ASSESSMENT OF EFFECTS OF CHEMICAL MECHANISM UNCERTAINTY ON AIRSHED MODEL RESULTS

Report to the

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Narseh Kumar[1]
Frederick W. Lurmann[2]
and
William P. L. Carter[3]

Statewide Air Pollution Research Center
University of California
Riverside, California 92521

[1] Sonoma Technology, Inc., Santa Rosa, California, Co-Investigator
[2] Sonoma Technology, Inc., Santa Rosa, California, Co-Principal Investigator
[3] Statewide Air Pollution Research Center, Principal Investigator

Summary

The objective of this phase of the program was to determine the effect on Urban Airshed Model (UAM) simulations of using a different and more up-to-date chemical mechanism than the Carbon Bond IV mechanism which is presently incorporated in the regulatory model. The approach was to implement updated version of the SAPRC-90 mechanism of Carter (1990), designated the SAPRC-93 mechanism, in the UAM Flexible Chemical Mechanism (FCM) solver developed by Sonoma Technology, Inc (STI) in Phase I of this program (Kumar et al, 1995), and use it to simulate the August SCAQS episode. Significant differences were found in the results. A discussion and interpretation of these results is beyond the scope of this report.

Work Carried Out

Mechanism Implementation. The updated version of the SAPRC-90 chemical mechanism of Carter (1990), modified as described by Carter et al (1993) and Carter (1995), is listed in Appendix A. Files implementing this mechanism in the format required by the FCM solver of Kumar et al (1995) were prepared and made available for downloading from the Internet, as described in Appendix B. Some minor modifications had to be made to the emissions processing routines associated with the FCM software to implement this version of the mechanism. This updated mechanism is referred to as the SAPRC-93 mechanism in the subsequent discussion. The UAM program for this mechanism was re-compiled and the chemical parameter input files were prepared as described by Kumar et al (1995).

UAM Simulations. UAM emissions input files were created for the August SCAQS episode for both the SAPRC-93 and the UAM 6.21 version of the Carbon Bond IV (CB4) mechanisms. These were generated with the 1987 on-road motor vehicle exhaust hydrocarbons scaled up by a factor of four. This scale-up was done previously to obtain what is considered acceptable performance of the UAM 6.21 model simulations to the chamber data, and is not to imply that the authors necessarily consider that this is an appropriate representation of the actual emissions. A new set of initial and boundary condition files were created for both mechanisms for this episode. UAM-FCM was first performed using the photolysis rates calculated the actinic fluxes distributed with the mechanisms. Since actinic fluxes are part of the scenario and not the mechanism, this is not an appropriate comparison of mechanism effects. Therefore, these simulations were repeated with the photolysis rates calculated using the same actinic fluxes.

Subsequently, emissions files were recreated using the SAPRC-93 mechanism with the 1987 on-road motor vehicle exhaust emissions scaled by a factor of two, and UAM simulations were performed using these new emissions files. This was done to develop a more reasonable baseline case for sensitivity calculations, which were not carried out as part of this program, and will thus not be discussed further here.

UAM input files for both chemical mechanisms, along with the modified UAM-FCM software incorporating the updates developed during this phase, were transmitted to the CARB technical support division staff.

Results

An interpretation and complete discussion of the results of these simulations is beyond the scope of this report. Appendix C gives concentration-time plots for ozone predicted by the UAM with the SAPRC-93 and UAM 6.21 version of the Carbon Bond Mechanism in the simulation of ozone measured in various stations in the August SCAQS episode. Measured ozone data are also shown for comparison. These were calculated with the motor vehicle emissions scaled by a factor of 4, and with the photolysis rates being calculated using a consistent set of actinic fluxes. It can be seen that there is a significant effect of using the different mechanism in the model simulations, with the SAPRC-93 mechanism consistently predicting higher ozone levels in most stations, though by varying amounts depending on the station. Although the calculations using the CB4 mechanism has somewhat better overall performance statistics, it should be noted that the emissions were scaled to achieve satisfactory performance using this model, and different results (presumably with lower emissions scaling factors) would be expected had the emissions been scaled to optimize the fits using the SAPRC-93 mechanism.

Conclusions

The chemical mechanism used in UAM simulations of the August SCAQS episode has a non-negligible effect on ozone predictions. Additional sensitivity calculations are required to assess the extent to which this is due to improvements in our knowledge between the time the CB4 and the SAPRC-93 mechanisms were developed, problems or approximations incorporated in the condensations incorporated in CB4 which are treated less approximately in SAPRC-93. Additional sensitivity calculations are also necessary to determine the extent to which these differences may affect control strategy conclusions which might arise out of use the UAM in regulatory applications.

References

Carter, W. P. L. (1990): "A Detailed Mechanism for the Gas-Phase Atmospheric Reactions of Organic Compounds," Atmos. Environ., 24A, 481-518.

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Kumar, N., F. W. Lurmann, and W. P. L. Carter (1995), "Development of the Flexible Chemical Mechanism Version of the Urban Airshed Model," Report to California Air Resources Board, Agreement no. 93-716. Document No. STI-94470-1508-FR, Sonoma Technology, Inc. Santa Rosa, CA, August.

Appendix A. Listing of the SAPRC-93 Chemical Mechanism.

Table A-1. List of species in the SAPRC-93 chemical mechanism.

Name	Description
Constant Species.	
O2	Oxygen
M	Air
H2O	Water
Active Inorganic Species.	
O3	Ozone
NO	Nitric Oxide
NO2	Nitrogen Dioxide
NO3	Nitrate Radical
N2O5	Nitrogen Pentoxide
HONO	Nitrous Acid
HNO3	Nitric Acid
HNO4	Peroxynitric Acid
HO2H	Hydrogen Peroxide
Active Radical Species and Operators.	
HO2.	Hydroperoxide Radicals
RO2.	Operator to Calculate Total Organic Peroxy Radicals
RCO3.	Operator to Calculate Total Acetyl Peroxy Radicals
Active Reactive Organic Product Species.	
CO	Carbon Monoxide
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes
ACET	Acetone
MEK	Lumped Ketones
PHEN	Phenol
CRES	Cresols
BALD	Aromatic aldehydes (e.g., benzaldehyde)
GLY	Glyoxal
MGLY	Methyl Glyoxal
AFG1	Reactive Aromatic Fragmentation Products from benzene and naphthalene
AFG2	Other Reactive Aromatic Fragmentation Products
AFG3	Aromatic Fragmentation Products used in adjusted m-xylene mechanism
RNO3	Organic Nitrates
NPHE	Nitrophenols
ISOPROD	Lumped isoprene product species
PAN	Peroxy Acetyl Nitrate
PPN	Peroxy Propionyl Nitrate

Table 1, (continued)

Name	Description
GPAN	PAN Analogue formed from Glyoxal
PBZN	PAN Analogues formed from Aromatic Aldehydes
-OOH	Operator Representing Hydroperoxy Groups
Non-Reacting Species	
CO2	Carbon Dioxide
-C	"Lost Carbon"
-N	"Lost Nitrogen"
H2	Hydrogen
Steady State Species and Operators.	
HO.	Hydroxyl Radicals
O	Ground State Oxygen Atoms
O*1D2	Excited Oxygen Atoms
RO2-R.	Peroxy Radical Operator representing NO to NO_2 conversion with HO_2 formation.
RO2-N.	Peroxy Radical Operator representing NO consumption with organic nitrate formation.
RO2-NP.	Peroxy Radical Operator representing NO consumption with nitrophenol formation
R2O2.	Peroxy Radical Operator representing NO to NO_2 conversion.
CCO-O2.	Peroxy Acetyl Radicals
C2CO-O2.	Peroxy Propionyl Radicals
HCOCO-O2.	Peroxyacyl Radical formed from Glyoxal
BZ-CO-O2.	Peroxyacyl Radical formed from Aromatic Aldehydes
HOCOO.	Intermediate formed in Formaldehyde + HO_2 reaction
BZ-O.	Phenoxy Radicals
BZ(NO2)-O.	Nitratophenoxy Radicals
HOCOO.	Radical Intermediate formed in the HO_2 + Formaldehyde system.
(HCHO2)	Excited Criegee biradicals formed from $=CH_2$ groups
(CCHO2)	Excited Criegee biradicals formed from $=CHCH_3$ groups
(RCHO2)	Excited Criegee biradicals formed from =CHR groups, where R not CH_3
(C(C)CO2)	Excited Criegee biradicals formed from $=C(CH_3)_2$ groups
(C(R)CO2)	Excited Criegee biradicals formed from $=C(CH_3)R$ or CR_2 groups
(BZCHO2)	Excited Criegee biradicals formed from styrenes
Hydrocarbon species represented explicitly	
CH4	Methane (EKMA simulations only)
ETHE	Ethene
ISOP	Isoprene (EKMA Simulations only)
Lumped species whose parameters depend on the emissions mixtures.	
ALK1	Alkanes and other saturated compounds with $k_{OH} < 10^4$ ppm^{-1} min^{-1}.
ALK2	Alkanes and other saturated compounds with $k_{OH} \geq 10^4$ ppm^{-1} min^{-1}.
ARO1	Aromatics with $k_{OH} < 2x10^4$ ppm^{-1} min^{-1}.
ARO2	Aromatics with $k_{OH} \geq 2x10^4$ ppm^{-1} min^{-1}.

Table 1, (continued)

Name	Description
OLE1	Alkenes (other than ethene) with $k_{OH} < 7x10^4$ ppm^{-1} min^{-1}.
OLE2	Alkenes with $k_{OH} \geq 7x10^4$ ppm^{-1} min^{-1}.
OLE3	Biogenic alkenes other than isoprene.

Table A-2. List of reactions in the SAPRC-93 Chemical Mechanism.

Rxn.	Kinetic Parameters [a]				Reactions [b]
Label	k(300)	A	Ea	B	
Inorganic Reactions					
1	(Phot. Set = NO2)				NO2 + HV = NO + O
2	2.16E-05	2.16E-05	0.00	-4.30	O + O2 + M = O3 + M
3A	1.42E+04	9.54E+03	-0.24	-1.00	O + NO2 = NO + O2
3B	2.28E+03	(Falloff Kinetics)			O + NO2 = NO3 + M
	k0 =	3.23E-03	0.00	-4.00	
	kINF =	3.23E+04	0.00	-1.00	
		F= 0.60 n= 1.00			
4	2.76E+01	2.94E+03	2.78	-1.00	O3 + NO = NO2 + O2
5	4.94E-02	2.06E+02	4.97	-1.00	O3 + NO2 = O2 + NO3
6	4.11E+04	2.49E+04	-0.30	-1.00	NO + NO3 = 2 NO2
7	6.90E-10	1.19E-10	-1.05	-2.00	NO + NO + O2 = 2 NO2
8	1.84E+03	(Falloff Kinetics)			NO2 + NO3 = N2O5
	k0 =	7.90E-02	0.00	-6.30	
	kINF =	2.20E+03	0.00	-1.50	
		F= 0.60 n= 1.00			
9	2.26E-03	3.72E+13	22.26	1.00	N2O5 + #RCON8 = NO2 + NO3
10	1.47E-06	1.47E-06	0.00	-1.00	N2O5 + H2O = 2 HNO3
11	6.13E-01	3.67E+01	2.44	-1.00	NO2 + NO3 = NO + NO2 + O2
12A	(Phot. Set = NO3NO)				NO3 + HV = NO + O2
12B	(Phot. Set = NO3NO2)				NO3 + HV = NO2 + O
13A	(Phot. Set = O3O3P)				O3 + HV = O + O2
13B	(Phot. Set = O3O1D)				O3 + HV = O*1D2 + O2
14	3.23E+05	3.23E+05	0.00	-1.00	O*1D2 + H2O = 2 HO.
15	4.29E+04	2.82E+04	-0.25	-1.00	O*1D2 + M = O + M
16	7.05E+03	(Falloff Kinetics)			HO. + NO = HONO
	k0 =	2.51E-02	0.00	-4.60	
	kINF =	2.20E+04	0.00	-1.50	
		F= 0.60 n= 1.00			
17	(Phot. Set = HONO)				HONO + HV = HO. + NO
18	1.66E+04	(Falloff Kinetics)			HO. + NO2 = HNO3
	k0 =	9.34E-02	0.00	-5.20	
	kINF =	3.52E+04	0.00	-2.30	
		F= 0.60 n= 1.00			
19	1.51E+02	9.47E+00	-1.65	-1.00	HO. + HNO3 = H2O + NO3
21	3.52E+02	3.52E+02	0.00	-1.00	HO. + CO = HO2. + CO2
22	1.02E+02	2.35E+03	1.87	-1.00	HO. + O3 = HO2. + O2
23	1.21E+04	5.43E+03	-0.48	-1.00	HO2. + NO = HO. + NO2
24	2.00E+03	(Falloff Kinetics)			HO2. + NO2 = HNO4
	k0 =	6.46E-03	0.00	-5.20	
	kINF =	6.90E+03	0.00	-2.40	
		F= 0.60 n= 1.00			
25	3.24E-03	1.95E+13	21.66	1.00	HNO4 + #RCON24 = HO2. + NO2
27	6.77E+03	1.91E+03	-0.75	-1.00	HNO4 + HO. = H2O + NO2 + O2
28	3.05E+00	1.61E+01	0.99	-1.00	HO2. + O3 = HO. + 2 O2
29A	2.54E+03	3.23E+02	-1.23	-1.00	HO2. + HO2. = HO2H + O2
29B	1.80E-03	6.82E-05	-1.95	-2.00	HO2. + HO2. + M = HO2H + O2
29C	1.34E-01	1.11E-05	-5.60	-2.00	HO2. + HO2. + H2O = HO2H + O2 + H2O
29D	9.52E-02	2.37E-06	-6.32	-2.00	HO2. + HO2. + H2O = HO2H + O2 + H2O
30A	2.54E+03	3.23E+02	-1.23	-1.00	NO3 + HO2. = HNO3 + O2
30B	1.80E-03	6.82E-05	-1.95	-2.00	NO3 + HO2. + M = HNO3 + O2
30C	1.34E-01	1.11E-05	-5.60	-2.00	NO3 + HO2. + H2O = HNO3 + O2 + H2O

