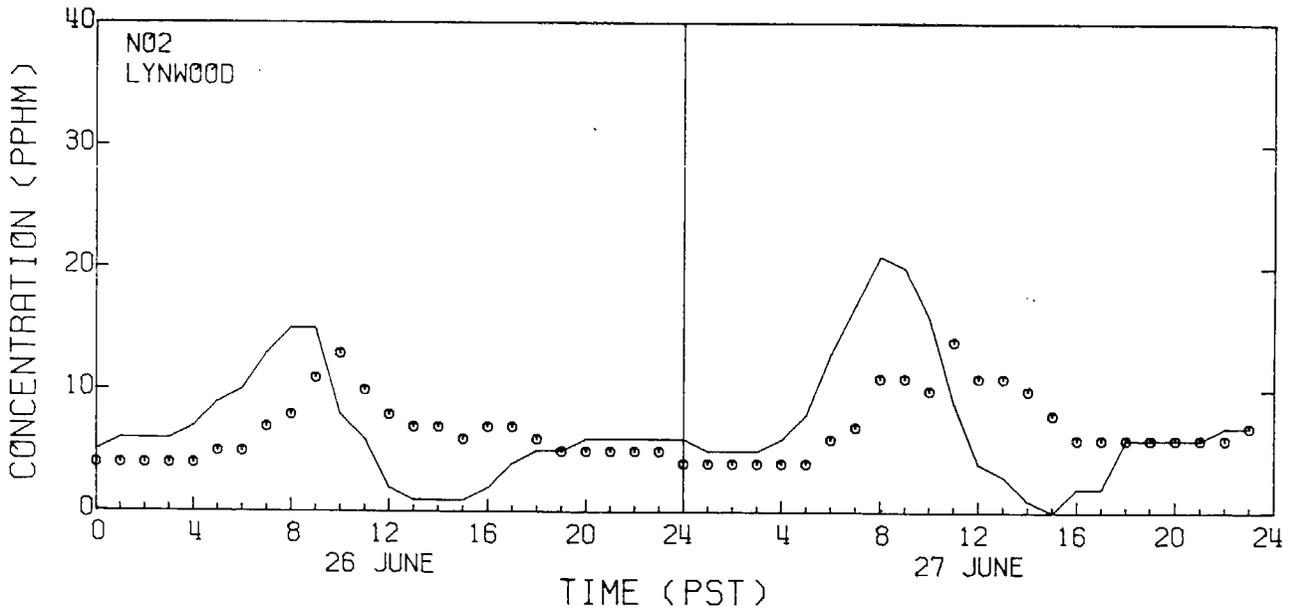
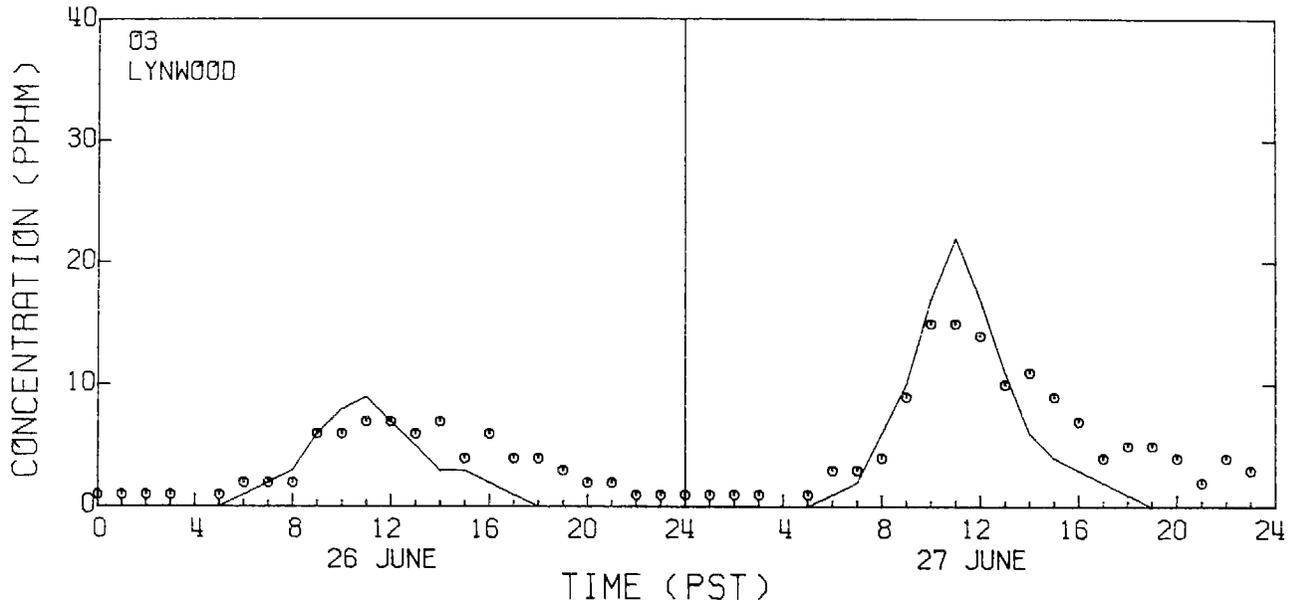


