APPENDIX A. LISTING OF THE SAPRC-90 MECHANISM

This appendix gives the full listing of the SAPRC-90 mechanism which was used in the reactivity calculations discussed in this report. Most aspects of the mechanism are documented by Carter (1990), but some changes were made to the mechanistic parameter assignments for individual detailed model species as indicated below. The parameter assignments for emissions processing are also given in this Appendix.

Table A-1 gives a listing of all the model species used in the SAPRC-90 mechanism for base case simulations. Note that although the individual species whose reactivities were calculated were not lumped with other species, lumping was done for most components of the base ROG surrogate. Some species in the base case mixture are represented explicitly, some are represented using the "lumped molecule" method (where a model species represents another compound on a mole-for-mole basis), and the rest are represented by lumped model species whose parameters are adjusted to fit the set of compounds they represent. These are the lumped higher alkane and/or aromatics (AARn, ALKn, or AROn), and the lumped higher alkenes (OLEn).

As indicated on the table, the lumping approach used for the EKMA simulations is not appropriate for gridded airshed model applications. In the EKMA simulations, three lumped model species were used for the higher alkanes and aromatics, and two lumped model species were used for the higher alkenes. While the alkene lumping is appropriate for most applications, the optimum alkene and aromatic lumping for EKMA is not appropriate for more physically detailed models. Although aromatics and alkanes have quite different reactivities, there is no significant approximation involved in lumping those which react at similar rates provided that they are input into the scenario at the same time. Since all components in the base ROG are input at the same time in EKMA simulations, the alkanes and aromatics can lumped together to permit more fine rate constant resolution with fewer model species. However, this is not appropriate for grid model calculations because alkanes and aromatics may be emitted at different times. Table A-1 indicates the recommended alkane and aromatic lumping for airshed model applications. Note that it requires one more lumped model species to achieve similar rate constant resolution as the EKMA lumping approach.

Table A-2 gives a listing of all the detailed model species in the SAPRC-90 mechanism. These are the classes of VOCs species whose reactivities can be separately calculated. The table also gives the number of carbons (nC), the molecular weight (Mwt), the OH radical rate constant at 300K [kOH(300)], the

Table A-1. List of model species used in the SAPRC-90 mechanism for base case simulations.

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.
RNO3	Organic Nitrates
NPHE	Nitrophenols
PAN	Peroxy Acetyl Nitrate
PPN	Peroxy Propionyl Nitrate
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

Table A-1, (continued)

Name	Description
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.
Hydrocarbon species represented explicitly	
CH4	Methane
ETHE	Ethene
ISOP	Isoprene
APIN	α-Pinene
UNKN	Unknown biogenics. (Represented by equal parts of α- and β-pinene.)
Lumped alkane and aromatic species used for EKMA model simulations. (Used in this work but not recommended for grid model applications. Number of carbons shown is derived from the base ROG mixture used in this work, and will differ if different mixtures are used.)	
AAR1	Alkanes and aromatics with kOH < 5.0E+3 ppm^{-1} min^{-1} (3.68 Carbons)
AAR2	Alkanes and aromatics with kOH between 5.0E+3 and 1.5E+4 ppm^{-1} min^{-1} (6.44 Carbons)
AAR3	Alkanes and aromatics with kOH > 1.5E+4 ppm^{-1} min^{-1} (9.14 Carbons)
Lumped alkane and aromatic species recommended for airshed model simulations. (Not used in this work but recommended for grid model applications. Number of carbons shown is derived from the base ROG mixture used in this work, and will differ if different mixtures are used.)	
ALK1	Alkanes with kOH < 1.0E+4 ppm^{-1} min^{-1} (4.58 Carbons)
ALK2	Alkanes with kOH > 1.0E+4 ppm^{-1} min^{-1} (8.06 Carbons)
ARO1	Aromatics with kOH < 2.0E+4 ppm^{-1} min^{-1} (7.45 Carbons)
ARO2	Aromatics with kOH > 2.0E+4 ppm^{-1} min^{-1} (8.89 Carbons)
Lumped higher alkenes	
OLE1	Alkenes with kOH < 7.0E+4 ppm^{-1} min^{-1} (Primarily terminal alkenes. 5.16 Carbons)
OLE2	Alkenes with kOH > 7.0E+4 ppm^{-1} min^{-1} (Primary internal alkenes. 5.64 Carbons)

Table A-2 Summary of detailed model species used for reactivity assessment or emissions processing.

DMSname	nC	Mwt	kOH(300) [a]	Repres. [b]	Unc [c]	Doc [d]	Description
CO	1	28.01	3.52E+2	Explicit	1	1	Carbon Monoxide
	Alkanes						
METHANE	1	16.04	1.28E+1	Explicit	2	1	Methane
ETHANE	2	30.07	4.02E+2	Grp=ALK1	2	1	Ethane
PROPANE	3	44.10	1.71E+3	Grp=ALK1	2	1	Propane
N-C4	4	58.12	3.76E+3	Grp=ALK1	1	2	n-Butane
N-C5	5	72.15	6.03E+3	Grp=ALK1	5	2	n-Pentane
N-C6	6	86.18	8.27E+3	Grp=ALK1	5	2	n-Hexane
N-C7	7	100.21	1.06E+4	Grp=ALK2	5	2	n-Heptane
N-C8	8	114.23	1.29E+4	Grp=ALK2	5	2	n-Octane
N-C9	9	128.26	1.50E+4	Grp=ALK2	5	2	n-Nonane
N-C10	10	142.29	1.71E+4	Grp=ALK2	7	2	n-Decane
N-C11	11	156.31	1.95E+4	Grp=ALK2	8	2	n-Undecane
N-C12	12	170.34	2.09E+4	Grp=ALK2	8	2	n-Dodecane
N-C13	13	184.37	2.36E+4	Grp=ALK2	8	3	n-Tridecane
N-C14	14	198.39	2.45E+4	Grp=ALK2	8	3	n-Tetradecane
N-C15	15	212.42	2.66E+4	Grp=ALK2	8	3	n-Pentadecane
2-ME-C3	4	58.12	3.46E+3	Grp=ALK1	7	2	Isobutane
2-ME-C4	5	72.15	5.79E+3	Grp=ALK1	7	2	Iso-Pentane
22-DM-C3	5	72.15	1.27E+3	Grp=ALK1	7	2	Neopentane
2-ME-C5	6	86.18	8.31E+3	Grp=ALK1	7	2	2-Methyl Pentane
3-ME-C5	6	86.18	8.46E+3	Grp=ALK1	7	2	3-Methylpentane
22-DM-C4	6	86.18	3.46E+3	Grp=ALK1	7	2	2,2-Dimethyl Butane
23-DM-C4	6	86.18	8.08E+3	Grp=ALK1	5	3	2,3-Dimethyl Butane
24-DM-C5	7	100.21	1.02E+4	Grp=ALK2	7	3	2,4-Dimethyl Pentane
3-ME-C6	7	100.21	1.06E+4	Grp=ALK2	7	3	3-Methyl Hexane
2-ME-C6	7	100.21	1.01E+4	Grp=ALK2	7	3	2-Methyl Hexane
23-DM-C5	7	100.21	1.07E+4	Grp=ALK2	7	3	2,3-Dimethyl Pentane
33-DM-C5	7	100.21	4.63E+3	Grp=ALK1	7	3	3,3-Dimethyl Pentane
223TM-C4	7	100.21	6.22E+3	Grp=ALK1	7	2	2,2,3-Trimethyl Butane
2-ME-C7	8	114.23	1.22E+4	Grp=ALK2	7	3	2-Methyl Heptane
3-ME-C7	8	114.23	1.27E+4	Grp=ALK2	7	3	3-Methyl Heptane
4-ME-C7	8	114.23	1.27E+4	Grp=ALK2	7	3	4-Methyl Heptane
23-DM-C6	8	114.23	1.28E+4	Grp=ALK2	7	3	2,3-Dimethyl Hexane
24-DM-C6	8	114.23	1.28E+4	Grp=ALK2	7	3	2,4-Dimethyl Hexane
25-DM-C6	8	114.23	1.22E+4	Grp=ALK2	7	3	2,5-Dimethyl Hexane
224TM-C5	8	114.23	5.46E+3	Grp=ALK1	7	2	2,2,4-Trimethyl Pentane
234TM-C5	8	114.23	1.28E+4	Grp=ALK2	7	3	2,3,4-Trimethyl Pentane
2233M-C4	8	114.23	1.62E+3	Grp=ALK1	7	2	2,2,3,3-Tetrame. Butane
24-DM-C7	9	128.26	1.48E+4	Grp=ALK2	7	3	2,4-Dimethyl Heptane
4-ET-C7	9	128.26	1.56E+4	Grp=ALK2	7	3	4-Ethyl Heptane
225TM-C6	9	128.26	9.04E+3	Grp=ALK1	7	3	2,2,5-Trimethyl Hexane
4-PR-C7	10	142.29	1.77E+4	Grp=ALK2	8	3	3,4-Propyl Heptane
35-DE-C7	11	156.31	2.12E+4	Grp=ALK2	8	3	3,5-Diethyl Heptane
36-DE-C8	12	170.34	2.33E+4	Grp=ALK2	8	3	2,6-Diethyl Octane
37-DE-C9	13	184.37	2.54E+4	Grp=ALK2	8	3	3,7-Diethyl Nonane
38DE-C10	14	198.39	2.74E+4	Grp=ALK2	8	3	3,8-Diethyl Decane
39DE-C11	15	212.42	2.95E+4	Grp=ALK2	8	3	3,9-Diethyl Undecane
CYCC5	5	70.14	7.62E+3	Grp=ALK1	7	2	Cyclopentane
ME-CYCC5	6	84.16	1.19E+4	Grp=ALK2	7	3	Methylcyclopentane
CYCC6	6	84.16	1.11E+4	Grp=ALK2	7	2	Cyclohexane

Table A-2 (continued)

DMSname	nC	Mwt	kOH(300) [a]	Repres. [b]	Unc [c]	Doc [d]	Description
ME-CYCC6	7	98.19	1.51E+4	Grp=ALK2	5	3	Methylcyclohexane
13DMCYC5	7	98.19	1.27E+4	Grp=ALK2	8	3	1,3-Dimeth. Cyclopentane
ET-CYCC5	7	98.19	1.32E+4	Grp=ALK2	8	3	Ethyl Cyclopentane
PR-CYCC5	8	112.22	1.52E+4	Grp=ALK2	8	3	Propyl Cyclopentane
ET-CYCC6	8	112.22	1.81E+4	Grp=ALK2	8	3	Ethylcyclohexane
13DMCYC6	8	112.22	1.78E+4	Grp=ALK2	8	3	1,3-Dimethyl Cyclohexane
1E4MCYC6	9	126.24	2.07E+4	Grp=ALK2	8	3	1-Eth.-4-Meth. Cyclohex.
13DECYC6	10	140.27	2.36E+4	Grp=ALK2	8	3	1,3-Diethyl-Cyclohexane
13E5MCC6	11	154.30	2.63E+4	Grp=ALK2	8	3	13-Dieth-5-Me. Cyclohex.
135ECYC6	12	168.32	2.92E+4	Grp=ALK2	8	3	1,3,5-Triethyl Cyclohex.
13E5PCC6	13	182.35	3.13E+4	Grp=ALK2	8	3	13-Dieth-5-Pent Cyclohx.
13P5ECC6	14	196.38	3.34E+4	Grp=ALK2	8	3	13-Diprop-5-Eth Cyclohx.
135PCYC6	15	210.41	3.55E+4	Grp=ALK2	8	3	135-Tripropyl Cyclohex.
BR-C5	5	72.15	5.79E+3	2-ME-C4	7		Branched C5 Alkanes
BR-C6	6	86.18	8.31E+3	2-ME-C5	7		Branched C6 Alkanes
BR-C7	7	100.21	1.06E+4	3-ME-C6	7		Branched C7 Alkanes
BR-C8	8	114.23	1.27E+4	4-ME-C7	7		Branched C8 Alkanes
BR-C9	9	128.26	1.56E+4	4-ET-C7	7		Branched C9 Alkanes
BR-C10	10	142.29	1.77E+4	4-PR-C7	8		Branched C10 Alkanes
BR-C11	11	156.31	2.12E+4	35-DE-C7	8		Branched C11 alkanes
BR-C12	12	170.34	2.33E+4	36-DE-C8	8		Branched C12 Alkanes
BR-C13	13	184.37	2.54E+4	37-DE-C9	8		Branched C13 Alkanes
BR-C14	14	198.39	2.74E+4	38DE-C10	8		Branched C14 Alkanes
BR-C15	15	212.42	2.95E+4	39DE-C11	18		Branched C15 Alkanes
BR-C16	16	226.44	2.95E+4	39DE-C11	18		Branched C16 Alkanes
BR-C17	17	240.46	2.95E+4	39DE-C11	18		Branched C17 Alkanes
BR-C18	18	254.49	2.95E+4	39DE-C11	18		Branched C18 Alkanes
CYC-C6	6	84.16	1.11E+4	CYCC6	7		C6 Cycloalkanes
CYC-C7	7	98.19	1.51E+4	ME-CYCC6	7		C7 Cycloalkanes
CYC-C8	8	112.22	1.81E+4	ET-CYCC6	8		C8 Cycloalkanes
CYC-C9	9	126.24	2.07E+4	1E4MCYC6	8		C9 Cycloalkanes
CYC-C10	10	140.27	2.36E+4	13DECYC6	8		C10 Cycloalkanes
CYC-C11	11	154.30	2.63E+4	13E5MCC6	8		C11 Cycloalkanes
CYC-C12	12	168.32	2.92E+4	135ECYC6	8		C12 Cycloalkanes
CYC-C13	13	182.35	3.13E+4	13E5PCC6	8		C13 Cycloalkanes
CYC-C14	14	196.38	3.34E+4	13P5ECC6	8		C14 Cycloalkanes
CYC-C15	15	210.41	3.55E+4	135PCYC6	8		C15 Cycloalkanes
BCYC-C9	9	124.23	2.07E+4	1E4MCYC6	8		C9 Bicycloalkanes
BCYC-C10	10	138.25	2.36E+4	13DECYC6	8		C10 Bicycloalkanes
BCYC-C11	11	152.28	2.63E+4	13E5MCC6	8		C11 Bicycloalkanes
BCYC-C12	12	166.30	2.92E+4	135ECYC6	8		C12 Bicycloalkanes
BCYC-C13	13	180.33	3.13E+4	13E5PCC6	8		C13 Bicycloalkanes
BCYC-C14	14	194.36	3.34E+4	13P5ECC6	8		C14 Bicycloalkanes
BCYC-C15	15	208.39	3.55E+4	135PCYC6	8		C15 Bicycloalkanes
	Alkenes						
ETHENE	2	28.05	1.24E+4*	Explicit	1	4	Ethene
PROPENE	3	42.08	3.82E+4*	Grp=OLE1	4	4	Propene
1-BUTENE	4	56.11	4.56E+4*	Grp=OLE1	4	4	1-Butene
C4-OLE1	4	56.11	4.56E+4*	1-BUTENE	7		C4 Terminal Alkanes
3M-1-BUT	5	70.14	4.61E+4*	Grp=OLE1	7	5	3-Methyl-1-Butene
1-PENTEN	5	70.14	4.56E+4*	Grp=OLE1	7	5	1-Pentene