Table 2 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
30D	9.52E-02	2.37E-06	-6.32	-2.00	NO3 + HO2. + H2O = HNO3 + O2 + H2O
31	(Phot. Set = H2O2)				HO2H + HV = 2 HO.
32	2.49E+03	4.84E+03	0.40	-1.00	HO2H + HO. = HO2. + H2O
33	1.45E+05	6.75E+04	-0.46	-1.00	HO. + HO2. = H2O + O2
N3N3	0.00E+00	0.00E+00	0.00	-1.00	NO3 + NO3 = 2 NO2 + O2
N3H2	0.00E+00	0.00E+00	0.00	-1.00	NO3 + HO2. = HO. + NO2 + O2
Peroxy Radical Operators					
B1	1.13E+04	6.16E+03	-0.36	-1.00	RO2. + NO = NO
B2	3.31E+04	(Falloff Kinetics)			RCO3. + NO = NO
	k0 =	2.03E+01	0.00	-9.10	
	kINF =	3.87E+04	0.00	-1.90	
		F= 0.27 n= 1.00			
B4	1.52E+04	(Falloff Kinetics)			RCO3. + NO2 = NO2
	k0 =	9.23E+00	0.00	-9.10	
	kINF =	1.76E+04	0.00	-1.90	
		F= 0.30 n= 1.00			
B5	7.19E+03	4.99E+02	-1.59	-1.00	RO2. + HO2. = HO2.
B6	7.19E+03	4.99E+02	-1.59	-1.00	RCO3. + HO2. = HO2.
B8	1.47E+00	1.47E+00	0.00	-1.00	RO2. + RO2. =
B9	1.60E+04	2.73E+03	-1.05	-1.00	RO2. + RCO3. =
B10	2.40E+04	4.11E+03	-1.05	-1.00	RCO3. + RCO3. =
B11	(Same k as Reaction B1)				RO2-R. + NO = NO2 + HO2.
B12	(Same k as Reaction B5)				RO2-R. + HO2. = -OOH
B13	(Same k as Reaction B8)				RO2-R. + RO2. = RO2. + 0.5 HO2.
B14	(Same k as Reaction B9)				RO2-R. + RCO3. = RCO3. + 0.5 HO2.
B19	(Same k as Reaction B1)				RO2-N. + NO = RNO3
B20	(Same k as Reaction B5)				RO2-N. + HO2. = -OOH + MEK - 1.5 -C
B21	(Same k as Reaction B8)				RO2-N. + RO2. = RO2. + 0.5 HO2. + MEK + 1.5 -C
B22	(Same k as Reaction B9)				RO2-N. + RCO3. = RCO3. + 0.5 HO2. + MEK + 1.5 -C
B15	(Same k as Reaction B1)				R2O2. + NO = NO2
B16	(Same k as Reaction B5)				R2O2. + HO2. =
B17	(Same k as Reaction B8)				R2O2. + RO2. = RO2.
B18	(Same k as Reaction B9)				R2O2. + RCO3. = RCO3.
B23	(Same k as Reaction B1)				RO2-XN. + NO = -N
B24	(Same k as Reaction B5)				RO2-XN. + HO2. = -OOH
B25	(Same k as Reaction B8)				RO2-XN. + RO2. = RO2. + 0.5 HO2.
B26	(Same k as Reaction B9)				RO2-XN. + RCO3. = RCO3. + HC2.
G2	(Same k as Reaction B1)				RO2-NP. + NO = NPHE
G3	(Same k as Reaction B5)				RO2-NP. + HO2. = -OOH + 6 -C
G4	(Same k as Reaction B8)				RO2-NP. + RO2. = RO2. + 0.5 HO2. + 6 -C
G5	(Same k as Reaction B9)				RO2-NP. + RCO3. = RCO3. + HC2. + 6 -C
Crigiee Biradicals					
RZ1	6.00E+01	(No T Dependence)			(HCHO2) = 0.7 HCOOH + 0.12 {HO. + HO2. + CO} + 0.18 {H2 + CO2}
RZ2	6.00E+01	(No T Dependence)			(CCHO2) = 0.25 CCOOH + 0.15 {CH4 + CO2} + 0.6 HO. + 0.3 {CCO-O2. + RCO3.} + 0.3 {RO2-R. + HCHO + CO + RO2.}
RZ3	6.00E+01	(No T Dependence)			(RCHO2) = 0.25 CCOOH + 0.15 CO2 + 0.6 HO. + 0.3 {C2CO-O2. + RCO3.} + 0.3 {RO2-R. + CCHO + CO + RO2.} + 0.55 -C
RZ4	6.00E+01	(No T Dependence)			(C(C)CO2) = HO. + R2O2. + HCHO + CCO-O2. + RCO3. + RO2.
RZ5	6.00E+01	(No T Dependence)			(C(R)CO2) = HO. + CCO-O2. + CCHO + R2O2. + RCO3. + RO2.
RZ6	6.00E+01	(No T Dependence)			(CYCCO2) = 0.3 {HO. + C2CO-O2. + R2O2. + RCO3. + RO2.} + 0.3 RCHO + 4.2 -C
RZ7	6.00E+01	(No T Dependence)			(BZCHO2) = 0.5 {BZ-O. + R2O2. + CO + HO.}
ISZ1	6.00E+01	(No T Dependence)			(C:CC(C)O2) = HO. + R2O2. + HCHO + C2CO-O2. + RO2. + RCO3.
ISZ2	6.00E+01	(No T Dependence)			(C:C(C)CHO2) = 0.75 RCHO + 0.25 ISOPROD + 0.5 -C
MAZ1	6.00E+01	(No T Dependence)			(C2(O2)CHO) = HO. + R2O2. + HCHO + HCOCO-O2. + RO2. + RCO3.
M1Z1	6.00E+01	(No T Dependence)			(HOCCHO2) = 0.6 HO. + 0.3 {CCO-O2. + RCO3.} + 0.3 {RO2-R. + HCHO + CO + RO2.} + 0.8 -C
M2Z1	6.00E+01	(No T Dependence)			(HCOCHO2) = 0.12 {HO2. + 2 CO + HO.} + 0.74 -C + 0.51 {CO2 + HCHO}
M2Z2	6.00E+01	(No T Dependence)			(C2(O2)COH) = HO. + MGLY + HO2. + R2O2. + RO2.
Organic Product Species					
B7	(Phot. Set = CO2H)				-OOH + HV = HO2. + HO.
B7A	2.65E+03	1.73E+03	-0.25	-1.00	HO. + -OOH = HO.
B7B	5.45E+03	2.63E+03	-0.44	-1.00	HO. + -OOH = RO2-R. + RO2.

Table 2 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
C1	(Phot. Set = HCHONEWR)				HCHO + HV = 2 HO2. + CO
C2	(Phot. Set = HCHONEWM)				HCHO + HV = H2 + CO
C3	1.43E+04	1.65E+03	-1.29	1.00	HCHO + HO. = HO2. + CO + H2O
C4	1.14E+02	1.42E+01	-1.24	-1.00	HCHO + HO2. = HOCOO.
C4A	1.06E+04	1.44E+14	13.91	0.00	HOCOO. = HO2. + HCHO
C4B	(Same k as Reaction B1)				HOCOO. + NO = -C + NO2 + HO2.
C9	9.36E-01	4.11E+03	5.00	-1.00	HCHO + NO3 = HNO3 + HO2. + CO
C10	2.30E+04	8.15E+03	-0.62	-1.00	CCHO + HO. = CCO-O2. + H2O + RCO3.
C11A	(Phot. Set = CCHOR)				CCHO + HV = CO + HO2. + HCHO + RO2-R. + RO2.
C12	4.17E+00	2.05E+03	3.70	-1.00	CCHO + NO3 = HNO3 + CCO-O2. + RCO3.
C13	(Same k as Reaction B2)				CCO-O2. + NO = CO2 + NO2 + HCHO + RO2-R. + RO2.
C14	(Same k as Reaction B4)				CCO-O2. + NO2 = PAN
C15	(Same k as Reaction B6)				CCO-O2. + HO2. = -OOH + CO2 + HCHO
C16	(Same k as Reaction B9)				CCO-O2. + RO2. = RO2. + 0.5 HO2. + CO2 + HCHO
C17	(Same k as Reaction B10)				CCO-O2. + RCO3. = RCO3. + HO2. + CO2 + HCHO
C18	3.90E-02	(Falloff Kinetics)			PAN = CCO-O2. + NO2 + RCO3.
	k0 =	7.19E+12	23.97	-1.00	
	kINF =	2.40E+18	27.08	0.00	
		F= 0.30	n= 1.00		
C25	2.89E+04	1.25E+04	-0.50	-1.00	RCHO + HO. = C2CO-O2. + RCO3.
C26	(Phot. Set = RCHO)				RCHO + HV = CCHO + RO2-R. + RO2. + CO + HO2.
C27	4.17E+00	2.05E+03	3.70	-1.00	NO3 + RCHO = HNO3 + C2CO-O2. + RCO3.
C28	(Same k as Reaction B2)				C2CO-O2. + NO = CCHO + RO2-R. + CO2 + NO2 + RO2.
C29	1.23E+04	1.23E+04	0.00	-1.00	C2CO-O2. + NO2 = PPN
C30	(Same k as Reaction B6)				C2CO-O2. + HO2. = -OOH + CCHO + CO2
C31	(Same k as Reaction B9)				C2CO-O2. + RO2. = RO2. + 0.5 HO2. + CCHO + CO2
C32	(Same k as Reaction B10)				C2CO-O2. + RCO3. = RCO3. + HO2. + CCHO + CO2
C33	4.07E-02	9.60E+18	27.97	0.00	PPN = C2CO-O2. + NO2 + RCO3.
C38	3.28E+02	7.06E+02	0.46	1.00	ACET + HO. = R2O2. + HCHO + CCO-O2. + RCO3. + RO2.
C39	(Phot. Set = ACET-93C)				ACET + HV = CCO-O2. + HCHO + RO2-R. + RCO3. + RO2.
C44	1.70E+03	4.29E+02	-0.82	1.00	MEK + HO. = H2O + 0.5 {CCHO + HCHO + CCO-O2. + C2CO-O2.} + RCO3. + 1.5 {R2O2. + RO2.}
C57	(Phot. Set = KETONE) (Overall Q.Y. = 0.1)				MEK + HV = CCO-O2. + CCHO + RO2-R. + RCO3. + RO2.
C95	3.03E+03	3.22E+04	1.41	-1.00	RNO3 + HO. = NO2 + 0.155 MEK + 1.05 RCHO + 0.48 CCHO + 0.16 HCHO + 0.11 -C + 1.39 {R2O2. + RO2.}
C58A	(Phot. Set = GLYOXAL1)				GLY + HV = 0.8 HO2. + 0.45 HCHO + 1.55 CO
C58B	(Phot. Set = GLYOXAL2) (Overall Q.Y. = 0.029)				GLY + HV = 0.13 HCHO + 1.87 CO
C59	1.67E+04	1.67E+04	0.00	-1.00	GLY + HO. = 0.6 HO2. + 1.2 CO + 0.4 {HCOCO-O2. + RCO3.}
C60	(Same k as Reaction C12)				GLY + NO3 = HNO3 + 0.6 HO2. + 1.2 CO + 0.4 {HCOCO-O2. + RCO3.}
C62	(Same k as Reaction B2)				HCOCO-O2. + NO = NO2 + CO2 + CO + HO2.
C63	(Same k as Reaction B4)				HCOCO-O2. + NO2 = GPAN
C65	(Same k as Reaction B6)				HCOCO-O2. + HO2. = -OOH + CO2 + CO
C66	(Same k as Reaction B9)				HCOCO-O2. + RO2. = RO2. + 0.5 HO2. + CO2 + CO
C67	(Same k as Reaction B10)				HCOCO-O2. + RCO3. = RCO3. + HO2. + CO2 + CO
C64	(Same k as Reaction C18)				GPAN = HCOCO-O2. + NO2 + RCO3.
C68A	(Phot. Set = MEGLYOX1)				MGLY + HV = HO2. + CO + CCO-O2. + RCO3.
C68B	(Phot. Set = MEGLYOX2)				MGLY + HV + 0.107 = HO2. + CO + CCO-O2. + RCO3.
C69	2.52E+04	2.52E+04	0.00	-1.00	MGLY + HO. = CO + CCO-O2. + RCO3.
C70	(Same k as Reaction C12)				MGLY + NO3 = HNO3 + CO + CCO-O2. + RCO3.
G46	3.86E+04	3.86E+04	0.00	-1.00	HO. + PHEN = 0.15 RO2-NP. + 0.85 RO2-R. + 0.2 GLY + 4.7 -C + RO2.
G51	5.28E+03	5.28E+03	0.00	-1.00	NO3 + PHEN = HNO3 + BZ-O.
G52	6.16E+04	6.16E+04	0.00	-1.00	HO. + CRES = 0.15 RO2-NP. + 0.85 RO2-R. + 0.2 MGLY + 5.5 -C + RO2.
G57	3.08E+04	3.08E+04	0.00	-1.00	NO3 + CRES = HNO3 + BZ-O. + -C
G30	1.89E+04	1.89E+04	0.00	-1.00	BALD + HO. = BZ-CO-O2. + RCO3.
G31	(Phot. Set = BZCHO)				BALD + HV + 0.05 = 7 -C
G32	3.83E+00	2.05E+03	3.75	-1.00	BALD + NO3 = HNO3 + BZ-CO-O2.
G33	(Same k as Reaction B2)				BZ-CO-O2. + NO = BZ-O. + CO2 + NO2 + R2O2. + RO2.

Table 2 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
G34	1.23E+04	1.23E+04	0.00	-1.00	BZ-CO-O2. + NO2 = PBZN
G36	(Same k as Reaction B6)				BZ-CO-O2. + HO2. = -OCH + CO2 + PHEN
G37	(Same k as Reaction B9)				BZ-CO-O2. + RO2. = RC2. + 0.5 HO2. + CO2 + PHEN
G38	(Same k as Reaction B10)				BZ-CO-O2. + RCO3. = RCO3. + HO2. + CO2 + PHEN
G35	1.30E-02	9.60E+16	25.90	0.00	PBZN = BZ-CO-O2. + NO2 + RCO3.
G43	5.19E+04	1.91E+04	-0.60	-1.00	BZ-O. + NO2 = NPHE
G44	(Same k as Reaction B5)				BZ-O. + HO2. = PHEN
G45	6.00E-02	(No T Dependence)			BZ-O. = PHEN
G58	5.28E+03	5.28E+03	0.00	-1.00	NPHE + NO3 = HNO3 + BZ(NO2)-O.
G59	(Same k as Reaction G43)				BZ(NO2)-O. + NO2 = 2 -N + 6 -C
G60	(Same k as Reaction B5)				BZ(NO2)-O. + HO2. = NPHE
G61	(Same k as Reaction G45)				BZ(NO2)-O. = NPHE
G7	1.67E+04	1.67E+04	0.00	-1.00	HO. + AFG1 = HCOCO-O2. + RCO3.
G8	(Phot. Set = ACROLEIN) (Overall Q.Y. = 0.029)				AFG1 + HV = HO2. + HCOCO-O2. + RCO3.
U2OH	2.52E+04	2.52E+04	0.00	-1.00	HO. + AFG2 = C2CO-O2. + RCO3.
U2HV	(Phot. Set = ACROLEIN) (Overall Q.Y. = 0.615)				AFG2 + HV = HO2. + CO + CCO-O2. + RCO3.
IPO3	1.04E-02	1.04E-02	0.00	-1.00	ISOPROD + O3 = 0.02 CCHO + 0.04 HCHO + 0.01 GLY + 0.84 MGLY + 0.09 MEK + 0.66 (HCHO2) + 0.09 (HCOCHO2) + 0.18 (HOCCHO2) + 0.06 (C2(O2)CHO) + 0.01 (C2(O2)COH) + -.39 -C
IPHV	(Phot. Set = ACROLEIN)				ISOPROD + HV + 0.0036 = 0.333 CO + 0.067 CCHO + 0.9 HCHO + 0.033 MEK + 0.333 HO2. + 0.7 RO2-R. + 0.267 CCO-O2. + 0.7 C2CO-O2. + 0.7 RO2. + 0.967 RCO3. + -.133 -C
IPN3	1.47E+00	1.47E+00	0.00	-1.00	ISOPROD + NO3 = 0.643 CO + 0.282 HCHO + 0.85 RNO3 + 0.357 RCHO + 0.925 HO2. + 0.075 C2CO-O2. + 0.075 R2O2. + 0.925 RO2. + 0.075 RCO3. + 0.075 HNO3 + -2.471 -C
Explicitly Represented Primary Emitted VOCs					
RCH4	1.28E+01	9.18E+02	2.55	1.00	CH4 + HO. = HCHO + RO2-R. + RO2.
ETOH	1.24E+04	2.88E+03	-0.87	-1.00	ETHE + HO. = RO2-R. + RO2. + 1.56 HCHO + 0.22 CCHO
ETO3	2.47E-03	1.34E+01	5.13	-1.00	ETHE + O3 = HCHO + (HCHO2)
ETN3	3.16E-01	7.97E+03	6.04	-1.00	ETHE + NO3 = R2O2. + RO2. + 2 HCHO + NO2
ETOA	1.09E+03	1.53E+04	1.57	-1.00	ETHE + O = RO2-R. + HO2. + RO2. + HCHO + CO
ISOH	1.45E+05	3.73E+04	-0.81	-1.00	ISOP + HO. = 0.088 RO2-N. + 0.912 RO2-R. + 0.629 HCHO + 0.912 ISOPROD + 0.079 R2O2. + 1.079 RO2. + 0.283 -C
ISO3	1.97E-02	1.15E+01	3.80	-1.00	ISOP + O3 = 0.4 HCHO + 0.6 ISOPROD + 0.55 (HCHO2) + 0.2 (C:CC(C)O2) + 0.2 (C:C(C)CHO2) + 0.05 -C
ISOA	5.28E+04	5.28E+04	0.00	-1.00	ISOP + O = 0.75 {ISOPROD + -C }+ 0.25 {C2CO-O2. + RCO3. + 2 HCHO + RO2-R. + RO2.}
ISN3	1.00E+03	4.45E+03	0.89	-1.00	ISOP + NO3 = 0.8 {RCHO + RNO3 + RO2-R.} + 0.2 {ISOPROD + R2O2. + NO2} + RO2. + -2.2 -C
ISN2	2.20E-04	2.20E-04	0.00	-1.00	ISOP + NO2 = 0.8 {RCHO + RNO3 + RO2-R.} + 0.2 {ISOPROD + R2O2. + NO} + RO2. + -2.2 -C
IPOH	4.93E+04	4.93E+04	0.00	-1.00	ISOPROD + HO. = 0.293 CO + 0.252 CCHO + 0.126 HCHO + 0.041 GLY + 0.021 RCHO + 0.168 MGLY + 0.314 MEK + 0.503 RO2-R. + 0.21 CCO-O2. + 0.288 C2CO-O2. + 0.21 R2O2. + 0.713 RO2. + 0.498 RCO3. + -.112 -C
Lumped species whose parameters depend on groups of species they represent (Parameters shown are based on emissions in August 27, 1987 SCAQS episode)					
A1OH	5.30E+03	3.29E+03	-0.28	0.00	ALK1 + HO. = 0.72 RO2-R. + 0.062 RO2-N. + 0.004 RO2-XN. + 0.214 HO2. + 0.412 R2O2. + 1.198 RO2. + 0.055 HCHO + 0.298 CCHO + 0.159 RCHO + 0.322 ACET + 0.374 MEK + 0.026 CO + 0.04 GLY + 0.149 -C
A2OH	1.49E+04	7.21E+03	-0.43	0.00	ALK2 + HO. = 0.71 RO2-R. + 0.215 RO2-N. + 0.001 RO2-XN. + 0.074 HO2. + 0.747 R2O2. + 1.672 RO2. + 0.058 HCHO + 0.086 CCHO + 0.309 RCHO + 0.001 ACET + 1.01 MEK + 0.015 CO + 0.017 CO2 + 1.19 -C
B1OH	8.67E+03	(No T Dependence)			AR01 + HO. = 0.741 RO2-R. + 0.259 HO2. + 0.741 RO2. + 0.013 PHEN + 0.246 CRES + 0.08 BALD + 0.123 GLY +