FIGURE C.32

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Lynwood

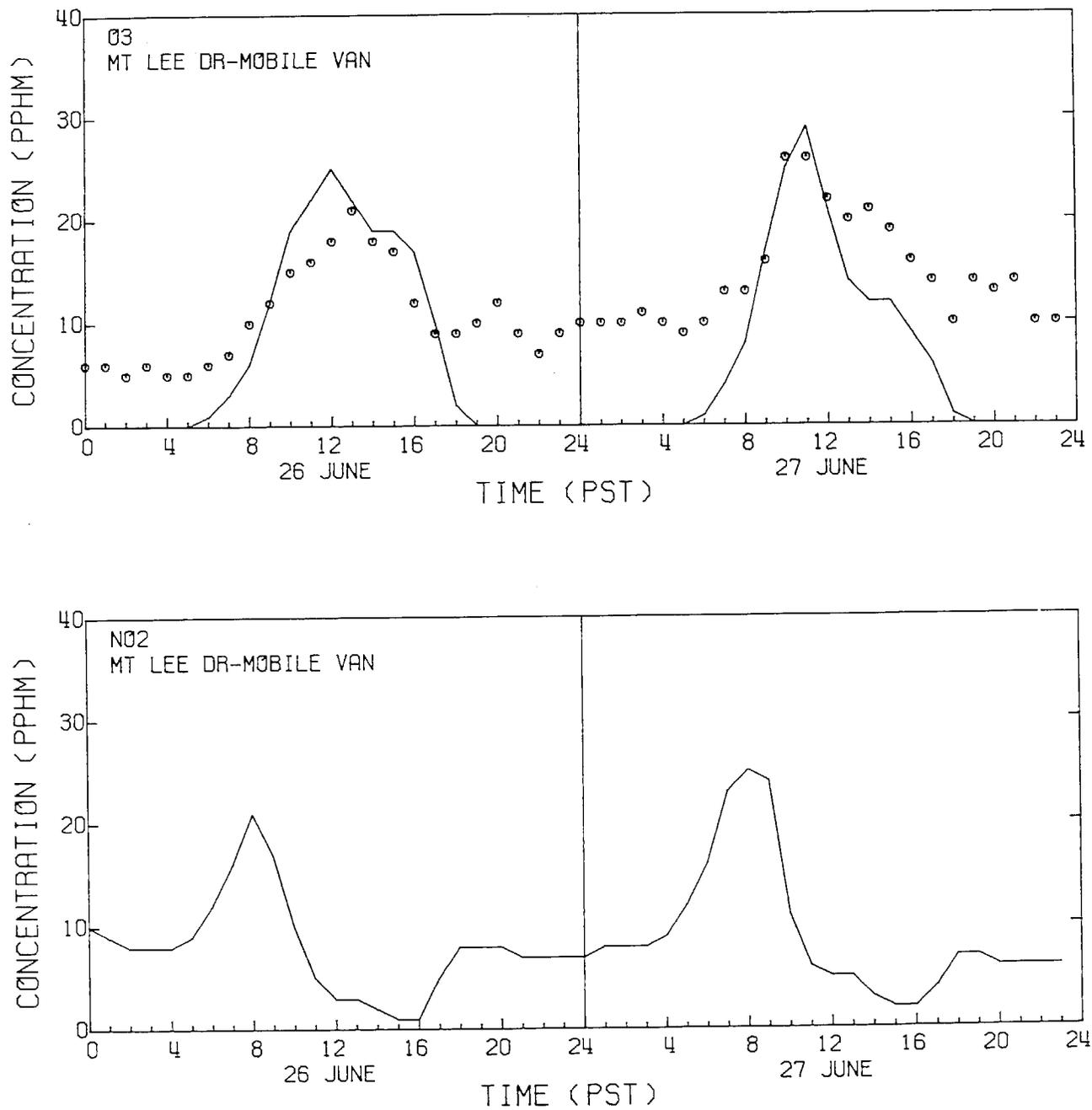


FIGURE C.33

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Mt Lee Dr-Mobile Van