Table A-2 (continued)

DMSname	nC	Mwt	kOH(300) [a]	Repres. [b]	Unc [c]	Doc [d]	Description
1-HEXENE	6	84.16	5.37E+4*	Grp=OLE1	4	5	1-Hexene
1-C7-OLE	7	98.19	5.37E+4*	Grp=OLE1	8	5	1-Heptene
1-C8-OLE	8	112.22	5.37E+4*	Grp=OLE1	8	5	1-Octene
1-C9-OLE	9	126.24	5.37E+4*	Grp=OLE1	8	5	1-Nonene
1C10-OLE	10	140.27	5.37E+4*	Grp=OLE1	8	5	C10 1-Alkenes
1C11-OLE	11	154.30	5.37E+4*	Grp=OLE1	8	5	C11 1-Alkenes
1C12-OLE	12	168.32	5.37E+4*	Grp=OLE1	8	5	C12 1-Alkenes
1C13-OLE	13	182.35	5.37E+4*	Grp=OLE1	8	5	C13 1-Alkenes
ISOBUTEN	4	56.11	7.46E+4*	Grp=OLE2	5	4	Isobutene
2M-1-BUT	5	70.14	8.80E+4*	Grp=OLE2	7	5	2-Methyl-1-Butene
T-2-BUTE	4	56.11	9.24E+4*	Grp=OLE2	5	4	trans-2-Butene
C-2-BUTE	4	56.11	8.19E+4*	Grp=OLE2	5	4	cis-2-Butene
2M-2-BUT	5	70.14	1.26E+5*	Grp=OLE2	7	5	2-Methyl-2-Butene
23M2-BUT	6	84.16	1.59E+5*	Grp=OLE2	7	5	2,3-Dimethyl-2-Butene
2-C5-OLE	5	70.14	9.62E+4*	Grp=OLE2	7	5	2-Pentenes
2-C6-OLE	6	84.16	9.62E+4*	Grp=OLE2	8	6	2-Hexenes
2-C7-OLE	7	98.19	9.62E+4*	Grp=OLE2	8	6	2-Heptenes
3-C8-OLE	8	112.22	9.62E+4*	Grp=OLE2	8	7	3-Octenes
3-C9-OLE	9	126.24	9.62E+4*	Grp=OLE2	8	7	3-Nonenes
3C10-OLE	10	140.27	9.62E+4*	Grp=OLE2	8	7	C10 3-Alkenes
3C11-OLE	11	154.30	9.62E+4*	Grp=OLE2	8	7	C11 3-Alkenes
3C12-OLE	12	168.32	9.62E+4*	Grp=OLE2	8	7	C12 3-Alkenes
3C13-OLE	13	182.35	9.62E+4*	Grp=OLE2	8	7	C13 3-Alkenes
13-BUTDE	4	54.09	9.67E+4*	Grp=OLE2	8	4	1,3-Butadiene
CYC-PNDE	5	66.10	9.62E+4*	2-C5-OLE	8		Cyclopentadiene
ISOPRENE	5	68.12	1.46E+5*	Grp=OLE2	6	4	Isoprene
CYC-PNTE	5	68.12	9.74E+4*	Grp=OLE2	8	8	Cyclopentene
CYC-HEXE	6	82.15	9.82E+4*	Grp=OLE2	8	8	Cyclohexene
A-PINENE	10	136.24	7.80E+4*	Grp=OLE2	5	8	a-Pinene
B-PINENE	10	136.24	1.15E+5*	Grp=OLE2	8	8	b-Pinene
3-CARENE	10	136.24	1.29E+5*	Grp=OLE2	8	8	3-Carene
C5-OLE1	5	70.14	4.56E+4*	1-PENTEN	7		C5 Terminal Alkanes
C6-OLE1	6	84.16	5.37E+4*	1-HEXENE	7		C6 Terminal Alkanes
C7-OLE1	7	98.19	5.37E+4*	1-C7-OLE	8		C7 Terminal Alkanes
C8-OLE1	8	112.22	5.37E+4*	1-C8-OLE	8		C8 Terminal Alkanes
C9-OLE1	9	126.24	5.37E+4*	1-C9-OLE	8		C9 Terminal Alkanes
C10-OLE1	10	140.27	5.37E+4*	1C10-OLE	8		C10 Terminal Alkanes
C11-OLE1	11	154.30	5.37E+4*	1C11-OLE	8		C11 Terminal Alkanes
C12-OLE1	12	168.32	5.37E+4*	1C12-OLE	8		C12 Terminal Alkanes
C13-OLE1	13	182.35	5.37E+4*	1C13-OLE	8		C13 Terminal Alkanes
C4-OLE2	4	56.11	9.24E+4*	T-2-BUTE	7		C4 Internal Alkenes
C5-OLE2	5	70.14	9.62E+4*	2-C5-OLE	7		C5 Internal Alkenes
C6-OLE2	6	84.16	9.62E+4*	2-C6-OLE	8		C6 Internal Alkenes
C7-OLE2	7	98.19	9.62E+4*	2-C7-OLE	8		C7 Internal Alkenes
C8-OLE2	8	112.22	9.62E+4*	3-C8-OLE	8		C8 Internal Alkenes
C9-OLE2	9	126.24	9.62E+4*	3-C9-OLE	8		C9 Internal Alkenes
C10-OLE2	10	140.27	9.62E+4*	3C10-OLE	8		C10 Internal Alkenes
C11-OLE2	11	154.30	9.62E+4*	3C11-OLE	8		C11 Internal Alkenes
C12-OLE2	12	168.32	9.62E+4*	3C12-OLE	8		C12 Internal Alkenes
C13-OLE2	13	182.35	9.62E+4*	3C13-OLE	8		C13 Internal Alkenes

Table A-2 (continued)

DMSname	nC	Mwt	kOH(300) [a]	Repres. [b]	Unc [c]	Doc [d]	Description
C6-OL2D	6	82.15	9.62E+4*	2-C6-OLE	8		C6 Cyclic or di-olefins
C7-OL2D	7	96.18	9.62E+4*	2-C7-OLE	8		C7 Cyclic or di-olefins
C8-OL2D	8	110.20	9.62E+4*	3-C8-OLE	8		C8 Cyclic or di-olefins
C9-OL2D	9	124.23	9.62E+4*	3-C9-OLE	8		C9 Cyclic or di-olefins
C10-OL2D	10	138.26	9.62E+4*	3C10-OLE	8		C10 Cyclic or di-olefins
C11-OL2D	11	152.29	9.62E+4*	3C11-OLE	8		C11 Cyclic or di-olefins
C12-OL2D	12	166.31	9.62E+4*	3C12-OLE	8		C12 Cyclic or di-olefins
C13-OL2D	13	180.34	9.62E+4*	3C13-OLE	8		C13 Cyclic or di-olefins
	Aromatic Hydrocarbons						
BENZENE	6	78.11	1.89E+3	Grp=ARO1	4	1	Benzene
TOLUENE	7	92.14	8.67E+3	Grp=ARO1	4	1	Toluene
C2-BENZ	8	106.17	1.04E+4	Grp=ARO1	7	1	Ethyl Benzene
N-C3-BEN	9	120.20	8.81E+3	Grp=ARO1	7	1	n-Propyl Benzene
I-C3-BEN	9	120.20	9.54E+3	Grp=ARO1	7	1	Isopropyl Benzene
C9-BEN1	9	120.20	8.67E+3	TOLUENE	7		C9 Monosub. Benzenes
S-C4-BEN	10	134.22	8.81E+3	Grp=ARO1	7	1	s-Butyl Benzene
C10-BEN1	10	134.22	8.67E+3	TOLUENE	8		C10 Monosub. Benzenes
C11-BEN1	11	148.25	8.67E+3	TOLUENE	8		C11 Monosub. Benzenes
C12-BEN1	12	162.28	8.67E+3	TOLUENE	8		C12 Monosub. Benzenes
C13-BEN1	13	176.30	8.67E+3	TOLUENE	8		C13 Monosub. Benzenes
O-XYLENE	8	106.17	2.01E+4	Grp=ARO2	4	1	o-Xylene
P-XYLENE	8	106.17	2.10E+4	Grp=ARO2	7	1	p-Xylene
M-XYLENE	8	106.17	3.46E+4	Grp=ARO2	4	1	m-Xylene
C8-BEN2	8	106.17	3.46E+4	M-XYLENE	7		C8 Disub. Benzenes
C9-BEN2	9	120.20	3.46E+4	M-XYLENE	8		C9 Disub. Benzenes
C10-BEN2	10	134.22	3.46E+4	M-XYLENE	8		C10 Disub. Benzenes
C11-BEN2	11	148.25	3.46E+4	M-XYLENE	8		C11 Disub. Benzenes
C12-BEN2	12	162.28	3.46E+4	M-XYLENE	8		C12 Disub. Benzenes
135-TMB	9	120.20	8.44E+4	Grp=ARO2	4	1	1,3,5-Trimethyl Benzene
123-TMB	9	120.20	4.80E+4	Grp=ARO2	7	1	1,2,3-Trimethyl Benzene
124-TMB	9	120.20	4.77E+4	Grp=ARO2	7	1	1,2,4-Trimethyl Benzene
C9-BEN3	9	120.20	8.44E+4	135-TMB	7		C9 Trisub. Benzenes
C10-BEN3	10	134.22	8.44E+4	135-TMB	8		C10 Trisub. Benzenes
C11-BEN3	11	148.25	8.44E+4	135-TMB	8		C11 Trisub. Benzenes
C12-BEN3	12	162.28	8.44E+4	135-TMB	8		C12 Trisub. Benzenes
C10-BEN4	10	134.22	8.44E+4	135-TMB	8		C10 Tetrasub. Benzenes
C11-BEN4	11	148.25	8.44E+4	135-TMB	8		C11 Tetrasub. Benzenes
C12-BEN4	12	162.28	8.44E+4	135-TMB	8		C12 Tetrasub. Benzenes
C11-BEN5	11	148.25	8.44E+4	135-TMB	8		C11 Pentasub. Benzenes
C12-BEN5	12	162.28	8.44E+4	135-TMB	8		C11 Pentasub. Benzenes
C12-BEN6	12	162.28	8.44E+4	135-TMB	8		C12 Hexaasub. Benzenes
INDAN	9	118.18	5.03E+4	TETRALIN	8		Indan
TETRALIN	10	132.21	5.03E+4	Grp=ARO2	5	1	Tetralin
C11-TET	11	146.24	5.03E+4	TETRALIN	8		C11 Tetralin or Indane
NAPHTHAL	10	128.17	3.17E+4	Grp=ARO2	5	1	Naphthalene
ME-NAPH	11	142.20	7.63E+4	Grp=ARO2	8	1	Methyl Naphthalenes
C12-NAP1	12	156.23	7.63E+4	ME-NAPH	8		C12 Monosub. Naphth.
C13-NAP1	13	170.26	7.63E+4	ME-NAPH	8		C13 Monosub. Naphth.
23-DMN	12	156.23	1.13E+5	Grp=ARO2	5	1	2,3-Dimethyl Naphth.
DM-NAPH	12	156.23	1.13E+5	23-DMN	8		Dimethyl Naphthalenes
C12-NAP2	12	156.23	1.13E+5	23-DMN	8		C12 Disub. Naphthalenes

Table A-2 (continued)

DMSname	nC	Mwt	kOH(300) [a]	Repres. [b]	Unc [c]	Doc [d]	Description
C13-NAP2	13	170.26	1.13E+5	23-DMN	8		C13 Disub. Naphthalenes
C13-NAP3	13	170.26	1.13E+5	23-DMN	8		C13 Trisub. Naphthalenes
STYRENE	8	104.15	8.41E+4	Grp=OLE2	8	9	Styrene
AME-STYR	9	118.18	8.41E+4	STYRENE	8		a-Methyl Styrene
C9-STYR	9	118.18	8.41E+4	STYRENE	8		C9 Styrenes
C10-STYR	10	132.21	8.41E+4	STYRENE	8		C10 Styrenes
Acetylenes							
ACETYLEN	2	26.04	1.15E+3	Grp=ALK1	5	1	Acetylene
ME-ACTYL	3	40.07	8.90E+3	Grp=ALK1	9	10	Methyl Acetylene
ET-ACTYL	4	54.09	4.56E+4	1-BUTENE	9		Ethyl Acetylene
Alcohols, Ethers, Esters, etc.							
MEOH	1	32.04	1.38E+3	Grp=ALK1	1	1	Methanol
ETOH	2	46.07	4.81E+3	Grp=ALK1	1	11	Ethanol
N-C3-OH	3	60.10	7.84E+3	Grp=ALK1	7	1	n-Propyl Alcohol
I-C3-OH	3	60.10	7.64E+3	Grp=ALK1	7	1	Isopropyl Alcohol
I-C4-OH	4	74.12	9.47E+3	Grp=ALK1	7	12	Isobutyl Alcohol
N-C4-OH	4	74.12	1.22E+4	Grp=ALK2	7	1	n-Butyl Alcohol
T-C4-OH	4	74.12	1.66E+3	Grp=ALK1	7	1	t-Butyl Alcohol
S-C4-OH	4	74.12	1.40E+4	Grp=ALK2	7	13	s-Butyl Alcohol
C5OH	5	88.15	1.59E+4	Grp=ALK2	7	14	Pentyl Alcohol
1-C7OH	7	116.21	2.00E+4	Grp=ALK2	7	15	1-Heptanol
2-ETC6OH	8	130.23	1.91E+4	Grp=ALK2	7	16	2-Ethyl-1-Hexanol
ME-O-ME	2	46.07	4.42E+3	Grp=ALK1	7	11	Dimethyl Ether
ET-O-ET	4	74.12	1.94E+4	Grp=ALK2	3	17	Diethyl Ether
MTBE	5	88.15	4.17E+3	Grp=ALK1	1	11	Methyl t-Butyl Ether
ETBE	6	102.18	1.10E+4	Grp=ALK2	7	11	Ethyl t-Butyl Ether
S-098106	5	88.15	2.47E+4	Grp=ALK2	7	18	Ethyl Isopropyl Ether
S-098108	8	128.19	3.88E+4	Grp=ALK2	8	19	2-Butyltetrahydrofuran
S-098107	8	130.23	2.77E+4	Grp=ALK2	7	20	Dibutyl Ether
ET-GLYCL	2	62.07	1.13E+4	Grp=ALK2	7	21	Ethylene Glycol
PR-GLYCL	3	76.10	1.76E+4	Grp=ALK2	7	22	Propylene Glycol
12-C4OH2	4	90.12	2.26E+4	Grp=ALK2	7	23	1,2-Butandiol
C6-GLYCL	6	118.18	2.67E+4	Grp=ALK2	7	24	1,2-Dihydroxy Hexane
MEO-ETOH	3	76.10	1.95E+4	Grp=ALK2	7	25	2-Methoxy-Ethanol
ETO-ETOH	4	90.12	3.46E+4	Grp=ALK2	4	26	2-Ethoxy-Ethanol
ETOC3OH	5	104.15	2.95E+4	Grp=ALK2	7	27	1-Ethoxy-2-Propanol
BUO-ETOH	6	118.18	2.06E+4	Grp=ALK2	7	28	2-Butoxy-Ethanol
CARBITOL	6	134.17	7.46E+4	Grp=ALK2	4	26	2-(2-Ethoxyethoxy) EtOH
C8-CELSV	8	162.23	1.27E+4	Grp=ALK2	8	29	2-(2-Butoxyethoxy)-EtOH
Aldehydes							
FORMALD	1	30.03	1.43E+4*	Explicit	1	1	Formaldehyde
ACETALD	2	44.05	2.30E+4*	Explicit	4	1	Acetaldehyde
PROPALD	3	58.08	2.89E+4*	Explicit	5	1	C3 Aldehydes
C4-RCHO	4	72.11	2.89E+4*	PROPALD	7		C4 Aldehydes
C5-RCHO	5	86.14	2.89E+4*	PROPALD	8		C5 Aldehydes
C6-RCHO	6	100.16	2.89E+4*	PROPALD	8		C6 Aldehydes