Table 2 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
					0.124 MGLY + 0.096 AFG1 + 0.463 AFG2 + 2.519 -C
B2OH	4.38E+04	1.63E+04	-0.59	0.00	ARO2 + HO. = 0.819 RO2-R. + 0.003 RO2-NP. + 0.178 HO2. + 0.822 RO2. + 0.002 PHEN + 0.176 CRES + 0.036 BALD + 0.073 GLY + 0.439 MGLY + 0.006 AFG1 + 0.733 AFG2 + 3.167 -C
O1OH	4.41E+04	3.08E+03	-1.59	0.00	OLE1 + HO. = 0.946 RO2-R. + 0.054 RO2-N. + RO2. + 0.946 HCHO + 0.61 CCHO + 0.268 RCHO + 0.069 ACET + 0.351 -C
O1O3	1.56E-02	2.41E+00	3.00	0.00	OLE1 + O3 = 0.617 HCHO + 0.244 CCHO + 0.258 RCHO + 0.014 ACET + 0.139 -C + 0.383 (HCHO2) + 0.499 (CCHO2) + 0.056 (RCHO2) + 0.063 (C(C)CO2
O1N3	5.30E+01	1.21E+03	1.86	0.00	OLE1 + NO3 = R2O2. + RO2. + HCHO + 0.61 CCHO + 0.314 RCHO + 0.077 ACET + 0.404 -C + NO2
O1OA	7.22E+03	6.32E+03	-0.08	0.00	OLE1 + O = 0.4 HO2. + 0.5 RCHO + 0.5 MEK + 0.295 -C
O2OH	9.52E+04	6.71E+03	-1.58	0.00	OLE2 + HO. = 0.912 RO2-R. + 0.088 RO2-N. + RO2. + 0.193 HCHO + 1.025 CCHO + 0.465 RCHO + 0.066 ACET + 0.028 MEK + 0.016 BALD + 0.311 -C
O2O3	2.86E-01	2.93E+00	1.39	0.00	OLE2 + O3 = 0.126 HCHO + 0.551 CCHO + 0.333 RCHO + 0.031 ACET + 0.031 MEK + 0.007 BALD + 0.091 -C + 0.072 (HCHO2) + 0.625 (CCHO2) + 0.219 (RCHO2) + 0.073 (C(C)CO2 + 0.01 (BZCHO2)
O2N3	1.53E+03	1.21E+03	-0.14	0.00	OLE2 + NO3 = R2O2. + RO2. + 0.198 HCHO + 1.086 CCHO + 0.552 RCHO + 0.079 ACET + 0.031 MEK + 0.017 BALD + 0.3 -C + NO2
O2OA	3.80E+04	1.20E+04	-0.69	0.00	OLE2 + O = 0.4 HO2. + 0.5 RCHO + 0.5 MEK + 1.309 -C
O3OH	1.63E+05	4.33E+04	-0.79	0.00	OLE3 + HO. = 0.75 RO2-R. + 0.25 RO2-N. + RO2. + 0.266 HCHO + 0.242 RCHO + 0.508 MEK + 5.725 -C
O3O3	1.81E-01	1.40E-01	-0.15	0.00	OLE3 + O3 = 0.142 HCHO + 0.086 RCHO + 0.213 MEK + 5.622 -C + 0.213 (HCHO2) + 0.236 (RCHO2) + 0.551 (C(R)CO2
O3N3	1.26E+04	3.26E+03	-0.80	0.00	OLE3 + NO3 = R2O2. + RO2. + 0.355 HCHO + 0.322 RCHO + 0.678 MEK + 5.967 -C + NO2
O3OA	9.95E+04	3.69E+04	-0.59	0.00	OLE3 + O = 0.4 HO2. + 0.5 RCHO + 0.5 MEK + 6.5 -C

[a] Except as noted, expression for rate constant is $k = A\ e^{Ea/RT}\ (T/300)^B$. Rate constants and A factor are in ppm, min units. Units of Ea is kcal $mole^{-1}$. "Phot Set" means this is a photolysis reaction, with the absorption coefficients and quantum yields given in Table A-3. If an "overall Q.Y." value is given for a photolysis reaction, the rate constant calculated assuming unit quantum yield is multiplied by this value to yield the rate constant used in the reaction. In addition, if "#(number)" or "#(parameter)" is given as a reactant, then the value of that number or parameter is multiplied by the result in the "rate constant expression" columns to obtain the rate constant used. Furthermore, "#RCONnn" as a reactant means that the rate constant for the reaction is obtained by multiplying the rate constant given by that for reaction "nn". Thus, the rate constant given is actually an equilibrium constant.

[b] Format of reaction listing same as used in documentation of the detailed mechanism (Carter 1990).

[c] Rate constants and product yield parameters based on the mixture of species in the base ROG mixture which are being represented.

Table A-3. Absorption cross sections and quantum yields for photolysis reactions.

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
Photolysis File = NO2														
250.0	2.83E-20	1.000	255.0	1.45E-20	1.000	260.0	1.90E-20	1.000	265.0	2.05E-20	1.000	270.0	3.13E-20	1.000
275.0	4.02E-20	1.000	280.0	5.54E-20	1.000	285.0	6.99E-20	1.000	290.0	8.18E-20	0.999	295.0	9.67E-20	0.998
300.0	1.17E-19	0.997	305.0	1.66E-19	0.996	310.0	1.76E-19	0.995	315.0	2.25E-19	0.994	320.0	2.54E-19	0.993
325.0	2.79E-19	0.992	330.0	2.99E-19	0.991	335.0	3.45E-19	0.990	340.0	3.88E-19	0.989	345.0	4.07E-19	0.988
350.0	4.10E-19	0.987	355.0	5.13E-19	0.986	360.0	4.51E-19	0.984	365.0	5.78E-19	0.983	370.0	5.42E-19	0.981
375.0	5.35E-19	0.979	380.0	5.99E-19	0.975	381.0	5.98E-19	0.974	382.0	5.97E-19	0.973	383.0	5.96E-19	0.972
384.0	5.95E-19	0.971	385.0	5.94E-19	0.969	386.0	5.95E-19	0.967	387.0	5.96E-19	0.966	388.0	5.98E-19	0.964
389.0	5.99E-19	0.962	390.0	6.00E-19	0.960	391.0	5.98E-19	0.959	392.0	5.96E-19	0.957	393.0	5.93E-19	0.953
394.0	5.91E-19	0.950	395.0	5.89E-19	0.942	396.0	6.06E-19	0.922	397.0	6.24E-19	0.870	398.0	6.41E-19	0.820
399.0	6.59E-19	0.760	400.0	6.76E-19	0.695	401.0	6.67E-19	0.635	402.0	6.58E-19	0.560	403.0	6.50E-19	0.485
404.0	6.41E-19	0.425	405.0	6.32E-19	0.350	406.0	6.21E-19	0.290	407.0	6.10E-19	0.225	408.0	5.99E-19	0.185
409.0	5.88E-19	0.153	410.0	5.77E-19	0.130	411.0	5.88E-19	0.110	412.0	5.98E-19	0.094	413.0	6.09E-19	0.083
414.0	6.19E-19	0.070	415.0	6.30E-19	0.059	416.0	6.29E-19	0.048	417.0	6.27E-19	0.039	418.0	6.26E-19	0.030
419.0	6.24E-19	0.023	420.0	6.23E-19	0.018	421.0	6.18E-19	0.012	422.0	6.14E-19	0.008	423.0	6.09E-19	0.004
424.0	6.05E-19	0.000	425.0	6.00E-19	0.000									
Photolysis File = NO3NO														
585.0	2.77E-18	0.000	590.0	5.14E-18	0.250	595.0	4.08E-18	0.400	600.0	2.83E-18	0.250	605.0	3.45E-18	0.200
610.0	1.48E-18	0.200	615.0	1.96E-18	0.100	620.0	3.58E-18	0.100	625.0	9.25E-18	0.050	630.0	5.66E-18	0.050
635.0	1.45E-18	0.000	640.0	1.11E-18	0.000									
Photolysis File = NO3NO2														
400.0	0.00E+00	1.000	405.0	3.00E-20	1.000	410.0	4.00E-20	1.000	415.0	5.00E-20	1.000	420.0	8.00E-20	1.000
425.0	1.00E-19	1.000	430.0	1.30E-19	1.000	435.0	1.80E-19	1.000	440.0	1.90E-19	1.000	445.0	2.20E-19	1.000
450.0	2.80E-19	1.000	455.0	3.30E-19	1.000	460.0	3.70E-19	1.000	465.0	4.30E-19	1.000	470.0	5.10E-19	1.000
475.0	6.00E-19	1.000	480.0	6.40E-19	1.000	485.0	6.90E-19	1.000	490.0	8.80E-19	1.000	495.0	9.50E-19	1.000
500.0	1.01E-18	1.000	505.0	1.10E-18	1.000	510.0	1.32E-18	1.000	515.0	1.40E-18	1.000	520.0	1.45E-18	1.000
525.0	1.48E-18	1.000	530.0	1.94E-18	1.000	535.0	2.04E-18	1.000	540.0	1.81E-18	1.000	545.0	1.81E-18	1.000
550.0	2.36E-18	1.000	555.0	2.68E-18	1.000	560.0	3.07E-18	1.000	565.0	2.53E-18	1.000	570.0	2.54E-18	1.000
575.0	2.74E-18	1.000	580.0	3.05E-18	1.000	585.0	2.77E-18	1.000	590.0	5.14E-18	0.750	595.0	4.08E-18	0.600
600.0	2.83E-18	0.550	605.0	3.45E-18	0.400	610.0	1.45E-18	0.300	615.0	1.96E-18	0.250	620.0	3.58E-18	0.200
625.0	9.25E-18	0.150	630.0	5.66E-18	0.050	635.0	1.45E-18	0.000						
Photolysis File = O3O3P														
280.0	3.97E-18	0.100	281.0	3.60E-18	0.100	282.0	3.24E-18	0.100	283.0	3.01E-18	0.100	284.0	2.73E-18	0.100
285.0	2.44E-18	0.100	286.0	2.21E-18	0.100	287.0	2.01E-18	0.100	288.0	1.76E-18	0.100	289.0	1.58E-18	0.100
290.0	1.41E-18	0.100	291.0	1.26E-18	0.100	292.0	1.10E-18	0.100	293.0	9.89E-19	0.100	294.0	8.59E-19	0.100
295.0	7.70E-19	0.100	296.0	6.67E-19	0.100	297.0	5.84E-19	0.100	298.0	5.07E-19	0.100	299.0	4.52E-19	0.100
300.0	3.92E-19	0.100	301.0	3.42E-19	0.100	302.0	3.06E-19	0.100	303.0	2.60E-19	0.100	304.0	2.37E-19	0.100
305.0	2.01E-19	0.112	306.0	1.79E-19	0.149	307.0	1.56E-19	0.197	308.0	1.38E-19	0.259	309.0	1.25E-19	0.339
310.0	1.02E-19	0.437	311.0	9.17E-20	0.546	312.0	7.88E-20	0.652	313.0	6.77E-20	0.743	314.0	6.35E-20	0.816
315.0	5.10E-20	0.872	316.0	4.61E-20	0.916	317.0	4.17E-20	0.949	318.0	3.72E-20	0.976	319.0	2.69E-20	0.997
320.0	3.23E-20	1.000	330.0	6.70E-21	1.000	340.0	1.70E-21	1.000	350.0	4.00E-22	1.000	355.0	0.00E+00	1.000
400.0	0.00E+00	1.000	450.0	1.60E-22	1.000	500.0	1.34E-21	1.000	550.0	3.32E-21	1.000	600.0	5.06E-21	1.000
650.0	2.45E-21	1.000	700.0	8.70E-22	1.000	750.0	3.20E-22	1.000	800.0	1.60E-22	1.000	900.0	0.00E+00	1.000
Photolysis File = O3O1D														
280.0	3.97E-18	0.900	281.0	3.60E-18	0.900	282.0	3.24E-18	0.900	283.0	3.01E-18	0.900	284.0	2.73E-18	0.900
285.0	2.44E-18	0.900	286.0	2.21E-18	0.900	287.0	2.01E-18	0.900	288.0	1.76E-18	0.900	289.0	1.58E-18	0.900
290.0	1.41E-18	0.900	291.0	1.26E-18	0.900	292.0	1.10E-18	0.900	293.0	9.89E-19	0.900	294.0	8.59E-19	0.900
295.0	7.70E-19	0.900	296.0	6.67E-19	0.900	297.0	5.84E-19	0.900	298.0	5.07E-19	0.900	299.0	4.52E-19	0.900
300.0	3.92E-19	0.900	301.0	3.42E-19	0.900	302.0	3.06E-19	0.900	303.0	2.60E-19	0.900	304.0	2.37E-19	0.900
305.0	2.01E-19	0.888	306.0	1.79E-19	0.851	307.0	1.56E-19	0.803	308.0	1.38E-19	0.741	309.0	1.25E-19	0.661
310.0	1.02E-19	0.563	311.0	9.17E-20	0.454	312.0	7.88E-20	0.348	313.0	6.77E-20	0.257	314.0	6.35E-20	0.184
315.0	5.10E-20	0.128	316.0	4.61E-20	0.084	317.0	4.17E-20	0.051	318.0	3.72E-20	0.024	319.0	2.69E-20	0.003
320.0	3.23E-20	0.000												
Photolysis File = HONO														
311.0	0.00E+00	1.000	312.0	2.00E-21	1.000	313.0	4.20E-21	1.000	314.0	4.60E-21	1.000	315.0	4.20E-21	1.000
316.0	3.00E-21	1.000	317.0	4.60E-21	1.000	318.0	3.60E-20	1.000	319.0	6.10E-20	1.000	320.0	2.10E-20	1.000
321.0	4.27E-20	1.000	322.0	4.01E-20	1.000	323.0	3.93E-20	1.000	324.0	4.01E-20	1.000	325.0	4.04E-20	1.000
326.0	3.13E-20	1.000	327.0	4.12E-20	1.000	328.0	7.55E-20	1.000	329.0	6.64E-20	1.000	330.0	7.29E-20	1.000
331.0	8.70E-20	1.000	332.0	1.38E-19	1.000	333.0	5.91E-20	1.000	334.0	5.91E-20	1.000	335.0	6.45E-20	1.000
336.0	5.91E-20	1.000	337.0	4.58E-20	1.000	338.0	1.91E-19	1.000	339.0	1.63E-19	1.000	340.0	1.05E-19	1.000
341.0	8.70E-20	1.000	342.0	3.35E-19	1.000	343.0	2.01E-19	1.000	344.0	1.02E-19	1.000	345.0	8.54E-20	1.000
346.0	8.32E-20	1.000	347.0	8.20E-20	1.000	348.0	7.49E-20	1.000	349.0	7.13E-20	1.000	350.0	6.83E-20	1.000
351.0	1.74E-19	1.000	352.0	1.14E-19	1.000	353.0	3.71E-19	1.000	354.0	4.96E-19	1.000	355.0	2.46E-19	1.000
356.0	1.19E-19	1.000	357.0	9.35E-20	1.000	358.0	7.78E-20	1.000	359.0	7.29E-20	1.000	360.0	6.83E-20	1.000
361.0	6.90E-20	1.000	362.0	7.32E-20	1.000	363.0	9.00E-20	1.000	364.0	1.21E-19	1.000	365.0	1.33E-19	1.000
366.0	2.13E-19	1.000	367.0	3.52E-19	1.000	368.0	4.50E-19	1.000	369.0	2.93E-19	1.000	370.0	1.19E-19	1.000
371.0	9.46E-20	1.000	372.0	8.85E-20	1.000	373.0	7.44E-20	1.000	374.0	4.77E-20	1.000	375.0	2.70E-20	1.000
376.0	1.90E-20	1.000	377.0	1.50E-20	1.000	378.0	1.90E-20	1.000	379.0	5.80E-20	1.000	380.0	7.78E-20	1.000
381.0	1.14E-19	1.000	382.0	1.40E-19	1.000	383.0	1.72E-19	1.000	384.0	1.99E-19	1.000	385.0	1.90E-19	1.000
386.0	1.19E-19	1.000	387.0	5.65E-20	1.000	388.0	3.20E-20	1.000	389.0	1.90E-20	1.000	390.0	1.20E-20	1.000
391.0	5.00E-21	1.000	392.0	0.00E+00	1.000									
Photolysis File = H2O2														
250.0	8.30E-20	1.000	255.0	6.70E-20	1.000	260.0	5.20E-20	1.000	265.0	4.20E-20	1.000	270.0	3.20E-20	1.000
275.0	2.50E-20	1.000	280.0	2.00E-20	1.000	285.0	1.50E-20	1.000	290.0	1.13E-20	1.000	295.0	8.70E-21	1.000
300.0	6.60E-21	1.000	305.0	4.90E-21	1.000	310.0	3.70E-21	1.000	315.0	2.80E-21	1.000	320.0	2.00E-21	1.000
325.0	1.50E-21	1.000	330.0	1.20E-21	1.000	335.0	9.00E-22	1.000	340.0	7.00E-22	1.000	345.0	5.00E-22	1.000
350.0	3.00E-22	1.000	355.0	0.00E+00	1.000									