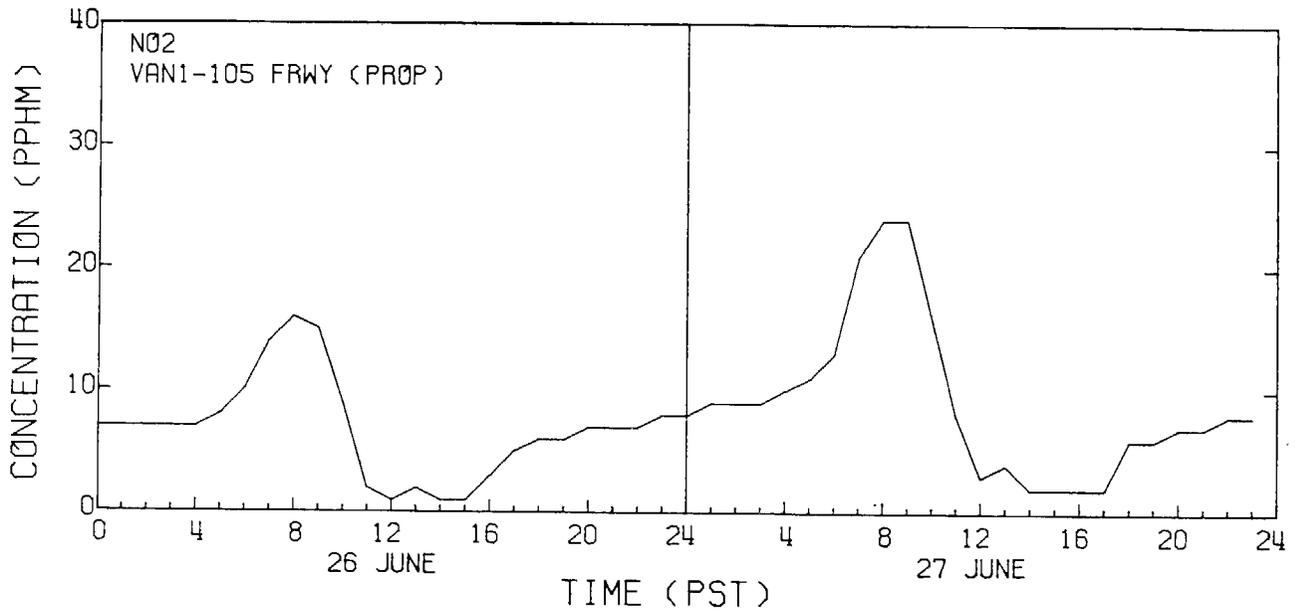
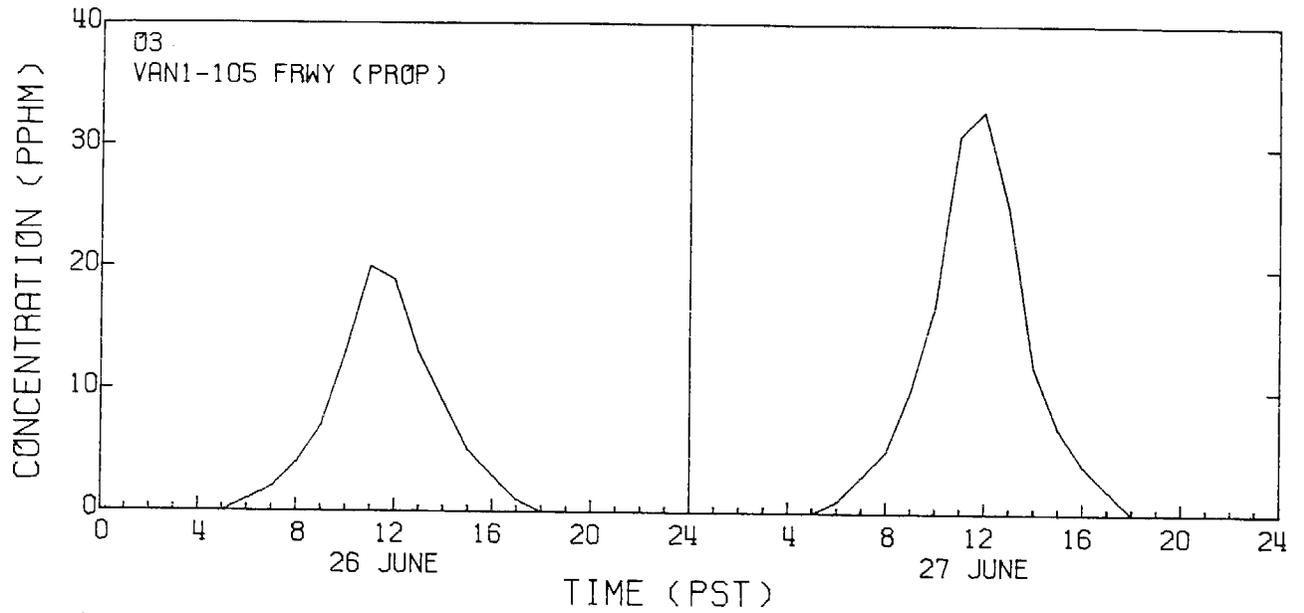


FIGURE C.34

Measured (o) and Predicted (-) Ozone and Nitrogen Dioxide  
Air Quality at Van1-105 Frwy (Prop)

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