Table A-2 (continued)

DMSname	nC	Mwt	kOH(300) [a]	Repres. [b]	Unc [c]	Doc [d]	Description
C7-RCHO	7	114.19	2.89E+4*	PROPALD	8		C7 Aldehydes
C8-RCHO	8	128.22	2.89E+4*	PROPALD	8		C8 Aldehydes
GLYOXAL	2	58.04	1.67E+4*	Explicit	3	1	Glyoxal
ACROLEIN	3	56.07	2.89E+4*	PROPALD	6		Acrolein
MEGLYOX	3	72.07	2.52E+4*	Explicit	3	1	Methyl Glyoxal
CROTALD	4	70.09	2.89E+4*	PROPALD	8		Crotonaldehyde
	Ketones						
ACETONE	3	58.08	3.39E+2*	Explicit	5	1	Acetone
MEK	4	72.11	1.70E+3*	Explicit	5	1	C4 Ketones
KET5	5	86.13	1.70E+3*	MEK	7		C5 Ketones
KET6	6	100.16	1.70E+3*	MEK	8		C6 Ketones
KET7	7	114.19	1.70E+3*	MEK	8		C7 Ketones
KET8	8	128.22	1.70E+3*	MEK	8		C8 Ketones
KET9	9	142.24	1.70E+3*	MEK	8		C9 Ketones
KET10	10	156.27	1.70E+3*	MEK	8		C10 Ketones
KET5C	5	84.12	1.70E+3*	MEK	8		C5 Cyclic Ketones
KET6C	6	98.15	1.70E+3*	MEK	8		C6 Cyclic Ketones
KET7C	7	112.17	1.70E+3*	MEK	8		C7 Cyclic Ketones
KET8C	8	126.20	1.70E+3*	MEK	8		C8 Cyclic Ketones
KET9C	9	140.23	1.70E+3*	MEK	8		C9 Cyclic Ketones
KET10C	10	154.25	1.70E+3*	MEK	8		C10 Cyclic Ketones
	Aromatic Oxygenates						
BENZALD	7	106.13	1.89E+4*	Explicit	5	1	Benzaldehyde
TOLUALD	8	120.15	1.89E+4*	BENZALD	7		Tolualdehyde
PHENOL	6	94.11	3.86E+4*	Explicit	7	1	Phenol
CRESOL	7	108.14	6.17E+4*	Explicit	5	1	Alkyl Phenols
	Various N-Containing Compounds						
ME-NITRT	1	61.04		Explicit	3	30	Methyl Nitrite

The assignments for the following compounds are not yet documented and must be considered to be preliminary and approximate. However, they should be suitable for processing emissions or assessing reactivities of complex mixtures where these are minor components. Measured or recommended rate constants were used when available, but they have not been updated since ~1988. Estimated rate constants are used when no reliable measurement data are available. The mechanistic parameter estimates are highly preliminary and in most cases very approximate. In view of the uncertainty of the mechanisms and the lack of data to test them, attempting to produce more elaborate assignments at this time would probably not yield significant improvements in reliability.

	Esters and oxides						
ME-ACET	3	74.08	2.50E+2	Grp=ALK1	0		Methyl Acetate
ME-ACRYL	4	86.09	4.56E+4	1-BUTENE	0		Methyl Acrylate
VIN-ACET	4	86.09	4.56E+4	1-BUTENE	0		Vinyl Acetate
ET-ACET	4	88.11	2.50E+3	Grp=ALK1	0		Ethyl Acetate
ET-ACRYL	5	100.11	4.56E+4	1-BUTENE	0		Ethyl Acrylate
PR-ACET	5	102.14	6.17E+3	Grp=ALK1	0		Propyl Acetate

Table A-2 (continued)

DMSname	nC	Mwt	kOH(300) [a]	Repres. [b]	Unc [c]	Doc [d]	Description
ME-IBUAT	5	102.13	8.66E+2	Grp=ALK1	0		Methyl Isobutyrate
IPR-ACET	5	104.00	4.54E+3	Grp=ALK1	0		Isopropyl Acetate
BU-ACET	6	116.16	6.31E+3	Grp=ALK1	0		n-Butyl Acetate
IBU-ACET	6	116.16	7.93E+3	Grp=ALK1	0		Isobutyl Acetate
CSV-ACET	6	132.00	2.88E+4	Grp=ALK2	0		2-Ethoxyethyl Acetate
IBU-IBTR	8	144.21	9.83E+3	Grp=ALK1	0		Isobutyl Isobutyrate
IC5IBUAT	9	158.24	9.91E+3	Grp=ALK1	0		Isoamyl Isobutyrate
S-098116	12	211.19	9.91E+3	Grp=ALK1	0		Subst. C7 Ester (C12)
S-098117	12	218.24	9.91E+3	Grp=ALK1	0		Subst. C9 Ester (C12)
ETOX	2	44.05	1.03E+2	Grp=ALK1	0		Ethylene Oxide
PROX	3	58.08	7.63E+2	Grp=ALK1	0		Propylene Oxide
FURAN	4	68.08	3.46E+4	M-XYLENE	6		Furan
Various N-Containing Compounds							
ET-AMINE	2	45.09	4.05E+4	Grp=ALK2	0		Ethyl Amine
ACRYLNIT	3	53.06	7.05E+3	Grp=ALK1	0		Acrylonitrile
TM-AMINE	3	59.11	8.90E+4	Grp=ALK2	0		Trimethyl Amine
NO2-BENZ	6	123.11	3.08E+2*	GrW=ARO1	0		Nitrobenzene
Halogenated Compounds							
S-043801	1	50.49	6.57E+1	Grp=ALK1	0		Methyl Chloride
S-043802	1	84.94	2.13E+2	Grp=ALK1	0		Dichloromethane
S-243819	1	94.95	6.02E+1	Grp=ALK1	0		Methyl Bromide
S-043803	1	119.39	1.55E+2	Grp=ALK1	0		Chloroform
CCL4	1	153.84	0.00E+0	INERT	1		Carbon Tetrachloride
S-043805	1	173.85	2.13E+2	Grp=ALK1	0		Methylene Bromide
S-043812	2	64.52	5.87E+2	Grp=ALK1	0		Ethyl Chloride
S-099018	2	96.95	2.64E+3	Grp=ALK1	0		Trans-1,2-Dichloroethene
S-043813	2	98.97	3.82E+2	Grp=ALK1	0		1,1-Dichloroethane
S-043820	2	131.66	4.84E+2	Grp=ALK1	0		1,1,2-Trichloroethane
S-043814	2	133.42	1.81E+1	Grp=ALK1	0		1,1,1-Trichloroethane
S-099016	3	112.99	1.45E+3	Grp=ALK1	0		1,2-Dichloropropane
S-098104	4	92.57	4.51E+3	Grp=ALK1	0		1-Chlorobutane
S-098105	8	148.68	1.26E+4	Grp=ALK2	0		3-(Chloromethyl)-Heptane
CL-ETHE	2	62.50	9.66E+3	GrW=ALK1	0		Vinyl Chloride
11CL2ETH	2	96.95	1.19E+4	Grp=ALK2	0		1,1-Dichloroethene
S-043815	2	99.00	3.38E+3	Grp=ALK1	0		Ethylene Dichloride
CL3-ETHE	2	131.40	0.00E+0	GrW=ALK1	0		Trichloroethylene
CL4-ETHE	2	165.85	0.00E+0	GrW=ALK1	0		Perchloroethylene
S-099014	2	187.88	3.38E+3	Grp=ALK1	0		Ethylene Dibromide
CL2IBUTE	4	125.01	4.64E+4	Grp=OLE1	0		2-(Cl-methyl)-3-Cl-Propene
CL-BEN	6	112.56	1.38E+3	Grp=ARO1	0		Monochlorobenzene
CL2-BEN	6	147.01	4.70E+2	Grp=ARO1	0		p-Dichlorobenzene

[a] Rate constant for reaction with OH radicals at 300K in units of ppm^{-1} min^{-1}. An "*" after the rate constant means that the mechanism includes other reactions of the compound besides OH reaction.

[b] The method used to represent the compound in the model, as follows:
"Explicit" = Explicitly represented in mechanism, even in mixtures. The "doc" code documents how the mechanism was derived.

"Grp=name" = Mechanistic parameters are assigned. The compound is represented explicitly when its reactivity is being calculated, but otherwise it is lumped with other similar species using the model species "name", whose rate constant and parameters are adjusted based on those for this and the other compounds this is lumped with. The "doc" code documents how the parameter assignments were derived.

"(model species)" = The compound is represented on a mole for mole basis by another detailed model species using the "lumped molecule" approach. If the model species has a different number of carbons, the additional carbons in this molecule are "lost", i.e., they are assumed not to affect the system.

[c] Uncertainty codes for the mechanism, parameter assignments, or the validity of the lumped molecule assignment are as follows:

1 Least uncertain mechanism, and tested against chamber data.
2 Mechanism probably not uncertain, but was not tested.
3 Laboratory data are available for the major reactions in the mechanism, but the mechanism was not tested.
4 Uncertain portions of the mechanism are adjusted or parameterized to fit chamber data.
5 The mechanism is uncertain, and only limited or uncertain data were available to test it.
6 The mechanism was not optimized to fit existing chamber data.
7 The mechanism was estimated and was not tested.
8 The mechanism was estimated and was not tested, and must be considered to be highly uncertain.
9 The mechanism was estimated and was not tested, and is likely to be incorrect. Suitable only for qualitative estimates at best, or for deriving parameters for model species when this is part of a mixture.
0 The mechanism is not documented. It should be considered to be preliminary and subject to change. Suitable only for deriving parameters for model species when this is a small part of a mixture.

[d] Documentation codes for the mechanism or model species assignments are as follows:

1 Documented by Carter (1990)
2 Rate constant recommended or tabulated by Atkinson (1989). Parameters calculated using the general procedures discussed by Carter (1990), with updates to the alkyl nitrate yield estimation method as given by Carter and Atkinson (1989).
3 Parameters and rate constants calculated using the general procedures discussed by Carter (1990), with updates to the alkyl nitrate yield estimation method as given by Carter and Atkinson (1989).
4 Mechanism and OH, O_3, and $O(^3P)$ rate constants as documented by Carter (1990). NO_3 rate constants given by Atkinson (1990). If no temperature dependence is given for the NO_3 reaction, the A factor is assumed to be the same as for the OH reaction.
5 Mechanism and rate constants estimated as documented by Carter (1990). NO_3 rate constant estimate updated.
6 Mechanism and rate constants estimated as documented by Carter (1990) except substitutent codes are 2 and 3. NO_3 rate constant estimate updated.
7 Mechanism and rate constants estimated as documented by Carter (1990) except substitutent codes are 3 and 3. NO_3 rate constant estimate updated.
8 Mechanism and rate constants estimated as documented by Carter (1990) except that the method for representing the ozone reactions of cycloalkenes changed so the yield of radicals is the same as for other internal alkenes. NO_3 rate constant estimate updated.
9 OH rate constant as estimated by Atkinson (1989), with the activation energy estimated. The O_3 rate constant was recommended by Atkinson

(private communication, 1991), and the NO_3 rate constant was from Atkinson and Aschmann (1988). The Arrhenius A factor for the NO_3 and the O_3 reactions were assumed to be the same as for 1-butene. The $O(^3P)$ rate constant was assumed to be the same as for cis-2-butene, because the OH rate constants are similar. The mechanism is estimated based on assuming all the reaction is at the double bond in a manner analogous to the general alkene mechanism.

10 Rate constant based on values tabulated by Atkinson (1989). The mechanism is highly simplified and used for only qualitative estimates.

11 The updates to the mechanism is documented by Carter (1991).

12 A new mechanism is used for isobutyl alcohol (2-methyl-1-propanol) since the one in Carter (1990) was in error. The rate constant and relative rates of reaction at the various possible positions were estimated using the method of Atkinson (1987). The mechanisms for the subsequent reactions of the radicals formed were estimated, in a manner generally analogous to the method used for estimating the alkane mechanisms.

13 Rate constant estimated. Reaction assumed to occur 85% alpha to the OH, 11% in the 2-position, and 4% at a methyl group. Subsequent reactions derived as discussed by Carter and Atkinson (1985).

14 The single measured kOH is tabulated by Atkinson (1989). Half of the reaction is estimated to occur alpha to the OH, forming HO_2 and the corresponding aldehyde. The rest is assumed to react to form the similar products as n-pentane, except that the total nitrate yield is assumed to be 2%, based on the adjusted value for MTBE (Carter, 1991; Carter et al., 1993)

15 The single measured kOH is tabulated by Atkinson (1989). 35% of the reaction is estimated to occur alpha to the OH, forming HO_2 and the corresponding aldehyde. The rest is assumed to react to form the same products as n-heptane, except that the total nitrate yield is reduced by a factor of 2, based on data for MTBE (Carter, 1991), ethoxyethanol and carbitol (Carter et al., 1993)

16 The kOH is estimated. 30% of the reaction is estimated to occur alpha to the OH, forming HO_2 and the corresponding aldehyde. The rest is assumed to react to form the same products as 3-methyl-heptane, except that the total nitrate yield is reduced by a factor of 2, based on data for MTBE (Carter, 1991), ethoxyethanol and carbitol (Carter et al., 1993)

17 Rate constant recommended by Atkinson (1989). The mechanism given by Wallington and Japar (1991), who showed that diethyl ether reacts to form formaldehyde and ethyl formate, is assumed. Ethyl formate is represented by MEK.

18 The rate constant is estimated. Neglecting reactions at the methyl groups, 30% of the reaction is assumed to occur on the ethyl side, and 70% on the isopropyl side. In both cases, the mechanism is assumed to be analogous to that of diethyl ether as discussed by Wallington and Japar (1991). After an NO to NO_2 conversion, a radical is formed which decomposes to yield methyl + isopropyl formate, or methyl + ethyl acetate. The methyl forms formaldehyde + HO_2 after a NO to NO_2 conversion. The formates and acetates are represented by MEK. The nitrate yield is assumed to be the same as MTBE.

19 The rate constant is estimated. The approximate mechanism is that propyl cyclohexane, except the nitrate yield is reduced by a factor of 2.