Table 3. (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
Photolysis File = CO2H														
210.0	3.75E-19	1.000	220.0	2.20E-19	1.000	230.0	1.38E-19	1.000	240.0	8.80E-20	1.000	250.0	5.80E-20	1.000
260.0	3.80E-20	1.000	270.0	2.50E-20	1.000	280.0	1.50E-20	1.000	290.0	9.00E-21	1.000	300.0	5.80E-21	1.000
310.0	3.40E-21	1.000	320.0	1.90E-21	1.000	330.0	1.10E-21	1.000	340.0	6.00E-22	1.000	350.0	4.00E-22	1.000
360.0	0.00E+00	1.000												
Photolysis File = HCHONEWR														
280.0	2.49E-20	0.590	280.5	1.42E-20	0.596	281.0	1.51E-20	0.602	281.5	1.32E-20	0.608	282.0	9.73E-21	0.614
282.5	6.76E-21	0.620	283.0	5.82E-21	0.626	283.5	9.10E-21	0.632	284.0	3.71E-20	0.638	284.5	4.81E-20	0.644
285.0	3.95E-20	0.650	285.5	2.87E-20	0.656	286.0	2.24E-20	0.662	286.5	1.74E-20	0.668	287.0	1.13E-20	0.674
287.5	1.10E-20	0.680	288.0	2.62E-20	0.686	288.5	4.00E-20	0.692	289.0	3.55E-20	0.698	289.5	2.12E-20	0.704
290.0	1.07E-20	0.710	290.5	1.35E-20	0.713	291.0	1.99E-20	0.717	291.5	1.56E-20	0.721	292.0	8.65E-21	0.724
292.5	5.90E-21	0.727	293.0	1.11E-20	0.731	293.5	6.26E-20	0.735	294.0	7.40E-20	0.738	294.5	5.36E-20	0.741
295.0	4.17E-20	0.745	295.5	3.51E-20	0.749	296.0	2.70E-20	0.752	296.5	1.75E-20	0.755	297.0	1.16E-20	0.759
297.5	1.51E-20	0.763	298.0	3.69E-20	0.766	298.5	4.40E-20	0.769	299.0	3.44E-20	0.773	299.5	2.02E-20	0.776
300.0	1.06E-20	0.780	300.4	7.01E-21	0.780	300.6	8.63E-21	0.779	300.8	1.47E-20	0.779	301.0	2.01E-20	0.779
301.2	2.17E-20	0.779	301.4	1.96E-20	0.779	301.6	1.54E-20	0.778	301.8	1.26E-20	0.778	302.0	1.03E-20	0.778
302.2	8.53E-21	0.778	302.4	7.13E-21	0.778	302.6	6.61E-21	0.777	302.8	1.44E-20	0.777	303.0	3.18E-20	0.777
303.2	3.81E-20	0.777	303.4	5.57E-20	0.777	303.6	6.91E-20	0.776	303.8	6.58E-20	0.776	304.0	6.96E-20	0.776
304.2	5.79E-20	0.776	304.4	5.24E-20	0.776	304.6	4.30E-20	0.775	304.8	3.28E-20	0.775	305.0	3.60E-20	0.775
305.2	5.12E-20	0.775	305.4	4.77E-20	0.775	305.6	4.43E-20	0.774	305.8	4.60E-20	0.774	306.0	4.01E-20	0.774
306.2	3.28E-20	0.774	306.4	2.66E-20	0.774	306.6	2.42E-20	0.773	306.8	1.95E-20	0.773	307.0	1.58E-20	0.773
307.2	1.37E-20	0.773	307.4	1.19E-20	0.773	307.6	1.01E-20	0.772	307.8	9.01E-21	0.772	308.0	8.84E-21	0.772
308.2	2.08E-20	0.772	308.4	2.39E-20	0.772	308.6	3.08E-20	0.771	308.8	3.39E-20	0.771	309.0	3.18E-20	0.771
309.2	3.06E-20	0.771	309.4	2.84E-20	0.771	309.6	2.46E-20	0.770	309.8	1.95E-20	0.770	310.0	1.57E-20	0.770
310.2	1.26E-20	0.767	310.4	9.26E-21	0.764	310.6	7.71E-21	0.761	310.8	6.05E-21	0.758	311.0	5.13E-21	0.755
311.2	4.82E-21	0.752	311.4	4.54E-21	0.749	311.6	6.81E-21	0.746	311.8	1.04E-20	0.743	312.0	1.43E-20	0.740
312.2	1.47E-20	0.737	312.4	1.35E-20	0.734	312.6	1.13E-20	0.731	312.8	9.86E-21	0.728	313.0	7.82E-21	0.725
313.2	6.48E-21	0.722	313.4	1.07E-20	0.719	313.6	2.39E-20	0.716	313.8	3.80E-20	0.713	314.0	5.76E-20	0.710
314.2	6.14E-20	0.707	314.4	7.45E-20	0.704	314.6	5.78E-20	0.701	314.8	5.59E-20	0.698	315.0	4.91E-20	0.695
315.2	4.37E-20	0.692	315.4	3.92E-20	0.689	315.6	2.89E-20	0.686	315.8	2.82E-20	0.683	316.0	2.10E-20	0.680
316.2	1.66E-20	0.677	316.4	2.05E-20	0.674	316.6	4.38E-20	0.671	316.8	5.86E-20	0.668	317.0	6.28E-20	0.665
317.2	5.07E-20	0.662	317.4	4.33E-20	0.659	317.6	4.17E-20	0.656	317.8	3.11E-20	0.653	318.0	2.64E-20	0.650
318.2	2.24E-20	0.647	318.4	1.70E-20	0.644	318.6	1.24E-20	0.641	318.8	1.11E-20	0.638	319.0	7.70E-21	0.635
319.2	6.36E-21	0.632	319.4	5.36E-21	0.629	319.6	4.79E-21	0.626	319.8	6.48E-21	0.623	320.0	1.48E-20	0.620
320.2	1.47E-20	0.614	320.4	1.36E-20	0.608	320.6	1.69E-20	0.601	320.8	1.32E-20	0.595	321.0	1.49E-20	0.589
321.2	1.17E-20	0.583	321.4	1.15E-20	0.577	321.6	9.64E-21	0.570	321.8	7.26E-21	0.564	322.0	5.94E-21	0.558
322.2	4.13E-21	0.552	322.4	3.36E-21	0.546	322.6	2.39E-21	0.539	322.8	2.01E-21	0.533	323.0	1.76E-21	0.527
323.2	2.82E-21	0.521	323.4	4.65E-21	0.515	323.6	7.00E-21	0.508	323.8	7.80E-21	0.502	324.0	7.87E-21	0.496
324.2	6.59E-21	0.490	324.4	5.60E-21	0.484	324.6	4.66E-21	0.477	324.8	4.21E-21	0.471	325.0	7.77E-21	0.465
325.2	2.15E-20	0.459	325.4	3.75E-20	0.453	325.6	4.10E-20	0.446	325.8	6.47E-20	0.440	326.0	7.59E-20	0.434
326.2	6.51E-20	0.428	326.4	5.53E-20	0.422	326.6	5.76E-20	0.415	326.8	4.43E-20	0.409	327.0	3.44E-20	0.403
327.2	3.22E-20	0.397	327.4	2.13E-20	0.391	327.6	1.91E-20	0.384	327.8	1.42E-20	0.378	328.0	9.15E-21	0.372
328.2	6.79E-21	0.366	328.4	4.99E-21	0.360	328.6	4.77E-21	0.353	328.8	1.75E-20	0.347	329.0	3.27E-20	0.341
329.2	3.99E-20	0.335	329.4	5.13E-20	0.329	329.6	4.00E-20	0.322	329.8	3.61E-20	0.316	330.0	3.38E-20	0.310
330.2	3.08E-20	0.304	330.4	2.16E-20	0.298	330.6	2.09E-20	0.291	330.8	1.41E-20	0.285	331.0	9.95E-21	0.279
331.2	7.76E-21	0.273	331.4	6.16E-21	0.267	331.6	4.06E-21	0.260	331.8	3.03E-21	0.254	332.0	2.41E-21	0.248
332.2	1.74E-21	0.242	332.4	1.33E-21	0.236	332.6	2.70E-21	0.229	332.8	1.65E-21	0.223	333.0	1.17E-21	0.217
333.2	9.84E-22	0.211	333.4	8.52E-22	0.205	333.6	6.32E-22	0.198	333.8	5.21E-22	0.192	334.0	1.46E-21	0.186
334.2	1.80E-21	0.180	334.4	1.43E-21	0.174	334.6	1.03E-21	0.167	334.8	7.19E-22	0.161	335.0	4.84E-22	0.155
335.2	2.73E-22	0.149	335.4	1.34E-22	0.143	335.6	1.62E-22	0.136	335.8	1.25E-22	0.130	336.0	4.47E-22	0.124
336.2	1.23E-21	0.118	336.4	2.02E-21	0.112	336.6	3.00E-21	0.105	336.8	2.40E-21	0.099	337.0	3.07E-21	0.093
337.2	2.29E-21	0.087	337.4	2.46E-21	0.081	337.6	2.92E-21	0.074	337.8	8.10E-21	0.068	338.0	1.82E-20	0.062
338.2	3.10E-20	0.056	338.4	3.24E-20	0.050	338.6	4.79E-20	0.043	338.8	5.25E-20	0.037	339.0	5.85E-20	0.031
339.2	4.33E-20	0.025	339.4	4.20E-20	0.019	339.6	3.99E-20	0.012	339.8	3.11E-20	0.006	340.0	2.72E-20	0.000
Photolysis File = HCHONEWM														
280.0	2.49E-20	0.350	280.5	1.42E-20	0.346	281.0	1.51E-20	0.341	281.5	1.32E-20	0.336	282.0	9.73E-21	0.332
282.5	6.76E-21	0.327	283.0	5.82E-21	0.323	283.5	9.10E-21	0.319	284.0	3.71E-20	0.314	284.5	4.81E-20	0.309
285.0	3.95E-20	0.305	285.5	2.87E-20	0.301	286.0	2.24E-20	0.296	286.5	1.74E-20	0.291	287.0	1.13E-20	0.287
287.5	1.10E-20	0.282	288.0	2.62E-20	0.278	288.5	4.00E-20	0.273	289.0	3.55E-20	0.269	289.5	2.12E-20	0.264
290.0	1.07E-20	0.260	290.5	1.35E-20	0.258	291.0	1.99E-20	0.256	291.5	1.56E-20	0.254	292.0	8.65E-21	0.252
292.5	5.90E-21	0.250	293.0	1.11E-20	0.248	293.5	6.26E-20	0.246	294.0	7.40E-20	0.244	294.5	5.36E-20	0.242
295.0	4.17E-20	0.240	295.5	3.51E-20	0.238	296.0	2.70E-20	0.236	296.5	1.75E-20	0.234	297.0	1.16E-20	0.232
297.5	1.51E-20	0.230	298.0	3.69E-20	0.228	298.5	4.40E-20	0.226	299.0	3.44E-20	0.224	299.5	2.02E-20	0.222
300.0	1.06E-20	0.220	300.4	7.01E-21	0.220	300.6	8.63E-21	0.221	300.8	1.47E-20	0.221	301.0	2.01E-20	0.221
301.2	2.17E-20	0.221	301.4	1.96E-20	0.221	301.6	1.54E-20	0.222	301.8	1.26E-20	0.222	302.0	1.03E-20	0.222
302.2	8.53E-21	0.222	302.4	7.13E-21	0.222	302.6	6.61E-21	0.223	302.8	1.44E-20	0.223	303.0	3.18E-20	0.223
303.2	3.81E-20	0.223	303.4	5.57E-20	0.223	303.6	6.91E-20	0.224	303.8	6.58E-20	0.224	304.0	6.96E-20	0.224
304.2	5.79E-20	0.224	304.4	5.24E-20	0.224	304.6	4.30E-20	0.225	304.8	3.28E-20	0.225	305.0	3.60E-20	0.225
305.2	5.12E-20	0.225	305.4	4.77E-20	0.225	305.6	4.43E-20	0.226	305.8	4.60E-20	0.226	306.0	4.01E-20	0.226
306.2	3.28E-20	0.226	306.4	2.66E-20	0.226	306.6	2.42E-20	0.227	306.8	1.95E-20	0.227	307.0	1.58E-20	0.227
307.2	1.37E-20	0.227	307.4	1.19E-20	0.227	307.6	1.01E-20	0.228	307.8	9.01E-21	0.228	308.0	8.84E-21	0.228
308.2	2.08E-20	0.228	308.4	2.39E-20	0.228	308.6	3.08E-20	0.229	308.8	3.39E-20	0.229	309.0	3.18E-20	0.229
309.2	3.06E-20	0.229	309.4	2.84E-20	0.229	309.6	2.46E-20	0.230	309.8	1.95E-20	0.230	310.0	1.57E-20	0.230
310.2	1.26E-20	0.233	310.4	9.26E-21	0.236	310.6	7.71E-21	0.239	310.8	6.05E-21	0.242	311.0	5.13E-21	0.245
311.2	4.82E-21	0.248	311.4	4.54E-21	0.251	311.6	6.81E-21	0.254	311.8	1.04E-20	0.257	312.0	1.43E-20	0.260
312.2	1.47E-20	0.263	312.4	1.35E-20	0.266	312.6	1.13E-20	0.269	312.8	9.86E-21	0.272	313.0	7.82E-21	0.275
313.2	6.48E-21	0.278	313.4	1.07E-20	0.281	313.6	2.39E-20	0.284	313.8	3.80E-20	0.287	314.0	5.76E-20	0.290
314.2	6.14E-20	0.293	314.4	7.45E-20	0.296	314.6	5.78E-20	0.299	314.8	5.59E-20	0.302	315.0	4.91E-20	0.305
315.2	4.37E-20	0.308	315.4	3.92E-20	0.311	315.6	2.89E-20	0.314	315.8	2.82E-20	0.317	316.0	2.10E-20	0.320
316.2	1.66E-20	0.323	316.4	2.05E-20	0.326	316.6	4.38E-20	0.329	316.8	5.86E-20	0.332	317.0	6.28E-20	0.335
317.2	5.07E-20	0.338	317.4	4.33E-20	0.341	317.6	4.17E-20	0.344	317.8	3.11E-20	0.347	318.0	2.64E-20	0.350
318.2	2.24E-20	0.353	318.4	1.70E-20	0.356	318.6	1.24E-20	0.359	318.8	1.11E-20	0.362	319.0	7.70E-21	0.365

Table 3. (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
319.2	6.36E-21	0.368	319.4	5.36E-21	0.371	319.6	4.79E-21	0.374	319.8	6.48E-21	0.377	320.0	1.48E-20	0.380
320.2	1.47E-20	0.386	320.4	1.36E-20	0.392	320.6	1.69E-20	0.399	320.8	1.32E-20	0.405	321.0	1.49E-20	0.411
321.2	1.17E-20	0.417	321.4	1.15E-20	0.423	321.6	9.64E-21	0.430	321.8	7.26E-21	0.436	322.0	5.94E-21	0.442
322.2	4.13E-21	0.448	322.4	3.36E-21	0.454	322.6	2.39E-21	0.461	322.8	2.01E-21	0.467	323.0	1.76E-21	0.473
323.2	2.82E-21	0.479	323.4	4.65E-21	0.485	323.6	7.00E-21	0.492	323.8	7.80E-21	0.498	324.0	7.87E-21	0.504
324.2	6.59E-21	0.510	324.4	5.60E-21	0.516	324.6	4.66E-21	0.523	324.8	4.21E-21	0.529	325.0	7.77E-21	0.535
325.2	2.15E-20	0.541	325.4	3.75E-20	0.547	325.6	4.10E-20	0.554	325.8	6.47E-20	0.560	326.0	7.59E-20	0.566
326.2	6.51E-20	0.572	326.4	5.53E-20	0.578	326.6	5.76E-20	0.585	326.8	4.43E-20	0.591	327.0	3.44E-20	0.597
327.2	3.22E-20	0.603	327.4	2.13E-20	0.609	327.6	1.91E-20	0.616	327.8	1.42E-20	0.622	328.0	9.15E-21	0.628
328.2	6.79E-21	0.634	328.4	4.99E-21	0.640	328.6	4.77E-21	0.647	328.8	1.75E-20	0.653	329.0	3.27E-20	0.659
329.2	3.99E-20	0.665	329.4	5.13E-20	0.671	329.6	4.00E-20	0.678	329.8	3.61E-20	0.684	330.0	3.38E-20	0.690
330.2	3.08E-20	0.694	330.4	2.16E-20	0.699	330.6	2.09E-20	0.703	330.8	1.41E-20	0.708	331.0	9.95E-21	0.712
331.2	7.76E-21	0.717	331.4	6.16E-21	0.721	331.6	4.06E-21	0.726	331.8	3.03E-21	0.730	332.0	2.41E-21	0.735
332.2	1.74E-21	0.739	332.4	1.33E-21	0.744	332.6	2.70E-21	0.748	332.8	1.65E-21	0.753	333.0	1.17E-21	0.757
333.2	9.84E-22	0.762	333.4	8.52E-22	0.766	333.6	6.32E-22	0.771	333.8	5.21E-22	0.775	334.0	1.46E-21	0.780
334.2	1.80E-21	0.784	334.4	1.43E-21	0.789	334.6	1.03E-21	0.793	334.8	7.19E-22	0.798	335.0	4.84E-22	0.802
335.2	2.73E-22	0.798	335.4	1.34E-22	0.794	335.6	0.00E+00	0.790	335.8	1.25E-22	0.786	336.0	4.47E-22	0.782
336.2	1.23E-21	0.778	336.4	2.02E-21	0.773	336.6	3.00E-21	0.769	336.8	2.40E-21	0.764	337.0	3.07E-21	0.759
337.2	2.29E-21	0.754	337.4	2.46E-21	0.749	337.6	2.92E-21	0.745	337.8	8.10E-21	0.740	338.0	1.82E-20	0.734
338.2	3.10E-20	0.729	338.4	3.24E-20	0.724	338.6	4.79E-20	0.719	338.8	5.25E-20	0.714	339.0	5.85E-20	0.709
339.2	4.33E-20	0.703	339.4	4.20E-20	0.698	339.6	3.99E-20	0.693	339.8	3.11E-20	0.687	340.0	2.72E-20	0.682
340.2	1.99E-20	0.676	340.4	1.76E-20	0.671	340.6	1.39E-20	0.666	340.8	1.01E-20	0.660	341.0	6.57E-21	0.655
341.2	4.83E-21	0.649	341.4	3.47E-21	0.643	341.6	2.23E-21	0.638	341.8	1.55E-21	0.632	342.0	3.70E-21	0.627
342.2	4.64E-21	0.621	342.4	1.08E-20	0.616	342.6	1.14E-20	0.610	342.8	1.79E-20	0.604	343.0	2.33E-20	0.599
343.2	1.72E-20	0.593	343.4	1.55E-20	0.588	343.6	1.46E-20	0.582	343.8	1.38E-20	0.576	344.0	1.00E-20	0.571
344.2	8.26E-21	0.565	344.4	6.32E-21	0.559	344.6	4.28E-21	0.554	344.8	3.22E-21	0.548	345.0	2.54E-21	0.542
345.2	1.60E-21	0.537	345.4	1.15E-21	0.531	345.6	8.90E-22	0.525	345.8	6.50E-22	0.520	346.0	5.09E-22	0.514
346.2	5.15E-22	0.508	346.4	3.45E-22	0.503	346.6	3.18E-22	0.497	346.8	3.56E-22	0.491	347.0	3.24E-22	0.485
347.2	3.34E-22	0.480	347.4	2.88E-22	0.474	347.6	2.84E-22	0.468	347.8	9.37E-22	0.463	348.0	9.70E-22	0.457
348.2	7.60E-22	0.451	348.4	6.24E-22	0.446	348.6	4.99E-22	0.440	348.8	4.08E-22	0.434	349.0	3.39E-22	0.428
349.2	1.64E-22	0.423	349.4	1.49E-22	0.417	349.6	8.30E-23	0.411	349.8	2.52E-23	0.406	350.0	2.57E-23	0.400
350.2	0.00E+00	0.394	350.4	5.16E-23	0.389	350.6	0.00E+00	0.383	350.8	2.16E-23	0.377	351.0	7.07E-23	0.371
351.2	3.45E-23	0.366	351.4	1.97E-22	0.360	351.6	4.80E-22	0.354	351.8	3.13E-21	0.349	352.0	6.41E-21	0.343
352.2	8.38E-21	0.337	352.4	1.55E-20	0.331	352.6	1.86E-20	0.326	352.8	1.94E-20	0.320	353.0	2.78E-20	0.314
353.2	1.96E-20	0.309	353.4	1.67E-20	0.303	353.6	1.75E-20	0.297	353.8	1.63E-20	0.291	354.0	1.36E-20	0.286
354.2	1.07E-20	0.280	354.4	9.82E-21	0.274	354.6	8.66E-21	0.269	354.8	6.44E-21	0.263	355.0	4.84E-21	0.257
355.2	3.49E-21	0.251	355.4	2.41E-21	0.246	355.6	1.74E-21	0.240	355.8	1.11E-21	0.234	356.0	7.37E-22	0.229
356.2	4.17E-22	0.223	356.4	1.95E-22	0.217	356.6	1.50E-22	0.211	356.8	8.14E-23	0.206	357.0	0.00E+00	0.200
Photolysis File = CCHOR														
260.0	2.00E-20	0.310	270.0	3.40E-20	0.390	280.0	4.50E-20	0.580	290.0	4.90E-20	0.530	295.0	4.50E-20	0.480
300.0	4.30E-20	0.430	305.0	3.40E-20	0.370	315.0	2.10E-20	0.170	320.0	1.80E-20	0.100	325.0	1.10E-20	0.040
330.0	6.90E-21	0.000												
Photolysis File = RCHO														
280.0	5.26E-20	0.960	290.0	5.77E-20	0.910	300.0	5.05E-20	0.860	310.0	3.68E-20	0.600	320.0	1.66E-20	0.360
330.0	6.49E-21	0.200	340.0	1.44E-21	0.080	345.0	0.00E+00	0.020						
Photolysis File = ACET-93C														
250.0	2.37E-20	0.760	260.0	3.66E-20	0.800	270.0	4.63E-20	0.640	280.0	5.05E-20	0.550	290.0	4.21E-20	0.300
300.0	2.78E-20	0.150	310.0	1.44E-20	0.050	320.0	4.80E-21	0.026	330.0	8.00E-22	0.017	340.0	1.00E-22	0.000
350.0	3.00E-23	0.000	360.0	0.00E+00	0.000									
Photolysis File = KETONE														
210.0	1.10E-21	1.000	220.0	1.20E-21	1.000	230.0	4.60E-21	1.000	240.0	1.30E-20	1.000	250.0	2.68E-20	1.000
260.0	4.21E-20	1.000	270.0	5.54E-20	1.000	280.0	5.92E-20	1.000	290.0	5.16E-20	1.000	300.0	3.44E-20	1.000
310.0	1.53E-20	1.000	320.0	4.60E-21	1.000	330.0	1.10E-21	1.000	340.0	0.00E+00	1.000			
Photolysis File = GLYOXAL1														
230.0	2.87E-21	1.000	235.0	2.87E-21	1.000	240.0	4.30E-21	1.000	245.0	5.73E-21	1.000	250.0	8.60E-21	1.000
255.0	1.15E-20	1.000	260.0	1.43E-20	1.000	265.0	1.86E-20	1.000	270.0	2.29E-20	1.000	275.0	2.58E-20	1.000
280.0	2.87E-20	1.000	285.0	3.30E-20	1.000	290.0	3.15E-20	1.000	295.0	3.30E-20	1.000	300.0	3.58E-20	1.000
305.0	2.72E-20	1.000	310.0	2.72E-20	1.000	312.5	2.87E-20	1.000	315.0	2.29E-20	1.000	320.0	1.43E-20	1.000
325.0	1.15E-20	1.000	327.5	1.43E-20	1.000	330.0	1.15E-20	1.000	335.0	2.87E-21	1.000	340.0	0.00E+00	1.000
Photolysis File = GLYOXAL2														
355.0	0.00E+00	1.000	360.0	2.29E-21	1.000	365.0	2.87E-21	1.000	370.0	8.03E-21	1.000	375.0	1.00E-20	1.000
380.0	1.72E-20	1.000	382.0	1.58E-20	1.000	384.0	1.49E-20	1.000	386.0	1.49E-20	1.000	388.0	2.87E-20	1.000
390.0	3.15E-20	1.000	391.0	3.24E-20	1.000	392.0	3.04E-20	1.000	393.0	2.23E-20	1.000	394.0	2.63E-20	1.000
395.0	3.04E-20	1.000	396.0	2.63E-20	1.000	397.0	2.43E-20	1.000	398.0	3.24E-20	1.000	399.0	3.04E-20	1.000
400.0	2.84E-20	1.000	401.0	3.24E-20	1.000	402.0	4.46E-20	1.000	403.0	5.27E-20	1.000	404.0	4.26E-20	1.000
405.0	3.04E-20	1.000	406.0	3.04E-20	1.000	407.0	2.84E-20	1.000	408.0	2.43E-20	1.000	409.0	2.84E-20	1.000
410.0	6.08E-20	1.000	411.0	5.07E-20	1.000	411.5	6.08E-20	1.000	412.0	4.86E-20	1.000	413.0	8.31E-20	1.000
413.5	6.48E-20	1.000	414.0	7.50E-20	1.000	414.5	8.11E-20	1.000	415.0	8.11E-20	1.000	415.5	6.89E-20	1.000
416.0	4.26E-20	1.000	417.0	4.86E-20	1.000	418.0	5.88E-20	1.000	419.0	6.69E-20	1.000	420.0	3.85E-20	1.000
421.0	5.67E-20	1.000	421.5	4.46E-20	1.000	422.0	5.27E-20	1.000	422.5	1.05E-19	1.000	423.0	8.51E-20	1.000
424.0	6.08E-20	1.000	425.0	7.29E-20	1.000	426.0	1.18E-19	1.000	426.5	1.30E-19	1.000	427.0	1.07E-19	1.000
428.0	1.66E-19	1.000	429.0	4.05E-20	1.000	430.0	5.07E-20	1.000	431.0	4.86E-20	1.000	432.0	4.05E-20	1.000
433.0	3.65E-20	1.000	434.0	4.05E-20	1.000	434.5	6.08E-20	1.000	435.0	5.07E-20	1.000	436.0	8.11E-20	1.000
436.5	1.13E-19	1.000	437.0	5.27E-20	1.000	438.0	1.01E-19	1.000	438.5	1.38E-19	1.000	439.0	7.70E-20	1.000
440.0	2.47E-19	1.000	441.0	8.11E-20	1.000	442.0	6.08E-20	1.000	443.0	7.50E-20	1.000	444.0	9.32E-20	1.000
445.0	1.13E-19	1.000	446.0	5.27E-20	1.000	447.0	2.43E-20	1.000	448.0	2.84E-20	1.000	449.0	3.85E-20	1.000
450.0	6.08E-20	1.000	451.0	1.09E-19	1.000	451.5	9.32E-20	1.000	452.0	1.22E-19	1.000	453.0	2.39E-19	1.000
454.0	1.70E-19	1.000	455.0	3.40E-19	1.000	455.5	4.05E-19	1.000	456.0	1.01E-19	1.000	457.0	1.62E-20	1.000