20 The lower of the two values tabulated by Atkinson (1989) is used because it is close to the estimated value, and because high values are more likely to be in error than low values. The reaction is estimated to occur 70% of the time next to the ether groups, yielding, in a process analogous to that for diethyl ether, butyl formate, propionaldehyde, HO_2 and 2 NO to NO_2 conversions. The ~15% reaction at the 3-position is

assumed to yield, after a NO to NO_2 conversion, an alkoxy radical which isomerizes to yield, after another NO to NO_2 conversion, a radical analogous to that formed after reaction by the ether position, which then decomposes to give propyl and a hyroxyformate. The propyl forms propionaldehyde and HO_2 after a NO to NO_2 conversion, the hydroxyformate is represented by MEK. The reactions at the other positions are assumed to proceed in a manner analogous to that for higher n-alkanes. The nitrate yield is assumed to be half that of n-octane, on the basis that the nitrate yield which fit the carbitol data was half that of n-hexane (Carter et al., 1993).

21 The single measured kOH is tabulated by Atkinson (1989). The reaction is assumed to occur alpha to one of the OH's, forming HO_2 and glycolaldehyde. The latter is represented in the model by acetaldehyde.

22 The single measured kOH is tabulated by Atkinson (1989). The reaction is assumed to occur alpha to one of the OH's, forming HO_2 and the corresponding hydroxy-substituted aldehyde and ketone, which are represented by RCHO or MEK, respectively. The ratio of reaction at the two positions is estimated.

23 The kOH is estimated. The reaction is assumed to occur alpha to one of the OH's, forming HO_2 and the corresponding hydroxy-substituted aldehyde and ketone, which are represented by RCHO or MEK, respectively. The ratio of reaction at the two positions is estimated.

24 The kOH is estimated. 20% of the reaction is estimated to occur at the 1-position, forming HO_2 and the corresponding hydroxy-aldehyde, which is represented by RCHO. 60% of the reaction is estimated to occur at the 2-position, forming HO_2 and the corresponding hydroxy-ketone, which is represented by MEK. The mechanism for the remaining 10% is estimated based on assumed reaction at the 3-position, where a beta-hydroxy alkoxy radical is formed after an NO to NO_2 conversion, which then is assumed to decompose to form HO_2, glycolaldehyde and butyraldehyde. Glycolaldehyde is represented by acetaldehyde. No nitrate formation is assumed, based on data for ethoxyethanol (Carter et al., 1993).

25 Rate constant based on the single determination tabulated by Atkinson (1989). 35% of the reaction is estimated to occur at the 1-position, giving HO_2 and ethoxyacetaldehyde, which is represented by RCHO. The remainder is assumed to react at the 2-position, giving, after a NO to NO_2 conversion, a beta-hydroxy alkoxy radical which decomposes to formaldehyde and methyl formate. The latter is represented by 0.18 MEK, as discussed by Carter (1991).

26 The rate constant and mechanism used is documented by Carter et al. (1993). Nitrate yield adjusted to fit results of incremental reactivity experiments.

27 The rate constant is estimated. 40% of the reaction is assumed to occur at the 2-position (alpha to the OH) forming HO_2 and a ketone. 30% is assumed to occur at the 3-position forming (after an NO to NO_2 conversion) an alkoxy radical which decomposes to yield acetaldehyde, HO_2, and a formate. 30% is assumed occur at the 5-position (on the ethoxy), forming, after an NO to NO_2 conversion, a radical which decomposes in a manner to the known reactions of diethyl ether and ETBE (Wallington and Japar, 1991), formaldehyde, a formate, HO_2, and an additional NO to NO_2 conversion. The ketone and formate products are represented by MEK. The nitrate yield from the peroxy radicals is assumed to be roughly half that derived for carbitol (Carter et al. 1993), or 4%.

28 The single measured value tabulated by Atkinson (1989) was used. The reaction was assumed to occur 40% of the time on each of the two positions by the ether linkage, and 20% of the time alpha to the OH. The reaction by the OH is assumed to form HO_2 and a higher aldehyde, which is represented by RCHO. The reactions by the ether group are assumed to proceed in a manner analogous to similar reactions in the

Table A-2 (continued)

ETBE and dimethyl ether systems (Wallington and Japar, 1991), and assumed for carbitol and ethoxy ethanol (Carter et al. 1993), resulting in the formation, after a NO to NO_2 conversion, of a radical which decomposes to yield a formate (which is represented by MEK) and either formaldehyde and HO_2 or ethyl radicals, which form acetaldehyde and HO_2 after a NO to NO_2 conversion. The nitrate yield is assumed to be half that of carbitol, or ~4%.

29 The rate constant is based on that of carbitol, increased by the amount estimated due to the additional $-CH_2-$ groups on this molecule. The tentative mechanism is that of carbitol, except with a higher nitrate yield because of the greater number of carbons. Since the nitrate yield which fits the carbitol reactivity data is approximately half that of n-hexane (Carter et. al, 1993), we assume the nitrate yield for this compound is roughly half that of n-octane, or 17%.

30 Absorption cross sections of Calvert and Pitts (1966), with quantum yields of unity assumed for photolysis reaction. OH radical rate constant of Tuazon et al. (1983); see also discussion in Atkinson (1989). Alkoxy radical reactions based on the recommendations of Atkinson (1990).

method used to represent the species in the model, and uncertainty classification and mechanism documentation notes for the various species. Footnotes to the table indicate the terminology used. The mechanism documentation notes indicate any changes or additions made to the assignments for the model species relative to the version documented by Carter (1990).

Table A-3 gives the reactions in the SAPRC-90 mechanism which were used in the base case simulations. Except for the lumped higher alkanes and/or aromatics and the lumped alkenes, the reactions are as documented by Carter (1990). The mechanisms for the lumped species which depend on the mixtures are given for the base ROG mixture used in this study, which is given in Appendix B. Reactions for the lumped alkanes and/or aromatics are given for both the EKMA lumping, which was used in this work, and the separate lumping of alkanes and aromatics as recommended for more physically detailed airshed models. The parameters are derived based on the parameters for the detailed model species. These parameters are given in Table A-4.

Table A-3 also gives the reactions of the dummy species used to compute kinetic reactivities of explicit model species, or to calculate the kinetic reactivity as a function of the OH radical rate constant. The reactions of these species, which have names of the type "Tnn" or "T_name", do not affect computed concentrations of other species in the system. These species are all input in equal amounts in the base case calculation, with relative amounts present initially and hourly emissions rates being the same as the base ROG and the test VOCs. The ratio of the final concentrations of these species, compared to the

Table A-3. Listing of SAPRC-91 Mechanism as used to in the Base Case Simulations.

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [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 [c]
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 [c]
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	(Same k as Reaction 29A)				NO3 + HO2. = HNO3 + O2
30B	(Same k as Reaction 29B)				NO3 + HO2. + M = HNO3 + O2
30C	(Same k as Reaction 29C)				NO3 + HO2. + H2O = HNO3 + O2 + H2O
30A	(Same k as Reaction 29D)				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
Peroxy Radical Operators					
B1	1.13E+04	6.16E+03	-0.36	-1.00	RO2. + NO = NO
B2	1.46E+04	7.49E+03	-0.40	-1.00	RCO3. + NO = NO
B4	1.06E+04	(Falloff Kinetics)			RCO3. + NO2 = NO2
	k0 =	7.00E+00	0.00	-6.00	
	kINF =	1.23E+04	0.00	-1.00	
		F= 0.27 n= 1.00			
B5	7.19E+03	4.99E+02	-1.59	-1.00	RO2. + HO2. = HO2. + RO2-HO2-PROD
B6	7.19E+03	4.99E+02	-1.59	-1.00	RCO3. + HO2. = HO2. + RO2-HO2-PROD
B8	1.47E+00	1.47E+00	0.00	-1.00	RO2. + RO2. = RO2-RO2-PROD
B9	1.60E+04	2.73E+03	-1.05	-1.00	RO2. + RCO3. = RO2-RO2-PROD
B10	2.40E+04	4.11E+03	-1.05	-1.00	RCO3. + RCO3. = RO2-RO2-PROD
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. + #.5 HO2.
B14	(Same k as Reaction B9)				RO2-R. + RCO3. = RCO3. + #.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

Table A-3 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
B21	(Same k as Reaction B8)				RO2-N. + RO2. = RO2. + #.5 HO2. + MEK + #1.5 -C
B22	(Same k as Reaction B9)				RO2-N. + RCO3. = RCO3. + #.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. + #.5 HO2.
B26	(Same k as Reaction B9)				RO2-XN. + RCO3. = RCO3. + HO2.
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. + #.5 HO2. + #6 -C
G5	(Same k as Reaction B9)				RO2-NP. + RCO3. = RCO3. + HO2. + #6 -C
Lumped Hydroperoxide Group					
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.
Formaldehyde					
C1	(Phot. Set = HCHOAVGR)				HCHO + HV = #2 HO2. + CO
C2	(Phot. Set = HCHOAVGM)				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
Acetaldehyde and PAN					
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. + #.5 HO2. + CO2 + HCHO
C17	(Same k as Reaction B10)				CCO-O2. + RCO3. = RCO3. + HO2. + CO2 + HCHO
C18	4.04E-02	(Falloff Kinetics)			PAN = CCO-O2. + NO2 + RCO3.
	k0 =	9.25E+13	25.41	-1.00	
	kINF =	1.32E+18	26.70	0.00	
		F= 0.27	n= 1.00		
C3+ Aldehydes and PPN					
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	RCHO + NO3 = 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. + #.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.
Acetone					
C38	3.39E+02	2.82E+02	-0.11	1.00	ACET + HO. = #.8 "MGLY + RO2-R." + #.2 "R2O2. + HCHO + CCO-O2. + RCO3." + RO2.
C39	(Phot. Set = ACETONE)				ACET + HV = CCO-O2. + HCHO + RO2-R. + RCO3. + RO2.
C4+ Ketones					
C44	1.70E+03	4.29E+02	-0.82	1.00	MEK + HO. = H2O + #.5 "CCHO + HCHO + CCO-O2. + C2CO-O2." + RCO3. + #1.5 "R2O2. + RO2."
C57	(Phot. Set = KETONE)				MEK + HV = CCO-O2. + CCHO + RO2-R. + RCO3. + RO2.
Organic Nitrates					
C95	3.03E+03	3.22E+04	1.41	-1.00	RNO3 + HO. = NO2 + #.155 MEK + #1.05 RCHO + #.48 CCHO + #.16 HCHO + #.11 -C + #1.39 "R2O2. + RO2."

Table A-3 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
Glyoxal and GPAN					
C58A	(Phot. Set = GLYOXAL1)				GLY + HV = #.8 HO2. + #.45 HCHO + #1.55 CO
C58B	(Phot. Set = GLYOXAL2)				GLY + HV = #.13 HCHO + #1.87 CO
C59	1.67E+04	1.67E+04	0.00	-1.00	GLY + HO. = #.6 HO2. + #1.2 CO + #.4 "HCOCO-O2. + RCO3."
C60	(Same k as Reaction C12)				GLY + NO3 = HNO3 + #.6 HO2. + #1.2 CO + #.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
C64	(Same k as Reaction C18)				GPAN = HCOCO-O2. + NO2 + RCO3.
C65	(Same k as Reaction B6)				HCOCO-O2. + HO2. = -OOH + CO2 + CO
C66	(Same k as Reaction B9)				HCOCO-O2. + RO2. = RO2. + #.5 HO2. + CO2 + CO
C67	(Same k as Reaction B10)				HCOCO-O2. + RCO3. = RCO3. + HO2. + CO2 + CO
Methyl Glyoxal					
C68	(Phot. Set = MEGLYOX)				MGLY + HV = 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.
Phenol and cresols					
G46	3.86E+04	3.86E+04	0.00	-1.00	HO. + PHEN = #.15 RO2-NP. + #.85 RO2-R. + #.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 = #.15 RO2-NP. + #.85 RO2-R. + #.2 MGLY + #5.5 -C + RO2.
G57	3.08E+04	3.08E+04	0.00	-1.00	NO3 + CRES = HNO3 + BZ-O. + -C
Benzaldehyde and PBzN					
G30	1.89E+04	1.89E+04	0.00	-1.00	BALD + HO. = BZ-CO-O2. + RCO3.
G31	(Phot. Set = BZCHO)				BALD + HV = #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.
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. = -OOH + CO2 + PHEN
G37	(Same k as Reaction B9)				BZ-CO-O2. + RO2. = RO2. + #.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.
Nitrophenols					
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
Aromatic Fragmentation Products					
G7	1.67E+04	1.67E+04	0.00	-1.00	HO. + AFG1 = HCOCO-O2. + RCO3.
G8	(Phot. Set = AROMUNKN)				AFG1 + HV + #ARP1/U = HO2. + HCOCO-O2. + RCO3.
G9	2.52E+04	2.52E+04	0.00	-1.00	HO. + AFG2 = C2CO-O2. + RCO3.
G10	(Phot. Set = AROMUNKN)				AFG2 + HV + #ARP2/U = HO2. + CO + CCO-O2. + RCO3.
Methane					
RCH4	1.28E+01	9.18E+02	2.55	1.00	CH4 + HO. = HCHO + RO2-R. + RO2.
Ethene					
D1	1.24E+04	2.88E+03	-0.87	-1.00	ETHE + HO. = #.22 CCHO + #1.56 HCHO + RO2-R. + RO2.
D6	2.75E-03	1.76E+01	5.23	-1.00	ETHE + O3 = HCHO + #.44 CO + #.56 -C + #.12 HO2.
D8	1.09E+03	1.53E+04	1.57	-1.00	ETHE + O = HCHO + CO + HO2. + RO2-R. + RO2.
D9	3.16E-01	7.97E+03	6.04	-1.00	ETHE + NO3 = NO2 + #2 HCHO + R2O2. + RO2.
Isoprene					
ISOH	1.46E+05	3.73E+04	-0.81	-1.00	ISOP + HO. = RO2-R. + HCHO + RCHO + RO2. + -C
ISO3	2.20E-02	1.81E+01	4.00	-1.00	ISOP + O3 = #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #.165 HO2. + #.06 HO. + #.135 RO2-R. + #.135 RO2. + #1.565 -C
ISN3	1.01E+03	4.45E+03	0.89	-1.00	ISOP + NO3 = NO2 + R2O2. + HCHO + RCHO + RO2. + -C
ISOA	8.81E+04	8.81E+04	0.00	-1.00	ISOP + O = #.4 HO2. + #.5 MEK + #.5 RCHO + #1.5 -C