Table 3. (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
458.0	1.22E-20	1.000	458.5	1.42E-20	1.000	459.0	4.05E-21	1.000	460.0	4.05E-21	1.000	460.5	6.08E-21	1.000
461.0	2.03E-21	1.000	462.0	0.00E+00	1.000									
Photolysis File = MEGLYOX1														
220.0	2.10E-21	1.000	225.0	2.10E-21	1.000	230.0	4.21E-21	1.000	235.0	7.57E-21	1.000	240.0	9.25E-21	1.000
245.0	8.41E-21	1.000	250.0	9.25E-21	1.000	255.0	9.25E-21	1.000	260.0	9.67E-21	1.000	265.0	1.05E-20	1.000
270.0	1.26E-20	1.000	275.0	1.43E-20	1.000	280.0	1.51E-20	1.000	285.0	1.43E-20	1.000	290.0	1.47E-20	1.000
295.0	1.18E-20	1.000	300.0	1.14E-20	1.000	305.0	9.25E-21	1.000	310.0	6.31E-21	1.000	315.0	5.47E-21	1.000
320.0	3.36E-21	1.000	325.0	1.68E-21	1.000	330.0	8.41E-22	1.000	335.0	0.00E+00	1.000			
Photolysis File = MEGLYOX2														
350.0	0.00E+00	1.000	354.0	4.21E-22	1.000	358.0	1.26E-21	1.000	360.0	2.10E-21	1.000	362.0	2.10E-21	1.000
364.0	2.94E-21	1.000	366.0	3.36E-21	1.000	368.0	4.21E-21	1.000	370.0	5.47E-21	1.000	372.0	5.89E-21	1.000
374.0	7.57E-21	1.000	376.0	7.99E-21	1.000	378.0	8.83E-21	1.000	380.0	1.01E-20	1.000	382.0	1.09E-20	1.000
384.0	1.35E-20	1.000	386.0	1.51E-20	1.000	388.0	1.72E-20	1.000	390.0	2.06E-20	1.000	392.0	2.10E-20	1.000
394.0	2.31E-20	1.000	396.0	2.48E-20	1.000	398.0	2.61E-20	1.000	400.0	2.78E-20	1.000	402.0	2.99E-20	1.000
404.0	3.20E-20	1.000	406.0	3.79E-20	1.000	408.0	3.95E-20	1.000	410.0	4.33E-20	1.000	412.0	4.71E-20	1.000
414.0	4.79E-20	1.000	416.0	4.88E-20	1.000	418.0	5.05E-20	1.000	420.0	5.21E-20	1.000	422.0	5.30E-20	1.000
424.0	5.17E-20	1.000	426.0	5.30E-20	1.000	428.0	5.21E-20	1.000	430.0	5.55E-20	1.000	432.0	5.13E-20	1.000
434.0	5.68E-20	1.000	436.0	6.22E-20	1.000	438.0	6.06E-20	1.000	440.0	5.47E-20	1.000	441.0	6.14E-20	1.000
442.0	5.47E-20	1.000	443.0	5.55E-20	1.000	443.5	6.81E-20	1.000	444.0	5.97E-20	1.000	445.0	5.13E-20	1.000
446.0	4.88E-20	1.000	447.0	5.72E-20	1.000	448.0	5.47E-20	1.000	449.0	6.56E-20	1.000	450.0	5.05E-20	1.000
451.0	3.03E-20	1.000	452.0	4.29E-20	1.000	453.0	2.78E-20	1.000	454.0	2.27E-20	1.000	456.0	1.77E-20	1.000
458.0	8.41E-21	1.000	460.0	4.21E-21	1.000	464.0	1.68E-21	1.000	468.0	0.00E+00	1.000			
Photolysis File = BZCHO														
299.0	1.78E-19	1.000	304.0	7.40E-20	1.000	306.0	6.91E-20	1.000	309.0	6.41E-20	1.000	313.0	6.91E-20	1.000
314.0	6.91E-20	1.000	318.0	6.41E-20	1.000	325.0	8.39E-20	1.000	332.0	7.65E-20	1.000	338.0	8.88E-20	1.000
342.0	8.88E-20	1.000	346.0	7.89E-20	1.000	349.0	7.89E-20	1.000	354.0	9.13E-20	1.000	355.0	8.14E-20	1.000
364.0	5.67E-20	1.000	368.0	6.66E-20	1.000	369.0	8.39E-20	1.000	370.0	8.39E-20	1.000	372.0	3.45E-20	1.000
374.0	3.21E-20	1.000	376.0	2.47E-20	1.000	377.0	2.47E-20	1.000	380.0	3.58E-20	1.000	382.0	9.90E-21	1.000
386.0	0.00E+00	1.000												
Photolysis File = ACROLEIN														
250.0	1.80E-21	1.000	252.0	2.05E-21	1.000	253.0	2.20E-21	1.000	254.0	2.32E-21	1.000	255.0	2.45E-21	1.000
256.0	2.56E-21	1.000	257.0	2.65E-21	1.000	258.0	2.74E-21	1.000	259.0	2.83E-21	1.000	260.0	2.98E-21	1.000
261.0	3.24E-21	1.000	262.0	3.47E-21	1.000	263.0	3.58E-21	1.000	264.0	3.93E-21	1.000	265.0	4.67E-21	1.000
266.0	5.10E-21	1.000	267.0	5.38E-21	1.000	268.0	5.73E-21	1.000	269.0	6.13E-21	1.000	270.0	6.64E-21	1.000
271.0	7.20E-21	1.000	272.0	7.77E-21	1.000	273.0	8.37E-21	1.000	274.0	8.94E-21	1.000	275.0	9.55E-21	1.000
276.0	1.04E-20	1.000	277.0	1.12E-20	1.000	278.0	1.19E-20	1.000	279.0	1.27E-20	1.000	280.0	1.27E-20	1.000
281.0	1.26E-20	1.000	282.0	1.26E-20	1.000	283.0	1.28E-20	1.000	284.0	1.33E-20	1.000	285.0	1.38E-20	1.000
286.0	1.44E-20	1.000	287.0	1.50E-20	1.000	288.0	1.57E-20	1.000	289.0	1.63E-20	1.000	290.0	1.71E-20	1.000
291.0	1.78E-20	1.000	292.0	1.86E-20	1.000	293.0	1.95E-20	1.000	294.0	2.05E-20	1.000	295.0	2.15E-20	1.000
296.0	2.26E-20	1.000	297.0	2.37E-20	1.000	298.0	2.48E-20	1.000	299.0	2.60E-20	1.000	300.0	2.73E-20	1.000
301.0	2.85E-20	1.000	302.0	2.99E-20	1.000	303.0	3.13E-20	1.000	304.0	3.27E-20	1.000	305.0	3.39E-20	1.000
306.0	3.51E-20	1.000	307.0	3.63E-20	1.000	308.0	3.77E-20	1.000	309.0	3.91E-20	1.000	310.0	4.07E-20	1.000
311.0	4.25E-20	1.000	312.0	4.39E-20	1.000	313.0	4.44E-20	1.000	314.0	4.50E-20	1.000	315.0	4.59E-20	1.000
316.0	4.75E-20	1.000	317.0	4.90E-20	1.000	318.0	5.05E-20	1.000	319.0	5.19E-20	1.000	320.0	5.31E-20	1.000
321.0	5.43E-20	1.000	322.0	5.52E-20	1.000	323.0	5.60E-20	1.000	324.0	5.67E-20	1.000	325.0	5.67E-20	1.000
326.0	5.62E-20	1.000	327.0	5.63E-20	1.000	328.0	5.71E-20	1.000	329.0	5.76E-20	1.000	330.0	5.80E-20	1.000
331.0	5.95E-20	1.000	332.0	6.23E-20	1.000	333.0	6.39E-20	1.000	334.0	6.38E-20	1.000	335.0	6.24E-20	1.000
336.0	6.01E-20	1.000	337.0	5.79E-20	1.000	338.0	5.63E-20	1.000	339.0	5.56E-20	1.000	340.0	5.52E-20	1.000
341.0	5.54E-20	1.000	342.0	5.53E-20	1.000	343.0	5.47E-20	1.000	344.0	5.41E-20	1.000	345.0	5.40E-20	1.000
346.0	5.48E-20	1.000	347.0	5.90E-20	1.000	348.0	6.08E-20	1.000	349.0	6.00E-20	1.000	350.0	5.53E-20	1.000
351.0	5.03E-20	1.000	352.0	4.50E-20	1.000	353.0	4.03E-20	1.000	354.0	3.75E-20	1.000	355.0	3.55E-20	1.000
356.0	3.45E-20	1.000	357.0	3.46E-20	1.000	358.0	3.49E-20	1.000	359.0	3.41E-20	1.000	360.0	3.23E-20	1.000
361.0	2.95E-20	1.000	362.0	2.81E-20	1.000	363.0	2.91E-20	1.000	364.0	3.25E-20	1.000	365.0	3.54E-20	1.000
366.0	3.30E-20	1.000	367.0	2.78E-20	1.000	368.0	2.15E-20	1.000	369.0	1.59E-20	1.000	370.0	1.19E-20	1.000
371.0	8.99E-21	1.000	372.0	7.22E-21	1.000	373.0	5.86E-21	1.000	374.0	4.69E-21	1.000	375.0	3.72E-21	1.000
376.0	3.57E-21	1.000	377.0	3.55E-21	1.000	378.0	2.83E-21	1.000	379.0	1.69E-21	1.000	380.0	8.29E-24	1.000
381.0	0.00E+00	1.000												

Appendix B. SAPRC-93 Mechanism Files

The computer data files implementing the SAPRC-93 mechanism in the FCM format (Kumar et al, 1995) are available on the Internet to interested researchers via anonymous FTP at address FTP://cert.ucr.edu/pub/carter/mech. Table B-1 lists the files which are included in this set, and a brief description of each.

Table B-1 List and description of computer data files implementing the SAPRC-93 mechanism in FCM format.

File	Description
Chemical Mechanism files	
SAPRC93.RXN	SAPRC-93 general mechanism (without isoprene chemistry)
ISOP-1.RXN	The most condensed (one product) version of the isoprene mechanism. This is the default because it should perform satisfactorily except for applications where isoprene product predictions are required. Requires SAPRC93.RXN or equivalent.
ISOP-4.RXN	This is the four product condensed version of the isoprene mechanism which can be used when methacrolein and MVK predictions are desired. Requires SAPRC93.RXN or equivalent. (Edit SAPRC93.PRP as indicated in the comments there to use it.)
ISOP-D.RXN	This is the detailed isoprene mechanism as documented by Carter and Atkinson (1996). Requires SAPRC93.RXN or equivalent. (Edit SAPRC93.PRP as indicated in the comments there to use it.)
*.PHF	Photolysis absorption cross section and quantum yields used.
SAPRC93.LPC	Lumping control file for SAPRC-93 mechanism for airshed models. (Two lumped alkanes, two lumped aromatics, ethene explicit, two lumped higher non-biogenic alkenes, isoprene explicit, one lumped terpene.)
ALKOTH.GEN	Mechanistic parameters for alkanes and other compounds which are lumped with alkanes, such as alcohols, etc.
AROMATIC.GEN	Mechanistic parameters for aromatics
ALKENEA.GEN	Mechanistic parameters for alkenes except for isoprene and terpenes
ALKENET.GEN	Mechanistic parameters for terpenes
LUMPMOLE.LPM	Lumped molecule assignments of applicable detailed model species.

Table B-1 (continued)

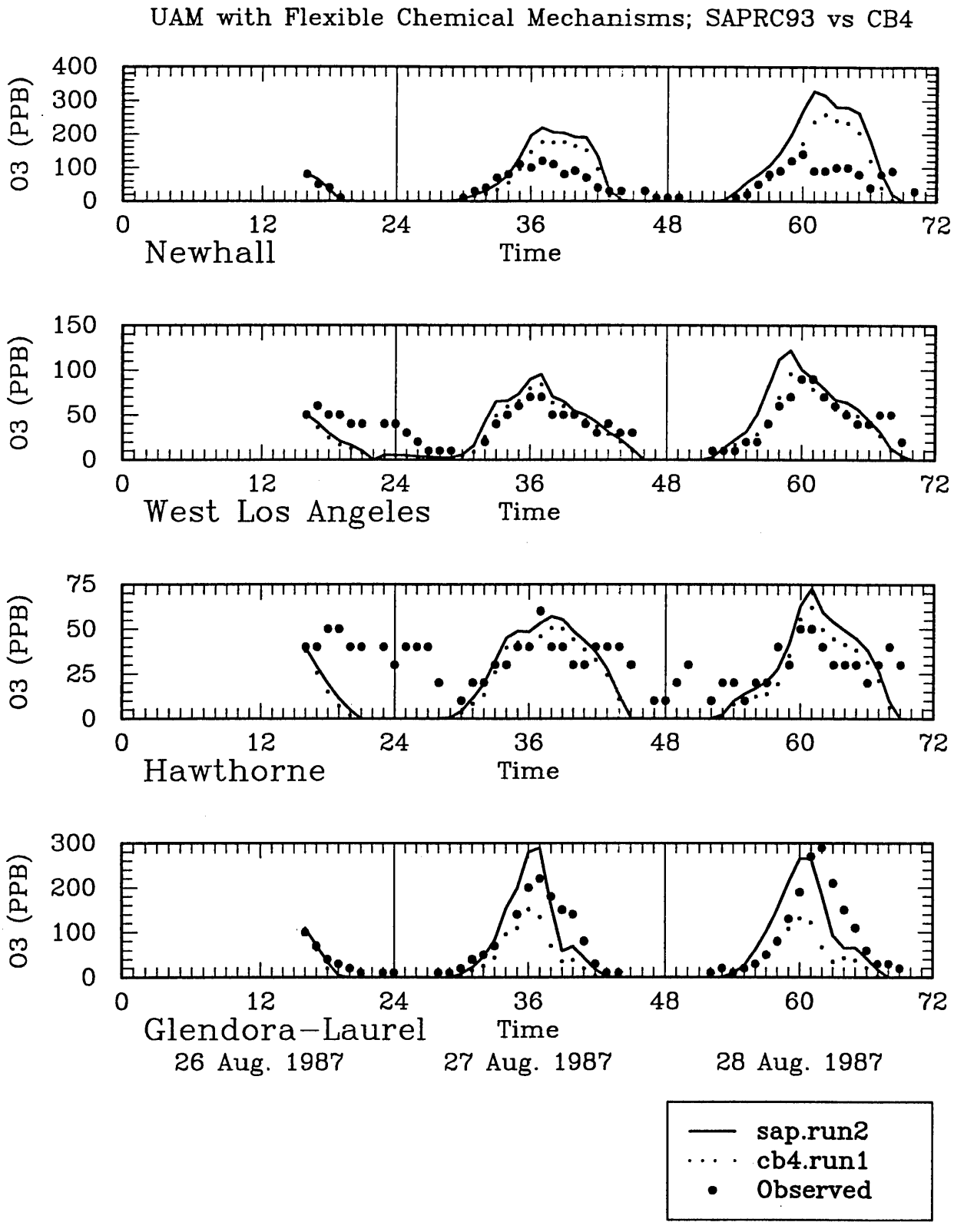
File	Description
Other Mechanism Preparation Input Files (compatible with FCM)	
SAPRC93.PRP	Main mechanism preparation file for FCM, using SAPRC93.RXN, ISOP-*.RXN, and the *.PHF files. As distributed it specifies use of the one product condensed isoprene mechanism, but can be edited to use another alternative. See comments in the file.
DUMMY.RXN	Specifies parameters output by emissions processing program which are ignored in the mechanism. Used by SAPRC93.PRP.
Other Emissions Assignment input files	
DMS.PRM	Lists and gives molecular weights, carbon numbers, and other information about all detailed model species used when processing emissions.
SAROAD.PRM	Assigns detailed model species to emissions classified using SAROAD numbers.
OLDNAMES.LPM	Renames detailed model species in older profiles to be consistent with nomenclature system currently used by mechanism parameter files.
Input files used by FCM processing example.	
PREPUAM.INP	List of file names and options used by all FCM programs.
LA082787.EMI	Example emissions profile (mass emissions of species identified by SAROAD numbers from the August, 27, 1987 SCAQS episode.)
STDZA640.JZS	Actinic flux data as computed by Jeffries and used in scenarios for calculating reactivity scales. Needed by PREPUAM to compute photolysis rates as a function of zenith angle from PREP output.
PETERSON.JZS	Actinic flux data as given by Peterson. Most similar to that probably used to derive photolysis rates for the UAM. Can be used as an alternative to STDZA640.JZS by changing the JZS reference in PREPUAM.INP.
RESIST.DAT	Used by PREPUAM to provide UAM with surface resistance values for the model species. Mechanism and scenario dependent.
Output files for FCM example: PREP output:	
SAPRC93.MOD	Mechanism data file
SAPRC93.PRO	Mechanism listing file
SAPRC93.F	Mechanism-dependent subroutine to be linked with the airshed model.
CONSTR.F	Parameter initialization subroutine to be linked with PREPUAM. (Not supported in this version, and should contain no executable code. This is output for future compatibility.)