Table A-3 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
Alpha-Pinene					
APOH	7.80E+04	1.78E+04	-0.88	-1.00	APIN + HO. = RO2-R. + RCHO + RO2. + #7 -C
APO3	1.47E-01	1.45E+00	1.37	-1.00	APIN + O3 = #.05 HCHO + #.2 CCHO + #.5 RCHO + #.61 MEK + #.075 CO + #.05 CCO-O2. + #.05 C2CO-O2. + #.1 RCO3. + #.105 HO2. + #.16 HO. + #.135 RO2-R. + #.15 R2O2. + #.285 RO2. + #5.285 -C
APN3	8.95E+03	1.75E+03	-0.97	-1.00	APIN + NO3 = NO2 + R2O2. + RCHO + RO2. + #7 -C
APOA	4.40E+04	4.40E+04	0.00	-1.00	APIN + O = #.4 HO2. + #.5 MEK + #.5 RCHO + #6.5 -C
Unknown Biogenics (Average of parameters of a-pinene and b-pinene)					
UNOH	9.64E+04	9.64E+04	0.00	-1.00	UNKN + HO. = RO2-R. + RO2. + #.5 HCHO + RCHO + #6.5 -C
UNO3	8.59E-02	8.59E-02	0.00	-1.00	UNKN + O3 = #.135 RO2-R. + #.135 HO2. + #.075 R2O2. + #.21 RO2. + #.025 CCO-O2. + #.025 C2CO-O2. + #.05 RCO3. + #.275 HCHO + #.175 CCHO + #.5 RCHO + #.41 MEK + #.185 CO + #5.925 -C + #.11 HO.
UNN3	6.31E+03	6.31E+03	0.00	-1.00	UNKN + NO3 = R2O2. + RO2. + #.5 HCHO + RCHO + #6.5 -C + NO2
UNOA	4.26E+04	4.26E+04	0.00	-1.00	UNKN + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
Lumped alkane and aromatic species whose parameters depend on the mixure being simulated.					
	The parameters given here are for the base ROG mixture used in this work. For EKMA models where all base ROGs are emitted with the same schedule, as is the case in all calculations in this work, the alkanes and aromatics with the same kOH ranges can be lumped together. Reactions with this lumping, used in this work, are given below. However, this is not a suitable lumping approach for airshed model applications where alkanes may be emitted in different places and times as aromatics. An alternative set of lumped reactions, where alkanes and aromatics are not lumped, is given for those who wish to use this mechanism in airshed model applications.				
	THE FOLLOWING SUITABLE FOR EKMA MODELS ONLY. NOT RECOMMENDED FOR AIRSHED MODELS.				
A1OH	2.89E+03	4.17E+03	0.22	0.00	AAR1 + HO. = #.917 RO2-R. + #.042 RO2-N. + #.007 RO2-XN. + #.034 HO2. + #.33 R2O2. + #1.295 RO2. + #.141 HCHO + #.315 CCHO + #.163 RCHO + #.254 ACET + #.25 MEK + #.024 CO + #.01 PHEN + #.065 GLY + #.021 AFG1 + #.188 -C
A2OH	8.80E+03	3.60E+03	-0.53	0.00	AAR2 + HO. = #.828 RO2-R. + #.109 RO2-N. + #.002 RO2-XN. + #.061 HO2. + #.635 R2O2. + #1.574 RO2. + #.013 HCHO + #.173 CCHO + #.205 RCHO + #.179 ACET + #.592 MEK + #.032 CO + #.007 CO2 + #.061 CRES + #.02 BALD + #.028 GLY + #.031 MGLY + #.096 AFG2 + #.973 -C
A3OH	4.32E+04	1.66E+04	-0.57	0.00	AAR3 + HO. = #.785 RO2-R. + #.079 RO2-N. + #.136 HO2. + #.198 R2O2. + #1.063 RO2. + #.003 HCHO + #.01 CCHO + #.046 RCHO + #.3 MEK + #.002 CO2 + #.136 CRES + #.027 BALD + #.046 GLY + #.36 MGLY + #.48 AFG2 + #3.63 -C
	THE FOLLOWING 4 SHOULD BE USED IN PLACE OF THE ABOVE 3 FOR AIRSHED MODELS.				
A1OH	5.12E+03	3.78E+03	-0.18	0.00	ALK1 + HO. = #.911 RO2-R. + #.074 RO2-N. + #.005 RO2-XN. + #.011 HO2. + #.575 R2O2. + #1.564 RO2. + #.065 HCHO + #.339 CCHO + #.196 RCHO + #.322 ACET + #.448 MEK + #.024 CO + #.025 GLY + #.051 -C
A2OH	1.36E+04	7.57E+03	-0.35	0.00	ALK2 + HO. = #.749 RO2-R. + #.249 RO2-N. + #.002 RO2-XN. + #.891 R2O2. + #1.891 RO2. + #.029 HCHO + #.048 CCHO + #.288 RCHO + #.028 ACET + #1.105 MEK + #.043 CO + #.018 CO2 + #1.268 -C
B1OH	8.67E+03	(No T Dependence)			ARO1 + HO. = #.742 RO2-R. + #.258 HO2. + #.742 RO2. + #.015 PHEN + #.244 CRES + #.08 BALD + #.124 GLY + #.123 MGLY + #.031 AFG1 + #.384 AFG2 + #3.271 -C
B2OH	4.79E+04	1.77E+04	-0.59	0.00	ARO2 + HO. = #.82 RO2-R. + #.18 HO2. + #.82 RO2. + #.18 CRES + #.036 BALD + #.068 GLY + #.462 MGLY + #.642 AFG2 + #3.933 -C
Lumped alkene species whose parameters depend on the mixure being simulated.					
	The parameters given here are for the base ROG mixture used in this work. The lumping approach is appropriate for airshed as well as EKMA models.				
O1OH	4.77E+04	3.28E+03	-1.59	0.00	OLE1 + HO. = #.871 RO2-R. + #.129 RO2-N. + RO2. + #.871 HCHO + #.256 CCHO + #.615 RCHO + #1.284 -C
O1O3	1.68E-02	2.78E+00	3.03	0.00	OLE1 + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.544 HCHO + #.253 CCHO + #.353 RCHO + #.189 MEK + #.295 CO + #1.995 -C + #.06 HO.
O1N3	1.71E+01	3.28E+03	3.12	0.00	OLE1 + NO3 = R2O2. + RO2. + HCHO + #.294 CCHO + #.706 RCHO + #1.451 -C + NO2
O1OA	6.07E+03	6.67E+03	0.06	0.00	OLE1 + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.657 -C

Table A-3 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
O2OH	9.89E+04	7.33E+03	-1.54	0.00	OLE2 + HO. = #.93 RO2-R. + #.07 RO2-N. + RO2. + #.321 HCHO + #.647 CCHO + #.605 RCHO + #.111 ACET + #.061 MEK + #.056 BALD + #.889 -C
O2O3	2.31E-01	2.57E+00	1.43	0.00	OLE2 + O3 = #.195 RO2-R. + #.163 HO2. + #.032 R2O2. + #.228 RO2. + #.006 CCO-O2. + #.006 C2CO-O2. + #.012 RCO3. + #.283 HCHO + #.453 CCHO + #.325 RCHO + #.06 ACET + #.364 MEK + #.193 CO + #.03 BALD + #.012 MGLY + #1.282 -C + #.12 HO. + #.015 BZ-O.
O2N3	1.54E+03	7.67E+02	-0.41	0.00	OLE2 + NO3 = R2O2. + RO2. + #.346 HCHO + #.696 CCHO + #.651 RCHO + #.119 ACET + #.066 MEK + #.06 BALD + #.908 -C + NO2
O2OA	4.21E+04	1.45E+04	-0.63	0.00	OLE2 + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #2.14 -C

Counter species used for computing integrated O3

NOTE: IntO3 is declared as a "non diluting" model species, which means that a dilution term is not included in its kinetic differential equations. Thus INTO3 is simply the integral of $[O_3]$ over time.

IO3	1.00E+00	(No T Dependence)	O3 = O3 + IntO3

Counter species used to compute kinetic reactivities

The following reactions are only included in base case calculations. The base case calculation has the counter species TRACE, T.3 through T3C, and T_HCHO through T_ETHE added to the scenario in the same way test species are when their incremental reactivities are calculated.

Counter species used to determine final concentrations of species which do not react chemically. (The software requires a dummy reaction for it to be integrated.)

R.T	0.00E+00	(No T Dependence)	TRACE =

Counter species used for computing dependence of mechanistic reactivity on kOH.

R.3	3.00E+02	(No T Dependence)	HO. + T.3 = HO. + T.3PROD
R01	1.00E+03	(No T Dependence)	HO. + T01 = HO. + T01PROD
R03	3.00E+03	(No T Dependence)	HO. + T03 = HO. + T03PROD
R10	1.00E+04	(No T Dependence)	HO. + T10 = HO. + T10PROD
R30	3.00E+04	(No T Dependence)	HO. + T30 = HO. + T30PROD
R1C	1.00E+05	(No T Dependence)	HO. + T1C = HO. + T1CPROD
R3C	3.00E+05	(No T Dependence)	HO. + T3C = HO. + T3CPROD

Counter species used for computing mechansitic reactivities for formaldehyde, acetaldehyde and other species which are represented explicitly.

R.3A	(Phot. Set = HCHOAVGR)				HV + T_HCHO = R_HCHO
R.3B	(Phot. Set = HCHOAVGM)				HV + T_HCHO = R_HCHO
R.3C	1.43E+04	1.65E+03	-1.29	1.00	HO. + T_HCHO = HO. + R_HCHO
R.3C	1.14E+02	1.42E+01	-1.24	-1.00	HO2. + T_HCHO = HO2. + R_HCHO
R.3C	9.36E-01	4.11E+03	5.00	-1.00	NO3 + T_HCHO = NO3 + R_HCHO
R01A	2.30E+04	8.15E+03	-0.62	-1.00	HO. + T_CCHO = HO. + R_HCHO
R01B	(Phot. Set = CCHOR)				HV + T_CCHO = R_HCHO
R01C	4.17E+00	2.05E+03	3.70	-1.00	NO3 + T_CCHO = NO3 + R_HCHO
R03A	2.89E+04	1.25E+04	-0.50	-1.00	HO. + T_RCHO = HO. + R_RCHO
R03B	(Phot. Set = RCHO)				HV + T_RCHO = R_RCHO
R03C	4.17E+00	2.05E+03	3.70	-1.00	NO3 + T_RCHO = NO3 + R_RCHO
R10A	3.39E+02	2.82E+02	-0.11	1.00	HO. + T_ACET = HO. + R_ACET
R10B	(Phot. Set = ACETONE)				HV + T_ACET = R_ACET
R30A	1.70E+03	4.29E+02	-0.82	1.00	HO. + T_MEK = HO. + R_MEK
R30B	(Phot. Set = KETONE)				HV + T_MEK = R_MEK
R3CA	1.24E+04	2.88E+03	-0.87	-1.00	HO. + T_ETHE = HO. + R_ETHE
R3CB	2.75E-03	1.76E+01	5.23	-1.00	O3 + T_ETHE = O3 + R_ETHE
R3CC	1.09E+03	1.53E+04	1.57	-1.00	O + T_ETHE = O + R_ETHE
R3CD	3.28E-01	2.88E+03	5.41	-1.00	NO3 + T_ETHE = NO3 + R_ETHE

[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-5.

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

[c] "#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.

Table A-4. Reactions of Detailed Model Species used for reactivity assessment or emissions processing.

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
Alkanes				
4.02E+02	1.88E+03	0.92	1.00	ETHANE + HO. = RO2-R. + CCHO + RO2.
1.71E+03	1.98E+03	0.09	1.00	PROPANE + HO. = #.039 RO2-XN. + #.961 RO2-R. + #.658 ACET + #.303 RCHO + #.116 -C + RO2.
3.76E+03	1.99E+03	-0.38	1.00	N-C4 + HO. = #.076 RO2-N. + #.924 RO2-R. + #.397 R2O2. + #.001 HCHO + #.571 CCHO + #.14 RCHO + #.533 MEK + #-0.076 -C + #1.397 RO2.
6.03E+03	2.77E+03	-0.46	1.00	N-C5 + HO. = #.12 RO2-N. + #.88 RO2-R. + #.544 R2O2. + #.007 HCHO + #.08 CCHO + #.172 RCHO + #.929 MEK + #.001 -C + #1.544 RO2.
8.27E+03	1.98E+04	0.52	-1.00	N-C6 + HO. = #.185 RO2-N. + #.815 RO2-R. + #.738 R2O2. + #.02 CCHO + #.105 RCHO + #1.134 MEK + #.186 -C + #1.738 RO2.
1.06E+04	2.88E+04	0.60	-1.00	N-C7 + HO. = #.267 RO2-N. + #.733 RO2-R. + #.727 R2O2. + #.056 RCHO + #1.241 MEK + #.535 -C + #1.727 RO2.
1.29E+04	4.62E+04	0.76	-1.00	N-C8 + HO. = #.333 RO2-N. + #.667 RO2-R. + #.706 R2O2. + #.002 RCHO + #1.333 MEK + #.998 -C + #1.706 RO2.
1.50E+04	3.19E+04	0.45	-1.00	N-C9 + HO. = #.373 RO2-N. + #.627 RO2-R. + #.673 R2O2. + #.001 RCHO + #1.299 MEK + #1.934 -C + #1.673 RO2.
1.71E+04	3.63E+04	0.45	-1.00	N-C10 + HO. = #.397 RO2-N. + #.603 RO2-R. + #.659 R2O2. + #.001 RCHO + #1.261 MEK + #2.969 -C + #1.659 RO2.
1.95E+04	4.12E+04	0.45	-1.00	N-C11 + HO. = #.411 RO2-N. + #.589 RO2-R. + #.654 R2O2. + #.001 RCHO + #1.241 MEK + #3.975 -C + #1.654 RO2.
2.09E+04	4.43E+04	0.45	-1.00	N-C12 + HO. = #.42 RO2-N. + #.58 RO2-R. + #.644 R2O2. + #.001 RCHO + #1.223 MEK + #5.004 -C + #1.644 RO2.
2.36E+04	4.99E+04	0.45	-1.00	N-C13 + HO. = #.427 RO2-N. + #.573 RO2-R. + #.638 R2O2. + #.001 RCHO + #1.211 MEK + #6.022 -C + #1.638 RO2.
2.45E+04	5.34E+04	0.47	-1.00	N-C14 + HO. = #.431 RO2-N. + #.569 RO2-R. + #.634 R2O2. + #.001 RCHO + #1.202 MEK + #7.033 -C + #1.634 RO2.
2.66E+04	5.76E+04	0.46	-1.00	N-C15 + HO. = #.434 RO2-N. + #.566 RO2-R. + #.631 R2O2. + #.001 RCHO + #1.196 MEK + #8.044 -C + #1.631 RO2.
3.46E+03	1.37E+03	-0.55	1.00	2-ME-C3 + HO. = #.027 RO2-N. + #.973 RO2-R. + #.744 R2O2. + #.744 HCHO + #.744 ACET + #.229 RCHO + #.202 -C + #1.744 RO2.
5.79E+03	7.50E+03	0.15	-1.00	2-ME-C4 + HO. = #.064 RO2-N. + #.002 RO2-XN. + #.933 RO2-R. + #.734 R2O2. + #.614 CCHO + #.611 ACET + #.133 RCHO + #.303 MEK + #.007 -C + #1.734 RO2.
1.27E+03	2.36E+03	0.37	1.00	22-DM-C3 + HO. = #.051 RO2-N. + #.949 RO2-R. + #.019 R2O2. + #.019 HCHO + #.01 ACET + #.939 RCHO + #1.878 -C + #1.019 RO2.
8.31E+03	1.21E+04	0.22	-1.00	2-ME-C5 + HO. = #.122 RO2-N. + #.005 RO2-XN. + #.873 RO2-R. + #.749 R2O2. + #.006 HCHO + #.023 CCHO + #.223 ACET + #.545 RCHO + #.724 MEK + #.137 -C + #1.749 RO2.
8.46E+03	9.81E+03	0.09	-1.00	3-ME-C5 + HO. = #.112 RO2-N. + #.888 RO2-R. + #.86 R2O2. + #.005 HCHO + #.523 CCHO + #.089 RCHO + #1.003 MEK + #.11 -C + #1.86 RO2.
3.46E+03	4.17E+04	1.48	-1.00	22-DM-C4 + HO. = #.153 RO2-N. + #.847 RO2-R. + #.96 R2O2. + #.295 HCHO + #.303 CCHO + #.295 ACET + #.372 RCHO + #.542 MEK + #.164 -C + #1.96 RO2.
8.08E+03	6.74E+03	-0.11	-1.00	23-DM-C4 + HO. = #.061 RO2-N. + #.039 RO2-XN. + #.901 RO2-R. + #.944 R2O2. + #1.584 ACET + #.128 RCHO + #.096 MEK + #.177 -C + #1.944 RO2.
1.01E+04	1.56E+04	0.26	-1.00	2-ME-C6 + HO. = #.196 RO2-N. + #.803 RO2-R. + #.858 R2O2. + #.03 HCHO + #.037 CCHO + #.036 ACET + #.118 RCHO + #1.265 MEK + #.393 -C + #1.858 RO2.
1.06E+04	1.37E+04	0.15	-1.00	3-ME-C6 + HO. = #.182 RO2-N. + #.002 RO2-XN. + #.815 RO2-R. + #.842 R2O2. + #.127 CCHO + #.329 RCHO + #1.119 MEK + #.369 -C + #1.842 RO2.

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
1.07E+04	9.09E+03	-0.10	-1.00	23-DM-C5 + HO. = #.128 RO2-N. + #.011 RO2-XN. + #.86 RO2-R. + #1.101 R2O2. + #.036 HCHO + #.253 CCHO + #.39 ACET + #.185 RCHO + #.96 MEK + #.252 -C + #2.101 RO2.
1.02E+04	1.01E+04	0.00	-1.00	24-DM-C5 + HO. = #.131 RO2-N. + #.002 RO2-XN. + #.867 RO2-R. + #.844 R2O2. + #.257 ACET + #.772 RCHO + #.682 MEK + #.531 -C + #1.844 RO2.
4.63E+03	2.04E+04	0.89	-1.00	33-DM-C5 + HO. = #.231 RO2-N. + #.769 RO2-R. + #.94 R2O2. + #.04 HCHO + #.289 CCHO + #.145 ACET + #.237 RCHO + #.907 MEK + #.453 -C + #1.94 RO2.
6.22E+03	1.19E+03	-0.98	1.00	223TM-C4 + HO. = #.107 RO2-N. + #.893 RO2-R. + #1.581 R2O2. + #.637 HCHO + #1.291 ACET + #.255 RCHO + #.255 MEK + #.165 -C + #2.581 RO2.
1.22E+04	1.97E+04	0.29	-1.00	2-ME-C7 + HO. = #.26 RO2-N. + #.74 RO2-R. + #.839 R2O2. + #.022 HCHO + #.025 CCHO + #.018 ACET + #.118 RCHO + #1.36 MEK + #.779 -C + #1.839 RO2.
1.27E+04	1.76E+04	0.19	-1.00	3-ME-C7 + HO. = #.245 RO2-N. + #.755 RO2-R. + #.867 R2O2. + #.072 CCHO + #.066 RCHO + #1.425 MEK + #.733 -C + #1.867 RO2.
1.27E+04	1.76E+04	0.19	-1.00	4-ME-C7 + HO. = #.244 RO2-N. + #.002 RO2-XN. + #.753 RO2-R. + #.803 R2O2. + #.352 RCHO + #1.204 MEK + #.906 -C + #1.803 RO2.
1.28E+04	1.25E+04	-0.01	-1.00	23-DM-C6 + HO. = #.175 RO2-N. + #.008 RO2-XN. + #.817 RO2-R. + #1.051 R2O2. + #.006 HCHO + #.01 CCHO + #.125 ACET + #.241 RCHO + #1.363 MEK + #.548 -C + #2.051 RO2.
1.28E+04	1.25E+04	-0.01	-1.00	24-DM-C6 + HO. = #.178 RO2-N. + #.822 RO2-R. + #.968 R2O2. + #.045 HCHO + #.122 CCHO + #.027 ACET + #.339 RCHO + #1.257 MEK + #.698 -C + #1.968 RO2.
1.22E+04	1.37E+04	0.07	-1.00	25-DM-C6 + HO. = #.188 RO2-N. + #.812 RO2-R. + #1.731 R2O2. + #.422 HCHO + #.518 ACET + #.165 RCHO + #1.008 MEK + #.563 -C + #2.731 RO2.
5.46E+03	2.36E+04	0.87	-1.00	224TM-C5 + HO. = #.188 RO2-N. + #.001 RO2-XN. + #.811 RO2-R. + #.878 R2O2. + #.115 HCHO + #.001 CCHO + #.254 ACET + #.745 RCHO + #.573 MEK + #1.65 -C + #1.878 RO2.
1.28E+04	8.88E+03	-0.22	-1.00	234TM-C5 + HO. = #.128 RO2-N. + #.016 RO2-XN. + #.855 RO2-R. + #1.312 R2O2. + #.066 HCHO + #.037 CCHO + #.518 ACET + #.332 RCHO + #1.075 MEK + #.368 -C + #2.312 RO2.
1.62E+03	2.15E+03	0.17	1.00	2233M-C4 + HO. = #.137 RO2-N. + #.863 RO2-R. + #1.074 R2O2. + #.863 RCHO + #1.074 MEK + #.432 -C + #2.074 RO2.
1.48E+04	1.60E+04	0.05	-1.00	24-DM-C7 + HO. = #.223 RO2-N. + #.001 RO2-XN. + #.776 RO2-R. + #.933 R2O2. + #.033 HCHO + #.02 CCHO + #.015 ACET + #.385 RCHO + #1.257 MEK + #1.586 -C + #1.933 RO2.
1.56E+04	1.89E+04	0.12	-1.00	4-ET-C7 + HO. = #.271 RO2-N. + #.002 RO2-XN. + #.727 RO2-R. + #.804 R2O2. + #.002 HCHO + #.059 CCHO + #.303 RCHO + #1.167 MEK + #1.949 -C + #1.804 RO2.
9.04E+03	1.47E+04	0.29	-1.00	225TM-C6 + HO. = #.27 RO2-N. + #.73 RO2-R. + #1.081 R2O2. + #.039 HCHO + #.36 ACET + #.434 RCHO + #.977 MEK + #1.32 -C + #2.081 RO2.
1.77E+04	2.28E+04	0.15	-1.00	4-PR-C7 + HO. = #.301 RO2-N. + #.002 RO2-XN. + #.696 RO2-R. + #.775 R2O2. + #.004 CCHO + #.328 RCHO + #1.139 MEK + #2.945 -C + #1.775 RO2.
2.12E+04	1.86E+04	-0.08	-1.00	35-DE-C7 + HO. = #.246 RO2-N. + #.754 RO2-R. + #1.273 R2O2. + #.021 HCHO + #.054 CCHO + #.09 RCHO + #1.862 MEK + #1.922 -C + #2.273 RO2.
2.33E+04	2.19E+04	-0.04	-1.00	36-DE-C8 + HO. = #.267 RO2-N. + #.733 RO2-R. + #1.35 R2O2. + #.002 HCHO + #.422 CCHO + #.012 RCHO + #1.647 MEK + #3.192 -C + #2.351 RO2.
2.54E+04	2.54E+04	0.00	-1.00	37-DE-C9 + HO. = #.285 RO2-N. + #.715 RO2-R. + #1.226 R2O2. + #.002 HCHO + #.008 CCHO + #.111 RCHO + #1.819 MEK + #3.943 -C + #2.226 RO2.
2.74E+04	2.89E+04	0.03	-1.00	38DE-C10 + HO. = #.298 RO2-N. + #.702 RO2-R. + #1.122 R2O2. + #.002 HCHO + #.003 RCHO + #1.82 MEK + #5.223 -C + #2.122 RO2.

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
2.95E+04	3.26E+04	0.06	-1.00	39DE-C11 + HO. = #.31 RO2-N. + #.69 RO2-R. + #1.103 R2O2. + #.001 HCHO + #.003 RCHO + #1.79 MEK + #6.285 -C + #2.103 RO2.
7.62E+03	2.81E+03	-0.59	1.00	CYCC5 + HO. = #.127 RO2-N. + #.873 RO2-R. + #1.745 R2O2. + #.873 RCHO + #.218 MEK + #.873 CO + #2.745 RO2.
1.11E+04	3.51E+03	-0.68	1.00	CYCC6 + HO. = #.193 RO2-N. + #.807 RO2-R. + #.352 R2O2. + #.003 HCHO + #.333 RCHO + #.816 MEK + #.003 CO2 + #.765 -C + #1.352 RO2.
1.19E+04	1.84E+04	0.26	-1.00	ME-CYCC5 + HO. = #.153 RO2-N. + #.847 RO2-R. + #1.978 R2O2. + #.283 HCHO + #.697 RCHO + #.49 MEK + #.564 CO + #.189 CO2 + #.153 -C + #2.978 RO2.
1.51E+04	1.96E+04	0.16	-1.00	ME-CYCC6 + HO. = #.216 RO2-N. + #.784 RO2-R. + #.928 R2O2. + #.092 HCHO + #.001 CCHO + #.466 RCHO + #.987 MEK + #.003 CO + #.046 CO2 + #.432 -C + #1.928 RO2.
1.27E+04	1.40E+04	0.06	-1.00	13DMCYC5 + HO. = #.16 RO2-N. + #.84 RO2-R. + #2.118 R2O2. + #.517 HCHO + #.478 RCHO + #.825 MEK + #.284 CO + #.344 CO2 + #.32 -C + #3.118 RO2.
1.32E+04	1.79E+04	0.18	-1.00	ET-CYCC5 + HO. = #.207 RO2-N. + #.793 RO2-R. + #1.849 R2O2. + #.009 HCHO + #.34 CCHO + #.523 RCHO + #.674 MEK + #.336 CO + #.261 CO2 + #.41 -C + #2.849 RO2.
1.52E+04	2.18E+04	0.22	-1.00	PR-CYCC5 + HO. = #.269 RO2-N. + #.005 RO2-XN. + #.726 RO2-R. + #1.668 R2O2. + #.003 HCHO + #.054 CCHO + #.741 RCHO + #.762 MEK + #.23 CO + #.229 CO2 + #.814 -C + #2.668 RO2.
1.78E+04	1.70E+04	-0.03	-1.00	13DMCYC6 + HO. = #.215 RO2-N. + #.785 RO2-R. + #1.386 R2O2. + #.17 HCHO + #.001 CCHO + #.499 RCHO + #1.131 MEK + #.002 CO + #.084 CO2 + #.646 -C + #2.386 RO2.
1.81E+04	2.11E+04	0.09	-1.00	ET-CYCC6 + HO. = #.265 RO2-N. + #.735 RO2-R. + #1.282 R2O2. + #.186 HCHO + #.293 CCHO + #.347 RCHO + #.811 MEK + #.01 CO + #.185 CO2 + #1.424 -C + #2.282 RO2.
2.07E+04	1.89E+04	-0.05	-1.00	1E4MCYC6 + HO. = #.247 RO2-N. + #.753 RO2-R. + #1.782 R2O2. + #.278 HCHO + #.25 CCHO + #.457 RCHO + #1.022 MEK + #.264 CO2 + #1.263 -C + #2.782 RO2.
2.36E+04	2.08E+04	-0.08	-1.00	13DECYC6 + HO. = #.267 RO2-N. + #.733 RO2-R. + #1.596 R2O2. + #.211 HCHO + #.37 CCHO + #.175 RCHO + #1.151 MEK + #.006 CO + #.208 CO2 + #2.37 -C + #2.596 RO2.
2.63E+04	1.96E+04	-0.17	-1.00	13E5MCC6 + HO. = #.238 RO2-N. + #.762 RO2-R. + #1.89 R2O2. + #.226 HCHO + #.368 CCHO + #.159 RCHO + #1.53 MEK + #.001 CO + #.184 CO2 + #2.068 -C + #2.89 RO2.
2.92E+04	2.16E+04	-0.18	-1.00	135ECYC6 + HO. = #.251 RO2-N. + #.749 RO2-R. + #1.722 R2O2. + #.202 HCHO + #.392 CCHO + #.136 RCHO + #1.408 MEK + #.001 CO + #.166 CO2 + #3.55 -C + #2.722 RO2.
3.13E+04	2.47E+04	-0.14	-1.00	13E5PCC6 + HO. = #.267 RO2-N. + #.001 RO2-XN. + #.732 RO2-R. + #1.469 R2O2. + #.129 HCHO + #.216 CCHO + #.25 RCHO + #1.391 MEK + #.001 CO + #.107 CO2 + #4.682 -C + #2.469 RO2.
3.34E+04	2.79E+04	-0.11	-1.00	13P5ECC6 + HO. = #.281 RO2-N. + #.001 RO2-XN. + #.718 RO2-R. + #1.277 R2O2. + #.077 HCHO + #.097 CCHO + #.329 RCHO + #1.359 MEK + #.001 CO + #.066 CO2 + #5.835 -C + #2.277 RO2.
3.55E+04	3.12E+04	-0.08	-1.00	135PCYC6 + HO. = #.293 RO2-N. + #.002 RO2-XN. + #.705 RO2-R. + #1.128 R2O2. + #.041 HCHO + #.023 CCHO + #.38 RCHO + #1.312 MEK + #.001 CO + #.038 CO2 + #7.02 -C + #2.128 RO2.
Alkenes				
1.24E+04	2.88E+03	-0.87	-1.00	ETHENE + HO. = RO2-R. + RO2. + #1.56 HCHO + #.22 CCHO
2.75E-03	1.76E+01	5.23	-1.00	ETHENE + O3 = #.12 HO2. + HCHO + #.44 CO + #.56 -C
3.16E-01	7.97E+03	6.04	-1.00	ETHENE + NO3 = R2O2. + RO2. + #2 HCHO + NO2
1.09E+03	1.53E+04	1.57	-1.00	ETHENE + O = RO2-R. + HO2. + RO2. + HCHO + CO
3.82E+04	7.12E+03	-1.00	-1.00	PROPENE + HO. = RO2-R. + RO2. + HCHO + CCHO
1.74E-02	1.94E+01	4.18	-1.00	PROPENE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.65 HCHO + #.5 CCHO + #.14 MEK + #.295 CO + #.495 -C + #.06 HO.
1.44E+01	7.12E+03	3.70	-1.00	PROPENE + NO3 = R2O2. + RO2. + HCHO + CCHO + NO2
5.88E+03	1.73E+04	0.64	-1.00	PROPENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #-0.5 -C