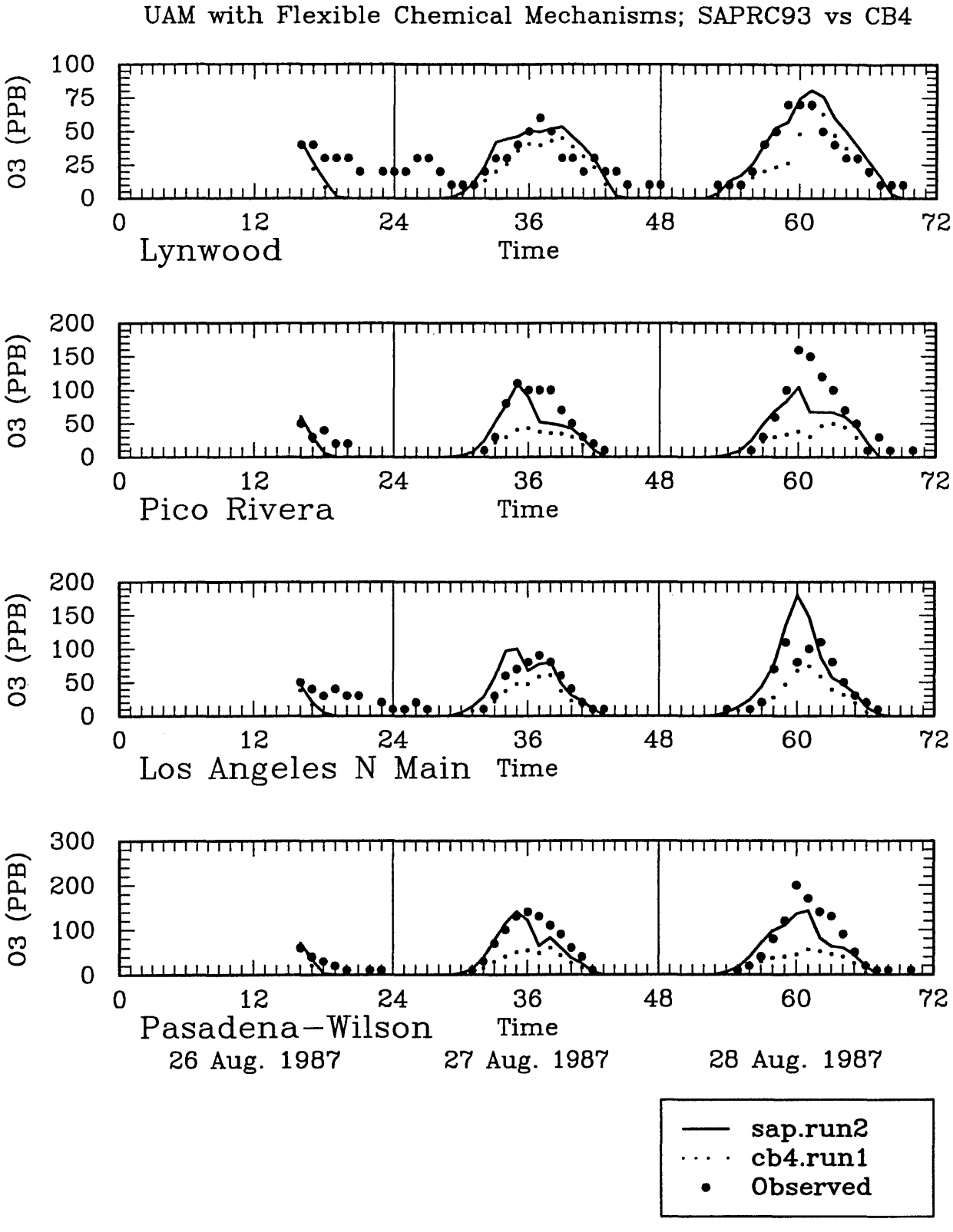
Table B-1 (continued)

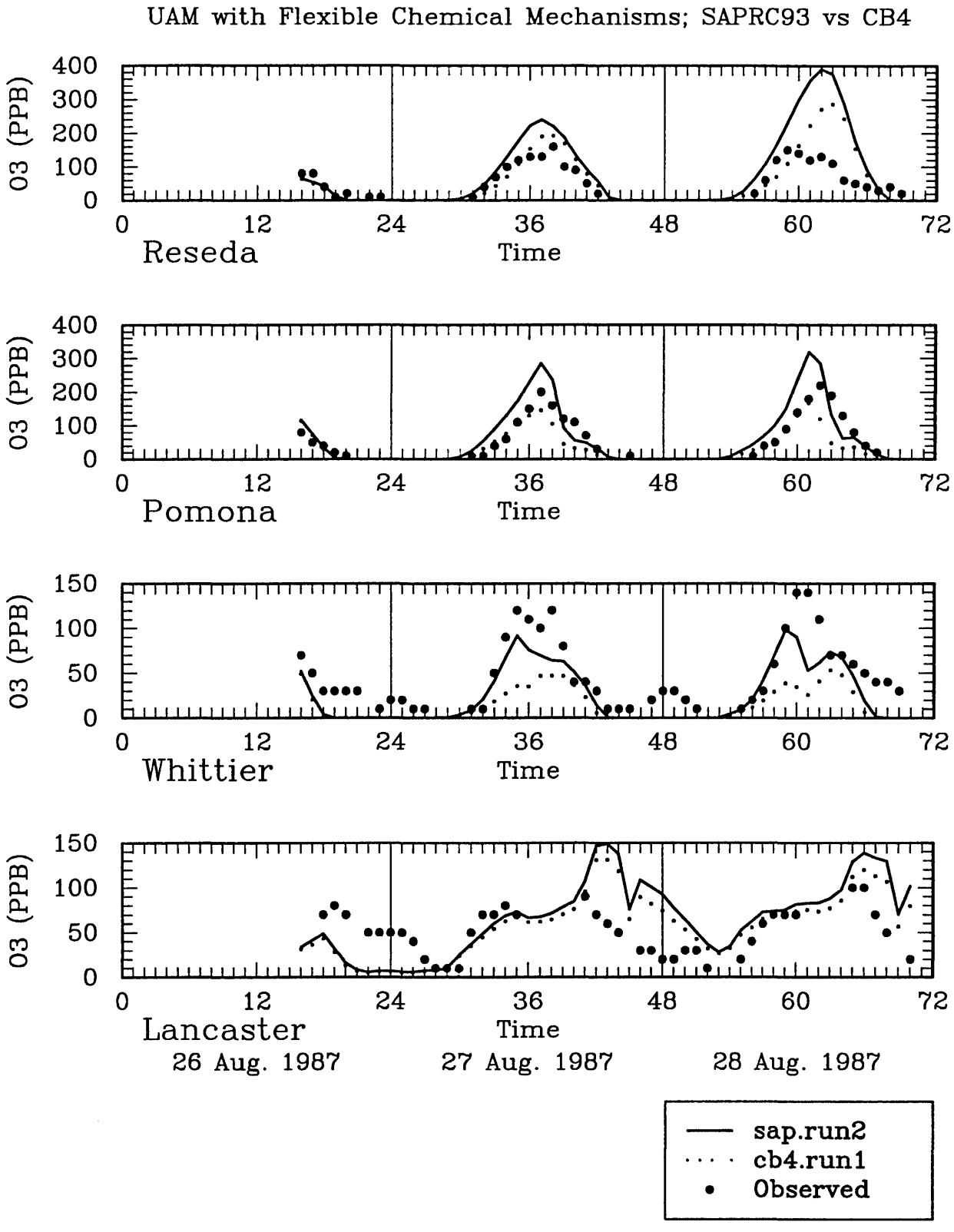
File	Description
Output files for FCM example: Emissions pre-processing output:	
TESTLA.CMP	Emissions data in LA082787.EMI given as molar emissions of detailed model species. Produced by EMITOCMP, and needed as input to PREPCOMP.
TESTLA.RXP	Mechanistic parameters optimized for the mixture given in TESTLA.CMP. Output by PREPCOMP and needed as input to PREPUAM to compute the emissions- dependent parameters needed by the model. Also used as input to CALGRID model for this purpose.
TESTLA.SAR	Assignments of SAROAD emissions classes to lumped species in the model. Should be compatible with the emissions processing routines developed for the CALGRID model, but this needs to be verified.
Output files for FCM example: PREPUAM output:	
CHEMOUT	Mechanism and parameter listing output.
BLCKDATA.F	One of three mechanistic dependent specification FORTRAN files which should be linked with the FCM/UAM model.
CHDATA.CMD	As above
CHPARM.CMD	As above
CHEMPARM	Chemical parameter input used by the FCM/UAM model.

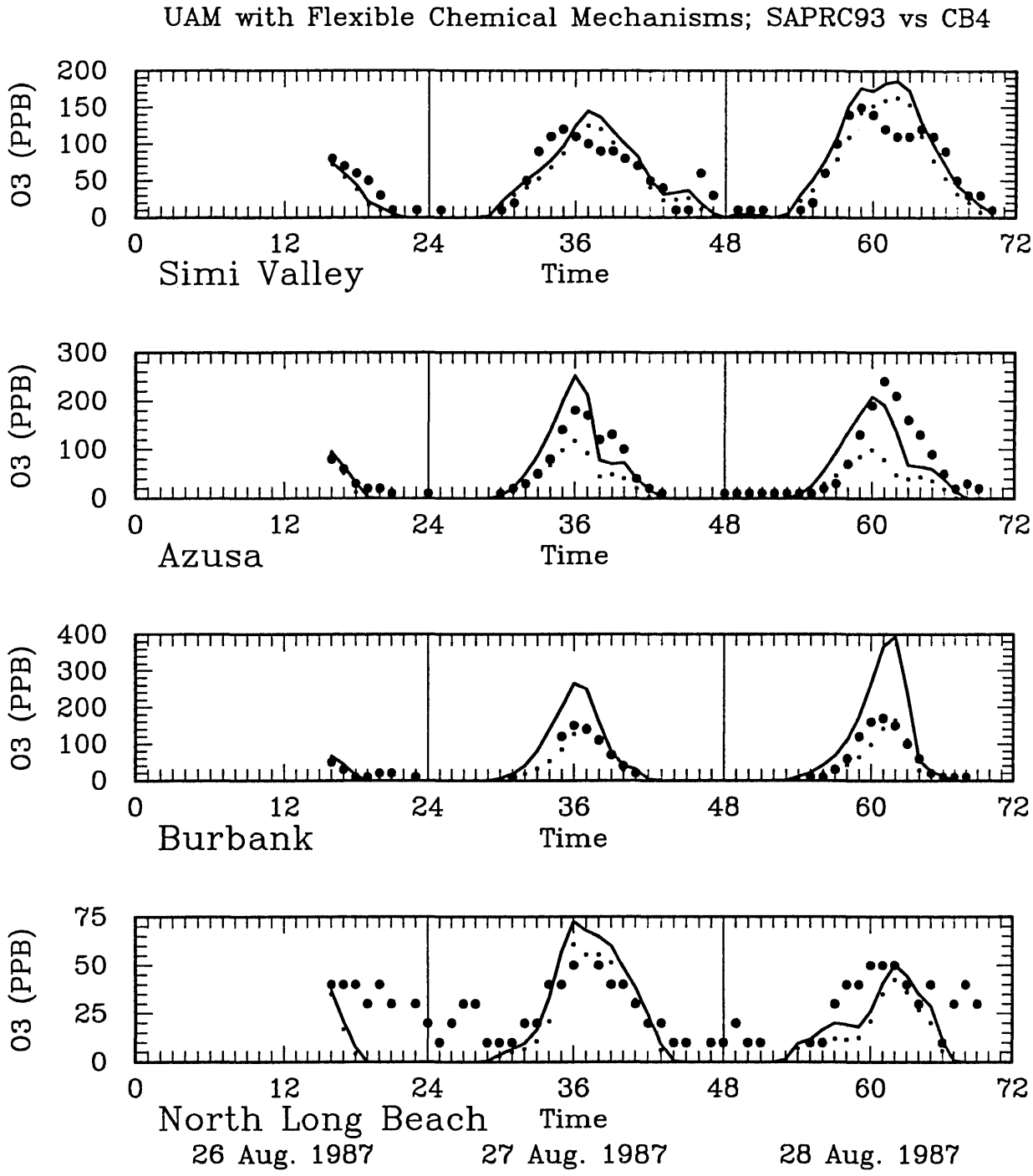
Appendix C. Representative Results of UAM Simulation

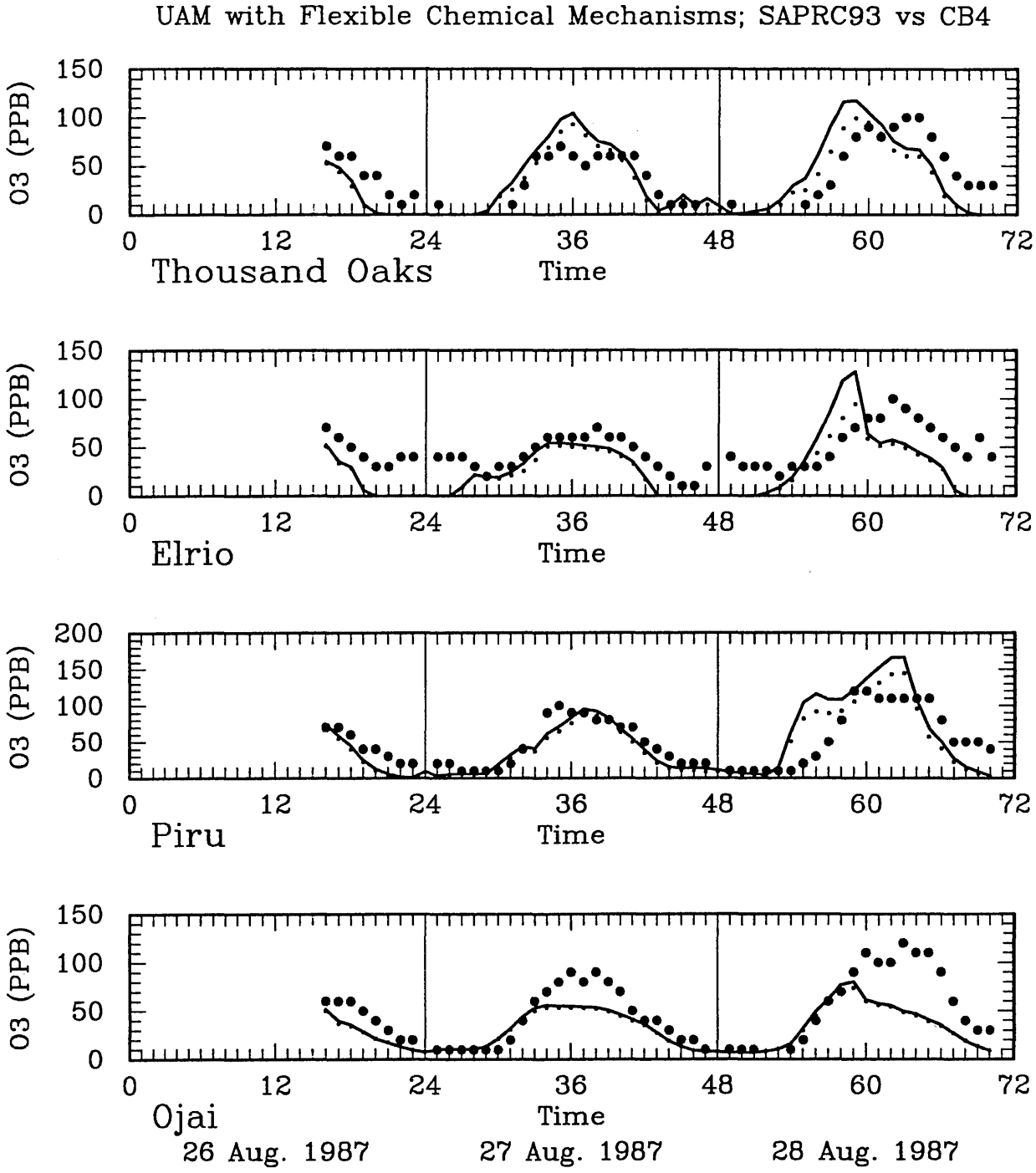
The following plots show the observed and calculated ozone simulations at the various monitoring stations for the 1987 SCAQS episode. The model simulations were calculated with the FCM version of the UAM using either the SAPRC-93 chemical mechanism (solid lines) or using the UAM 6.21 version of the Carbon Bond IV mechanism (dotted lines).