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
4.56E+04	9.61E+03	-0.93	-1.00	1-BUTENE + HO. = RO2-R. + RO2. + HCHO + RCHO
1.69E-02	5.08E+00	3.40	-1.00	1-BUTENE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1-BUTENE + NO3 = R2O2. + RO2. + HCHO + RCHO + NO2
6.19E+03	1.83E+04	0.65	-1.00	1-BUTENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #.5 -C
4.56E+04	8.51E+03	-1.00	-1.00	1-PENTEN + HO. = #.9 RO2-R. + #.1 RO2-N. + RO2. + #.9 HCHO + #.9 RCHO + #.9 -C
1.63E-02	5.08E+00	3.42	-1.00	1-PENTEN + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #1.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1-PENTEN + NO3 = R2O2. + RO2. + HCHO + RCHO + -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1-PENTEN + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1-HEXENE + HO. = #.775 RO2-R. + #.225 RO2-N. + RO2. + #.775 HCHO + #.775 RCHO + #1.775 -C
1.78E-02	5.08E+00	3.37	-1.00	1-HEXENE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #2.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1-HEXENE + NO3 = R2O2. + RO2. + HCHO + RCHO + #2 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1-HEXENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #2.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1-C7-OLE + HO. = #.73 RO2-R. + #.27 RO2-N. + RO2. + #.73 HCHO + #.73 RCHO + #2.73 -C
1.78E-02	5.08E+00	3.37	-1.00	1-C7-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #3.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1-C7-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #3 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1-C7-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #3.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1-C8-OLE + HO. = #.67 RO2-R. + #.33 RO2-N. + RO2. + #.67 HCHO + #.67 RCHO + #3.67 -C
1.78E-02	5.08E+00	3.37	-1.00	1-C8-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #4.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1-C8-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #4 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1-C8-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #4.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1-C9-OLE + HO. = #.64 RO2-R. + #.36 RO2-N. + RO2. + #.64 HCHO + #.64 RCHO + #4.64 -C
1.78E-02	5.08E+00	3.37	-1.00	1-C9-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #5.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1-C9-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #5 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1-C9-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #5.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1C10-OLE + HO. = #.62 RO2-R. + #.38 RO2-N. + RO2. + #.62 HCHO + #.62 RCHO + #5.62 -C
1.78E-02	5.08E+00	3.37	-1.00	1C10-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #6.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1C10-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #6 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1C10-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1C11-OLE + HO. = #.605 RO2-R. + #.395 RO2-N. + RO2. + #.605 HCHO + #.605 RCHO + #6.605 -C
1.78E-02	5.08E+00	3.37	-1.00	1C11-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #7.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1C11-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #7 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1C11-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #7.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1C12-OLE + HO. = #.6 RO2-R. + #.4 RO2-N. + RO2. + #.6 HCHO + #.6 RCHO + #7.6 -C
1.78E-02	5.08E+00	3.37	-1.00	1C12-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #8.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1C12-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #8 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1C12-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #8.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1C13-OLE + HO. = #.59 RO2-R. + #.41 RO2-N. + RO2. + #.59 HCHO + #.59 RCHO + #8.59 -C
1.78E-02	5.08E+00	3.37	-1.00	1C13-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #9.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1C13-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #9 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1C13-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #9.5 -C
5.37E+04	1.00E+04	-1.00	-1.00	1C14-OLE + HO. = #.588 RO2-R. + #.412 RO2-N. + RO2. + #.588 HCHO + #.588 RCHO + #9.588 -C
1.78E-02	5.08E+00	3.37	-1.00	1C14-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #10.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1C14-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #10 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1C14-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #10.5 -C

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
5.37E+04	1.00E+04	-1.00	-1.00	1C15-OLE + HO. = #.585 RO2-R. + #.415 RO2-N. + RO2. + #.585 HCHO + #.585 RCHO + #10.585 -C
1.78E-02	5.08E+00	3.37	-1.00	1C15-OLE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #11.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	1C15-OLE + NO3 = R2O2. + RO2. + HCHO + RCHO + #11 -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	1C15-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #11.5 -C
7.46E+04	1.39E+04	-1.00	-1.00	ISOBUTEN + HO. = RO2-R. + RO2. + HCHO + ACET
1.85E-02	5.21E+00	3.36	-1.00	ISOBUTEN + O3 = #.1 RO2-R. + #.06 HO2. + #.1 RO2. + #.5 HCHO + #.5 ACET + #.4 MEK + #.22 CO + #.1 MGLY + #-0.12 -C + #.1 HO.
4.99E+02	1.39E+04	1.98	-1.00	ISOBUTEN + NO3 = R2O2. + RO2. + HCHO + ACET + NO2
2.24E+04	2.58E+04	0.09	-1.00	ISOBUTEN + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #.5 -C
8.80E+04	1.64E+04	-1.00	-1.00	2M-1-BUT + HO. = RO2-R. + RO2. + HCHO + MEK
1.85E-02	5.21E+00	3.36	-1.00	2M-1-BUT + O3 = #.06 HO2. + #.15 R2O2. + #.15 RO2. + #.05 CCO-O2. + #.05 C2CO-O2. + #.1 RCO3. + #.55 HCHO + #.05 CCHO + #.9 MEK + #.22 CO + #.28 -C + #.1 HO.
4.99E+02	1.39E+04	1.98	-1.00	2M-1-BUT + NO3 = R2O2. + RO2. + HCHO + MEK + NO2
2.24E+04	2.58E+04	0.09	-1.00	2M-1-BUT + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.5 -C
9.24E+04	1.48E+04	-1.09	-1.00	T-2-BUTE + HO. = RO2-R. + RO2. + #2 CCHO
3.02E-01	1.33E+01	2.26	-1.00	T-2-BUTE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 HCHO + CCHO + #.28 MEK + #.15 CO + #.43 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	T-2-BUTE + NO3 = R2O2. + RO2. + #2 CCHO + NO2
3.43E+04	3.32E+04	-0.02	-1.00	T-2-BUTE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #.5 -C
8.19E+04	1.61E+04	-0.97	-1.00	C-2-BUTE + HO. = RO2-R. + RO2. + #2 CCHO
1.95E-01	5.17E+00	1.95	-1.00	C-2-BUTE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 HCHO + CCHO + #.28 MEK + #.15 CO + #.43 -C + #.12 HO.
5.09E+02	1.43E+02	-0.76	-1.00	C-2-BUTE + NO3 = R2O2. + RO2. + #2 CCHO + NO2
2.63E+04	1.78E+04	-0.23	-1.00	C-2-BUTE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #.5 -C
1.26E+05	2.82E+04	-0.89	-1.00	2M-2-BUT + HO. = RO2-R. + RO2. + CCHO + ACET
6.33E-01	9.06E+00	1.59	-1.00	2M-2-BUT + O3 = #.235 RO2-R. + #.105 HO2. + #.235 RO2. + #.15 HCHO + #.5 CCHO + #.5 ACET + #.54 MEK + #.075 CO + #.1 MGLY + #-0.185 -C + #.16 HO.
1.38E+04	2.82E+04	0.43	-1.00	2M-2-BUT + NO3 = R2O2. + RO2. + CCHO + ACET + NO2
6.94E+04	3.67E+04	-0.38	-1.00	2M-2-BUT + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.5 -C
4.61E+04	7.81E+03	-1.06	-1.00	3M-1-BUT + HO. = RO2-R. + RO2. + HCHO + RCHO + -C
1.69E-02	5.08E+00	3.40	-1.00	3M-1-BUT + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #1.565 -C + #.06 HO.
1.91E+01	9.61E+03	3.71	-1.00	3M-1-BUT + NO3 = R2O2. + RO2. + HCHO + RCHO + -C + NO2
6.19E+03	1.83E+04	0.65	-1.00	3M-1-BUT + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.5 -C
1.59E+05	2.98E+04	-1.00	-1.00	23M2-BUT + HO. = RO2-R. + RO2. + #2 ACET
1.71E+00	5.45E+00	0.69	-1.00	23M2-BUT + O3 = #.2 RO2-R. + #.2 RO2. + ACET + #.8 MEK + #.2 MGLY + #-0.8 -C + #.2 HO.
8.33E+04	2.98E+04	-0.61	-1.00	23M2-BUT + NO3 = R2O2. + RO2. + #2 ACET + NO2
1.14E+05	8.19E+03	-1.57	-1.00	23M2-BUT + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #2.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	2-C5-OLE + HO. = #.9 RO2-R. + #.1 RO2-N. + RO2. + #.9 CCHO + #.9 RCHO
3.93E-01	1.13E+01	2.00	-1.00	2-C5-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.15 HCHO + #.65 CCHO + #.5 RCHO + #.35 MEK + #.15 CO + #.5 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	2-C5-OLE + NO3 = R2O2. + RO2. + CCHO + RCHO + NO2
4.40E+04	4.40E+04	0.00	-1.00	2-C5-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	2-C6-OLE + HO. = #.775 RO2-R. + #.225 RO2-N. + RO2. + #.775 CCHO + #.775 RCHO + -C
3.93E-01	1.13E+01	2.00	-1.00	2-C6-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.15 HCHO + #.65 CCHO + #.5 RCHO + #.35 MEK + #.15 CO + #1.5 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	2-C6-OLE + NO3 = R2O2. + RO2. + CCHO + RCHO + -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	2-C6-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #2.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	2-C7-OLE + HO. = #.73 RO2-R. + #.27 RO2-N. + RO2. + #.73 CCHO + #.73 RCHO + #2 -C
3.93E-01	1.13E+01	2.00	-1.00	2-C7-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.15 HCHO + #.65 CCHO + #.5 RCHO + #.35 MEK + #.15 CO + #2.5 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	2-C7-OLE + NO3 = R2O2. + RO2. + CCHO + RCHO + #2 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	2-C7-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #3.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	3-C8-OLE + HO. = #.67 RO2-R. + #.33 RO2-N. + RO2. + #1.34 RCHO + #2.33 -C
3.93E-01	1.13E+01	2.00	-1.00	3-C8-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #2.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3-C8-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #2 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3-C8-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #4.5 -C