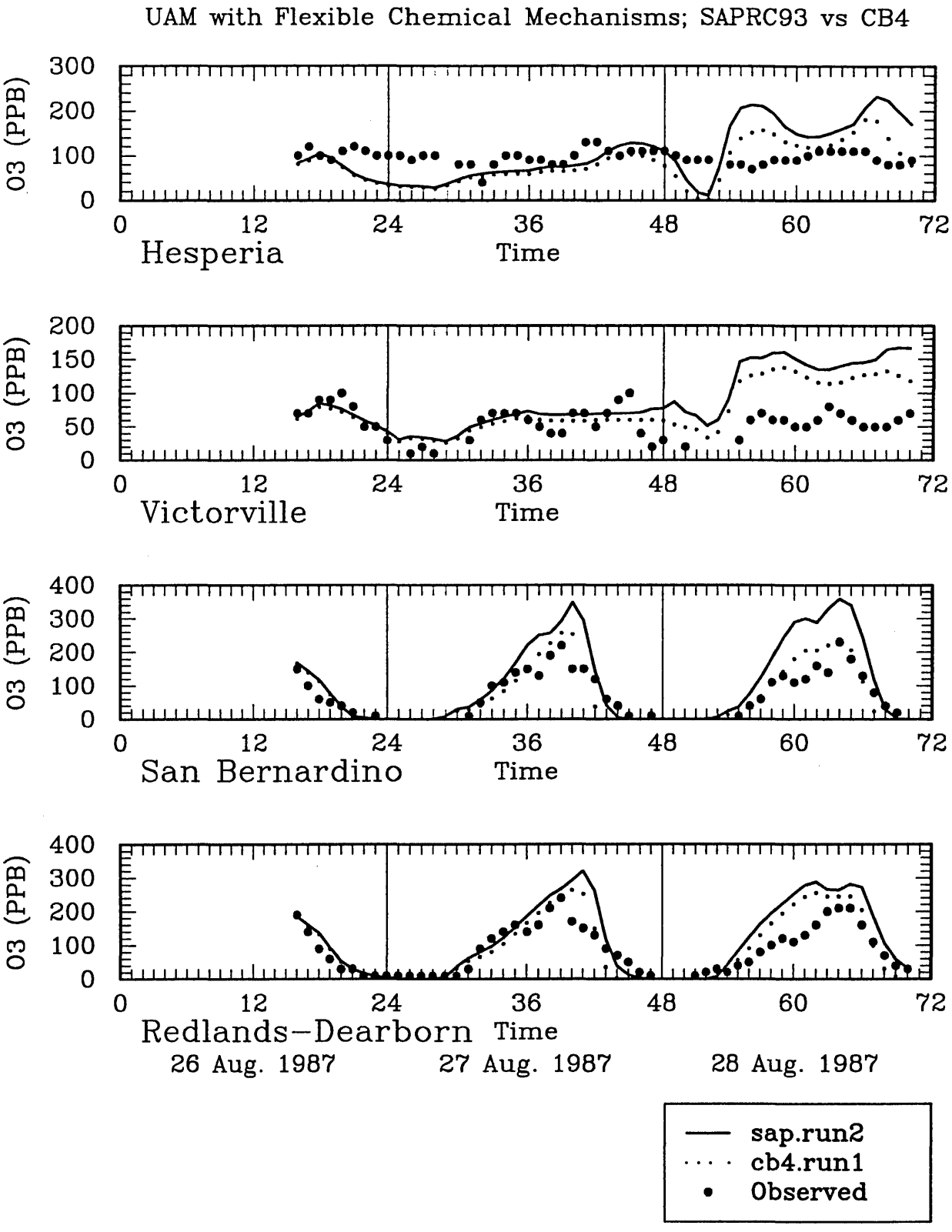

UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
400
300
200
100
0
0
12
24
36
48
60
72
Newhall
Time
03 (PPB)
150
100
50
0
West Los Angeles
Time
03 (PPB)
75
50
25
0
Hawthorne
Time
03 (PPB)
300
200
100
0
Glendora–Laurel
Time
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed

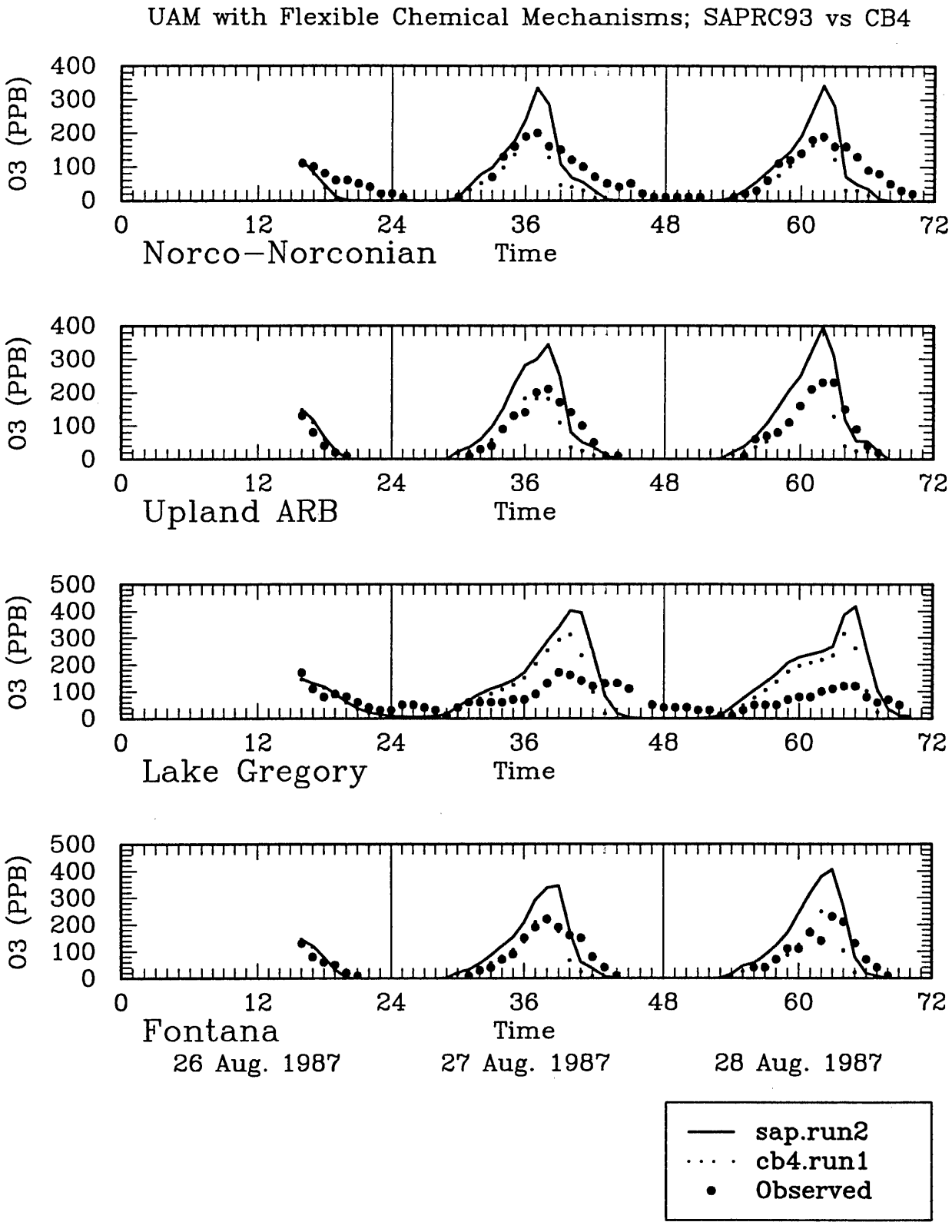

UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
100
75
50
25
0
0
12
24
36
48
60
72
Lynwood
Time
03 (PPB)
200
150
100
50
0
Pico Rivera
Time
03 (PPB)
Los Angeles N Main
Time
03 (PPB)
300
200
100
Pasadena–Wilson
Time
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed

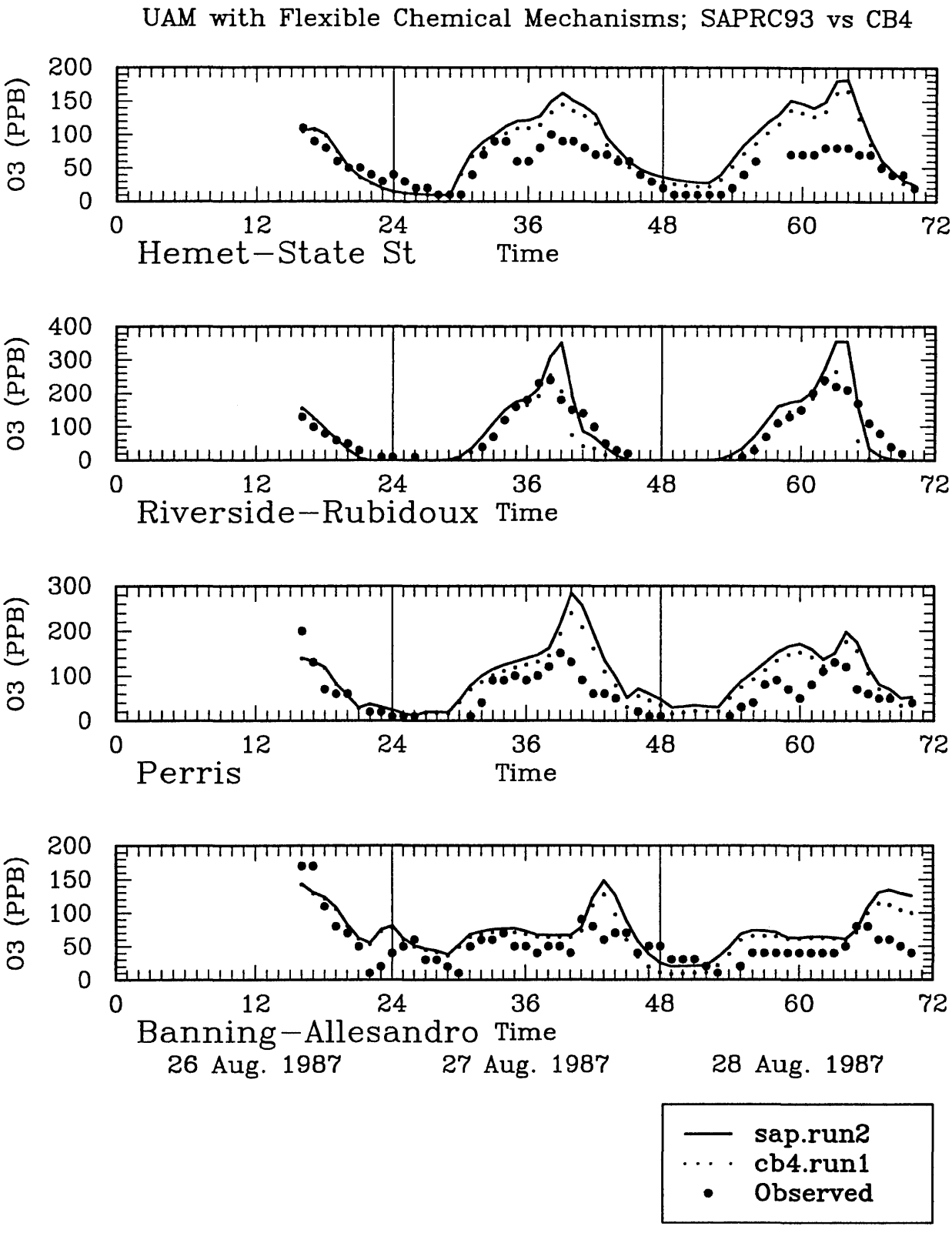

UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
400
300
200
100
0
0
12
24
36
48
60
72
Time
Reseda
Pomona
150
50
Whittier
Lancaster
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed

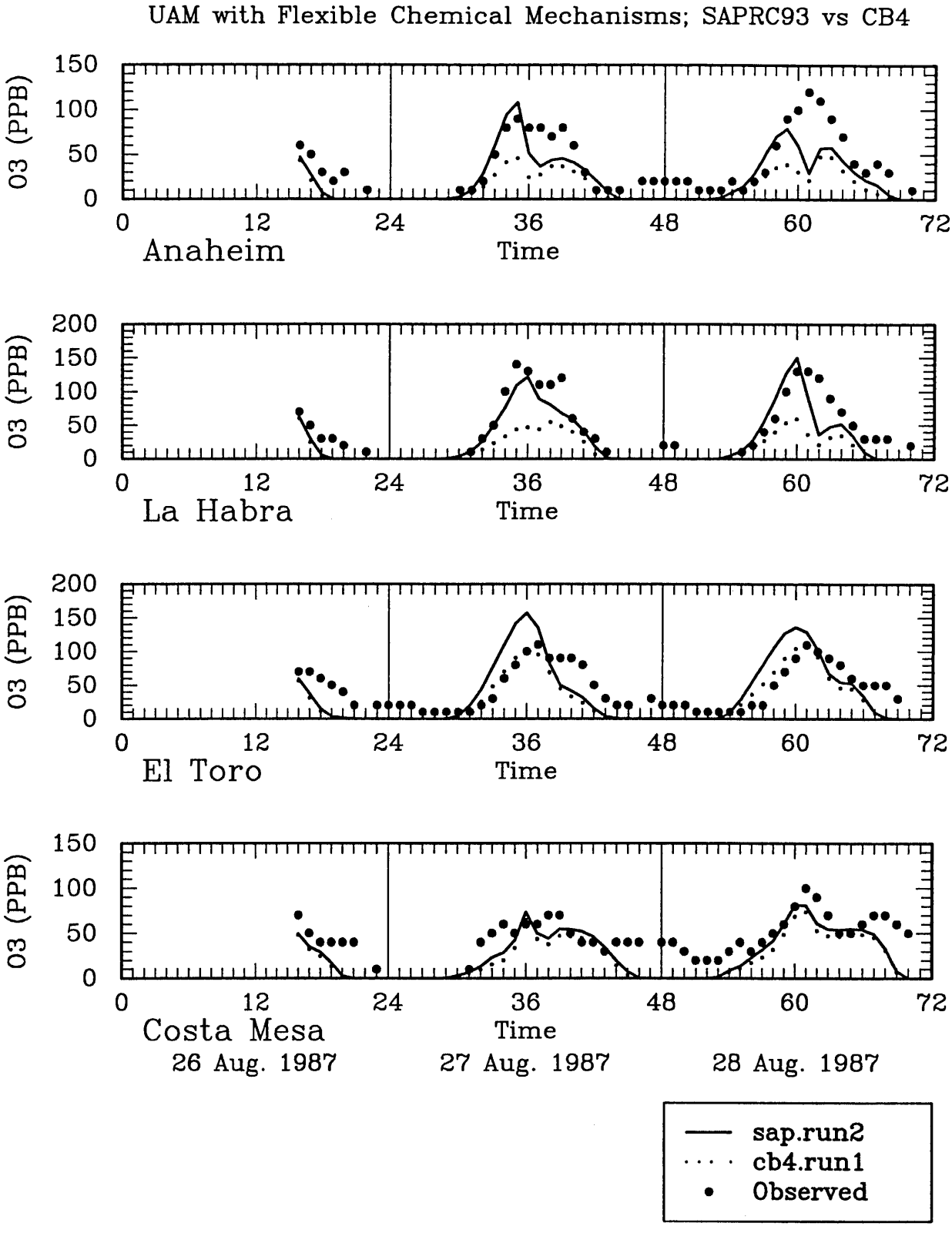

UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
200
150
100
50
0
0
12
24
36
48
60
72
Simi Valley
Time
03 (PPB)
300
200
100
0
Azusa
Time
03 (PPB)
400
300
200
100
0
Burbank
Time
03 (PPB)
75
50
25
0
North Long Beach
Time
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed


UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
150
100
50
0
0
12
24
36
48
60
72
Time
Thousand Oaks
Elrio
200
Piru
Ojai
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed


UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
300
200
100
0
0
12
24
36
48
60
72
Hesperia
Time
03 (PPB)
200
150
100
50
0
Victorville
Time
03 (PPB)
400
300
200
100
0
San Bernardino
Time
03 (PPB)
Redlands–Dearborn
Time
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed


UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
400
300
200
100
0
0
12
24
36
48
60
72
Time
Norco–Norconian
Upland ARB
Lake Gregory
Fontana
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed


UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
O3 (PPB)
200
150
100
50
0
0
12
24
36
48
60
72
Hemet–State St
Time
O3 (PPB)
400
300
200
100
0
Riverside–Rubidoux
Time
O3 (PPB)
300
200
100
0
Perris
Time
O3 (PPB)
200
150
100
50
0
Banning–Allesandro
Time
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed


UAM with Flexible Chemical Mechanisms; SAPRC93 vs CB4
03 (PPB)
150
100
50
0
0
12
24
36
48
60
72
Anaheim
Time
03 (PPB)
200
150
100
50
0
La Habra
Time
03 (PPB)
El Toro
Time
03 (PPB)
Costa Mesa
Time
26 Aug. 1987
27 Aug. 1987
28 Aug. 1987
sap.run2
cb4.run1
Observed