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
9.62E+04	1.80E+04	-1.00	-1.00	3-C9-OLE + HO. = #.64 RO2-R. + #.36 RO2-N. + RO2. + #1.28 RCHO + #3.36 -C
3.93E-01	1.13E+01	2.00	-1.00	3-C9-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #3.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3-C9-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #3 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3-C9-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #5.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	3C10-OLE + HO. = #.62 RO2-R. + #.38 RO2-N. + RO2. + #1.24 RCHO + #4.38 -C
3.93E-01	1.13E+01	2.00	-1.00	3C10-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #4.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3C10-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #4 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3C10-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	3C11-OLE + HO. = #.605 RO2-R. + #.395 RO2-N. + RO2. + #1.21 RCHO + #5.395 -C
3.93E-01	1.13E+01	2.00	-1.00	3C11-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #5.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3C11-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #5 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3C11-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #7.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	3C12-OLE + HO. = #.6 RO2-R. + #.4 RO2-N. + RO2. + #1.2 RCHO + #6.4 -C
3.93E-01	1.13E+01	2.00	-1.00	3C12-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #6.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3C12-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #6 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3C12-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #8.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	3C13-OLE + HO. = #.59 RO2-R. + #.41 RO2-N. + RO2. + #1.18 RCHO + #7.41 -C
3.93E-01	1.13E+01	2.00	-1.00	3C13-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #7.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3C13-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #7 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3C13-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #9.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	3C14-OLE + HO. = #.588 RO2-R. + #.412 RO2-N. + RO2. + #1.176 RCHO + #8.412 -C
3.93E-01	1.13E+01	2.00	-1.00	3C14-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #8.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3C14-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #8 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3C14-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #10.5 -C
9.62E+04	1.80E+04	-1.00	-1.00	3C15-OLE + HO. = #.585 RO2-R. + #.415 RO2-N. + RO2. + #1.17 RCHO + #9.415 -C
3.93E-01	1.13E+01	2.00	-1.00	3C15-OLE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + RCHO + #.42 MEK + #.15 CO + #9.57 -C + #.12 HO.
5.76E+02	1.61E+02	-0.76	1.00	3C15-OLE + NO3 = R2O2. + RO2. + #2 RCHO + #9 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3C15-OLE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #11.5 -C
9.82E+04	1.83E+04	-1.00	-1.00	CYC-HEXE + HO. = RO2-R. + RO2. + RCHO + #3 -C
1.50E-01	5.17E+00	2.11	-1.00	CYC-HEXE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + #.5 RCHO + #.42 MEK + #.15 CO + #2.07 -C + #.12 HO.
5.25E+02	1.61E+04	2.04	-1.00	CYC-HEXE + NO3 = R2O2. + RO2. + RCHO + #3 -C + NO2
3.22E+04	1.78E+04	-0.35	-1.00	CYC-HEXE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #2.5 -C
9.74E+04	1.82E+04	-1.00	-1.00	CYC-PNTE + HO. = RO2-R. + RO2. + RCHO + #2 -C
5.96E-01	5.17E+00	1.29	-1.00	CYC-PNTE + O3 = #.27 RO2-R. + #.21 HO2. + #.27 RO2. + #.3 CCHO + #.5 RCHO + #.42 MEK + #.15 CO + #1.07 -C + #.12 HO.
5.25E+02	1.61E+04	2.04	-1.00	CYC-PNTE + NO3 = R2O2. + RO2. + RCHO + #2 -C + NO2
3.51E+04	1.78E+04	-0.41	-1.00	CYC-PNTE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.5 -C
9.67E+04	2.17E+04	-0.89	-1.00	13-BUTDE + HO. = RO2-R. + RO2. + HCHO + RCHO
1.16E-02	4.84E+01	4.97	-1.00	13-BUTDE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #.565 -C + #.06 HO.
1.52E+02	2.17E+04	2.96	-1.00	13-BUTDE + NO3 = R2O2. + RO2. + HCHO + RCHO + NO2
3.08E+04	3.08E+04	0.00	-1.00	13-BUTDE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #.5 -C
1.46E+05	3.73E+04	-0.81	-1.00	ISOPRENE + HO. = RO2-R. + RO2. + HCHO + RCHO + -C
2.20E-02	1.81E+01	4.00	-1.00	ISOPRENE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #1.565 -C + #.06 HO.
1.01E+03	4.45E+03	0.89	-1.00	ISOPRENE + NO3 = R2O2. + RO2. + HCHO + RCHO + -C + NO2
8.81E+04	8.81E+04	0.00	-1.00	ISOPRENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #1.5 -C
7.80E+04	1.78E+04	-0.88	-1.00	A-PINENE + HO. = RO2-R. + RO2. + RCHO + #7 -C
1.47E-01	1.45E+00	1.37	-1.00	A-PINENE + O3 = #.135 RO2-R. + #.105 HO2. + #.15 R2O2. + #.285 RO2. + #.05 CCO-O2. + #.05 C2CO-O2. + #.1 RCO3. + #.05 HCHO + #.2 CCHO + #.5 RCHO + #.61 MEK + #.075 CO + #5.285 -C + #.16 HO.
8.95E+03	1.75E+03	-0.97	-1.00	A-PINENE + NO3 = R2O2. + RO2. + RCHO + #7 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	A-PINENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
1.15E+05	3.49E+04	-0.71	-1.00	B-PINENE + HO. = RO2-R. + RO2. + HCHO + RCHO + #6 -C
2.48E-02	5.21E+00	3.19	-1.00	B-PINENE + O3 = #.135 RO2-R. + #.165 HO2. + #.135 RO2. + #.5 HCHO + #.15 CCHO + #.5 RCHO + #.21 MEK + #.295 CO + #6.565 -C + #.06 HO.
3.68E+03	3.68E+03	0.00	-1.00	B-PINENE + NO3 = R2O2. + RO2. + HCHO + RCHO + #6 -C + NO2
4.11E+04	4.11E+04	0.00	-1.00	B-PINENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
2.51E+05	2.51E+05	0.00	-1.00	D-LIMONE + HO. = RO2-R. + RO2. + RCHO + #7 -C
3.08E-01	3.08E-01	0.00	-1.00	D-LIMONE + O3 = #.135 RO2-R. + #.105 HO2. + #.15 R2O2. + #.285 RO2. + #.05 CCO-O2. + #.05 C2CO-O2. + #.1 RCO3. + #.05 HCHO + #.2 CCHO + #.5 RCHO + #.61 MEK + #.075 CO + #5.285 -C + #.16 HO.
1.79E+04	1.79E+04	0.00	-1.00	D-LIMONE + NO3 = R2O2. + RO2. + RCHO + #7 -C + NO2
1.76E+05	1.76E+05	0.00	-1.00	D-LIMONE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
4.93E+05	4.93E+05	0.00	-1.00	TERPINEN + HO. = RO2-R. + RO2. + RCHO + #7 -C
1.27E+01	1.27E+01	0.00	-1.00	TERPINEN + O3 = #.135 RO2-R. + #.105 HO2. + #.15 R2O2. + #.285 RO2. + #.05 CCO-O2. + #.05 C2CO-O2. + #.1 RCO3. + #.05 HCHO + #.2 CCHO + #.5 RCHO + #.61 MEK + #.075 CO + #5.285 -C + #.16 HO.
1.42E+05	1.42E+05	0.00	-1.00	TERPINEN + NO3 = R2O2. + RO2. + RCHO + #7 -C + NO2
1.76E+05	1.76E+05	0.00	-1.00	TERPINEN + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
1.29E+05	1.29E+05	0.00	-1.00	3-CARENE + HO. = RO2-R. + RO2. + RCHO + #7 -C
6.87E-02	1.45E+00	1.82	-1.00	3-CARENE + O3 = #.135 RO2-R. + #.105 HO2. + #.15 R2O2. + #.285 RO2. + #.05 CCO-O2. + #.05 C2CO-O2. + #.1 RCO3. + #.05 HCHO + #.2 CCHO + #.5 RCHO + #.61 MEK + #.075 CO + #5.285 -C + #.16 HO.
1.34E+04	1.34E+04	0.00	-1.00	3-CARENE + NO3 = R2O2. + RO2. + RCHO + #7 -C + NO2
4.40E+04	4.40E+04	0.00	-1.00	3-CARENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
3.16E+05	3.16E+05	0.00	-1.00	MYRCENE + HO. = RO2-R. + RO2. + RCHO + ACET + #4 -C
7.12E-01	7.12E-01	0.00	-1.00	MYRCENE + O3 = #.235 RO2-R. + #.105 HO2. + #.235 RO2. + #.15 CCHO + #.5 RCHO + #.5 ACET + #.61 MEK + #.075 CO + #.1 MGLY + #3.885 -C + #.16 HO.
1.56E+04	1.56E+04	0.00	-1.00	MYRCENE + NO3 = R2O2. + RO2. + RCHO + ACET + #4 -C + NO2
2.94E+05	2.94E+05	0.00	-1.00	MYRCENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #6.5 -C
	Aromatics			
1.89E+03	3.67E+03	0.40	-1.00	BENZENE + HO. = #.236 PHEN + #.207 GLY + #.49 AFG1 + #.764 RO2-R. + #.236 HO2. + #3.19 -C + #.764 RO2.
8.67E+03	2.66E+03	-0.70	-1.00	TOLUENE + HO. = #.085 BALD + #.26 CRES + #.118 GLY + #.131 MGLY + #.41 AFG2 + #.74 RO2-R. + #.26 HO2. + #2.726 -C + #.74 RO2.
1.04E+04	1.04E+04	0.00	-1.00	C2-BENZ + HO. = #.085 BALD + #.26 CRES + #.118 GLY + #.131 MGLY + #.41 AFG2 + #.74 RO2-R. + #.26 HO2. + #3.726 -C + #.74 RO2.
9.54E+03	9.54E+03	0.00	-1.00	I-C3-BEN + HO. = #.085 BALD + #.26 CRES + #.118 GLY + #.131 MGLY + #.41 AFG2 + #.74 RO2-R. + #.26 HO2. + #4.726 -C + #.74 RO2.
8.81E+03	8.81E+03	0.00	-1.00	N-C3-BEN + HO. = #.085 BALD + #.26 CRES + #.118 GLY + #.131 MGLY + #.41 AFG2 + #.74 RO2-R. + #.26 HO2. + #4.726 -C + #.74 RO2.
8.81E+03	8.81E+03	0.00	-1.00	S-C4-BEN + HO. = #.085 BALD + #.26 CRES + #.118 GLY + #.131 MGLY + #.41 AFG2 + #.74 RO2-R. + #.26 HO2. + #5.726 -C + #.74 RO2.
3.46E+04	3.46E+04	0.00	-1.00	M-XYLENE + HO. = #.04 BALD + #.18 CRES + #.108 GLY + #.37 MGLY + #.666 AFG2 + #.82 RO2-R. + #.18 HO2. + #3.136 -C + #.82 RO2.
2.01E+04	2.01E+04	0.00	-1.00	O-XYLENE + HO. = #.04 BALD + #.18 CRES + #.108 GLY + #.37 MGLY + #.666 AFG2 + #.82 RO2-R. + #.18 HO2. + #3.136 -C + #.82 RO2.
2.10E+04	2.10E+04	0.00	-1.00	P-XYLENE + HO. = #.04 BALD + #.18 CRES + #.108 GLY + #.37 MGLY + #.666 AFG2 + #.82 RO2-R. + #.18 HO2. + #3.136 -C + #.82 RO2.
8.44E+04	8.44E+04	0.00	-1.00	135-TMB + HO. = #.03 BALD + #.18 CRES + #.62 MGLY + #.6 AFG2 + #.82 RO2-R. + #.18 HO2. + #3.87 -C + #.82 RO2.
4.80E+04	4.80E+04	0.00	-1.00	123-TMB + HO. = #.03 BALD + #.18 CRES + #.62 MGLY + #.6 AFG2 + #.82 RO2-R. + #.18 HO2. + #3.87 -C + #.82 RO2.
4.77E+04	4.77E+04	0.00	-1.00	124-TMB + HO. = #.03 BALD + #.18 CRES + #.62 MGLY + #.6 AFG2 + #.82 RO2-R. + #.18 HO2. + #3.87 -C + #.82 RO2.
3.17E+04	3.17E+04	0.00	-1.00	NAPHTHAL + HO. = #.17 PHEN + #.14 RO2-NP. + #.32 AFG1 + #.69 RO2-R. + #.17 HO2. + #7.5 -C + #.83 RO2.
1.13E+05	1.13E+05	0.00	-1.00	23-DMN + HO. = #.04 CRES + #.49 MGLY + #.16 RO2-NP. + #.85 AFG1 + #.8 RO2-R. + #.04 HO2. + #7.59 -C + #.96 RO2.

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
7.63E+04	7.63E+04	0.00	-1.00	ME-NAPH + HO. = #.085 PHEN + #.02 CRES + #.245 MGLY + #.15 RO2-NP. + #.585 AFG1 + #.745 RO2-R. + #.105 HO2. + #7.545 -C + #.895 RO2.
5.03E+04	5.03E+04	0.00	-1.00	TETRALIN + HO. = #.09 PHEN + #.12 RO2-NP. + #.164 AFG1 + #.79 RO2-R. + #.09 HO2. + #8.412 -C + #.91 RO2.
8.41E+04	1.57E+04	-1.00	-1.00	STYRENE + HO. = RO2-R. + RO2. + HCHO + BALD
2.60E-02	5.08E+00	3.14	-1.00	STYRENE + O3 = #.06 HO2. + #.25 R2O2. + #.25 RO2. + #.5 HCHO + #.47 CO + #.5 BALD + #2.03 -C + #.25 HO. + #.25 BZ-O.
2.27E+02	9.61E+03	2.23	-1.00	STYRENE + NO3 = R2O2. + RO2. + HCHO + BALD + NO2
2.63E+04	1.78E+04	-0.23	-1.00	STYRENE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #4.5 -C
	Acetylenes			
1.15E+03	2.50E+03	0.46	-1.00	ACETYLEN + HO. = #.7 RO2-R. + #.3 HO2. + #.3 CO + #.3 -C + #.7 GLY + #.7 RO2.
8.90E+03	8.90E+03	0.00	-1.00	ME-ACTYL + HO. = RO2-R. + RCHO + RO2.
	Alcohols and Ethers			
1.38E+03	8.44E+02	-0.29	1.00	MEOH + HO. = HO2. + HCHO
4.81E+03	8.16E+02	-1.06	1.00	ETOH + HO. = #.1 RO2-R. + #.9 HO2. + #.156 HCHO + #.922 CCHO + #.1 RO2.
7.84E+03	7.84E+03	0.00	-1.00	N-C3-OH + HO. = #.23 RO2-R. + #.77 HO2. + #.23 HCHO + #.23 CCHO + #.77 RCHO + #.23 RO2.
7.64E+03	9.67E+02	-1.23	1.00	I-C3-OH + HO. = HO2. + ACET
9.47E+03	9.47E+03	0.00	-1.00	I-C4-OH + HO. = #.43 RO2-R. + #.57 HO2. + #.37 HCHO + #.37 ACET + #.63 RCHO + #.63 -C + #.43 RO2.
1.22E+04	1.22E+04	0.00	-1.00	N-C4-OH + HO. = #.4 RO2-R. + #.6 HO2. + #.06 R2O2. + #.25 HCHO + #.12 CCHO + #.85 RCHO + #.09 MEK + #.6 -C + #.46 RO2.
1.66E+03	5.67E+02	-0.64	1.00	T-C4-OH + HO. = RO2-R. + HCHO + ACET + RO2.
1.40E+04	1.40E+04	0.00	-1.00	S-C4-OH + HO. = #.15 RO2-R. + #.85 HO2. + #.02 R2O2. + #.04 HCHO + #.22 CCHO + #.04 RCHO + #.85 MEK + #.17 RO2.
1.59E+04	1.59E+04	0.00	-1.00	C5OH + HO. = #.03 RO2-N. + #.47 RO2-R. + #.5 HO2. + #.27 R2O2. + #.04 CCHO + #.09 RCHO + #.46 MEK + #2.66 -C + #.77 RO2.
2.00E+04	2.00E+04	0.00	-1.00	1-C7OH + HO. = #.09 RO2-N. + #.56 RO2-R. + #.35 HO2. + #.47 R2O2. + #.04 RCHO + #.81 MEK + #3.19 -C + #1.12 RO2.
2.00E+04	2.00E+04	0.00	-1.00	1-C7OH + HO. = #.09 RO2-N. + #.56 RO2-R. + #.35 HO2. + #.47 R2O2. + #.04 RCHO + #.81 MEK + #3.19 -C + #1.12 RO2.
1.91E+04	1.91E+04	0.00	-1.00	2-ETC6OH + HO. = #.09 RO2-N. + #.61 RO2-R. + #.3 HO2. + #.61 R2O2. + #.05 CCHO + #.05 RCHO + MEK + #3.3 -C + #1.31 RO2.
4.42E+03	1.53E+04	0.74	-1.00	ME-O-ME + HO. = RO2-R. + #.18 MEK + #1.28 -C + RO2.
1.94E+04	1.16E+03	-1.68	1.00	ET-O-ET + HO. = RO2-R. + R2O2. + HCHO + MEK + #-1 -C + #2 RO2.
4.17E+03	9.00E+02	-0.91	1.00	MTBE + HO. = #.02 RO2-N. + #.98 RO2-R. + #.37 R2O2. + #.39 HCHO + #.41 MEK + #2.87 -C + #1.37 RO2.
1.10E+04	1.10E+04	0.00	-1.00	ETBE + HO. = #.03 RO2-N. + #.97 RO2-R. + #1.16 R2O2. + #1.16 HCHO + #.57 MEK + #2.41 -C + #2.16 RO2.
2.47E+04	2.47E+04	0.00	-1.00	S-098106 + HO. = #.02 RO2-N. + #.98 RO2-R. + #.98 R2O2. + #.98 HCHO + #.98 MEK + #1.98 RO2.
2.77E+04	2.77E+04	0.00	-1.00	S-098107 + HO. = #.17 RO2-N. + #.83 RO2-R. + #.9 R2O2. + #.06 CCHO + #.77 RCHO + #.77 MEK + #1.64 -C + #1.9 RO2.
3.88E+04	3.88E+04	0.00	-1.00	S-098108 + HO. = #.13 RO2-N. + #.87 RO2-R. + #1.67 R2O2. + #.06 CCHO + #.75 RCHO + #.77 MEK + #.23 CO + #.23 CO2 + #1.44 -C + #2.67 RO2.
1.13E+04	1.13E+04	0.00	-1.00	ET-GLYCL + HO. = HO2. + CCHO
1.76E+04	1.76E+04	0.00	-1.00	PR-GLYCL + HO. = HO2. + #.314 RCHO + #.686 MEK + #-0.686 -C
2.26E+04	2.26E+04	0.00	-1.00	12-C4OH2 + HO. = HO2. + #.25 RCHO + #.75 MEK + #.25 -C

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
2.67E+04	2.67E+04	0.00	-1.00	C6-GLYCL + HO. = #.2 RO2-R. + #.8 HO2. + #.1 CCHO + #.3 RCHO + #.7 MEK + #2.1 -C + #.2 RO2.
1.95E+04	6.61E+03	-0.65	-1.00	MEO-ETOH + HO. = #.65 RO2-R. + #.35 HO2. + #.65 HCHO + #.35 RCHO + #.12 MEK + #.82 -C + #.65 RO2.
3.46E+04	3.46E+04	0.00	-1.00	ETO-ETOH + HO. = #.76 RO2-R. + #.24 HO2. + #.33 R2O2. + #.76 HCHO + #.24 RCHO + #.63 MEK + #1.09 RO2.
2.95E+04	2.95E+04	0.00	-1.00	ETOC3OH + HO. = #.04 RO2-N. + #.56 RO2-R. + #.4 HO2. + #.3 R2O2. + #.3 HCHO + #.3 CCHO + MEK + #-0.1 -C + #.9 RO2.
2.06E+04	2.06E+04	0.00	-1.00	BUO-ETOH + HO. = #.04 RO2-N. + #.36 RO2-R. + #.6 HO2. + #.8 R2O2. + #.4 HCHO + #.4 CCHO + #.2 RCHO + #.8 MEK + #.8 -C + #1.2 RO2.
7.46E+04	7.46E+04	0.00	-1.00	CARBITOL + HO. = #.09 RO2-N. + #.79 RO2-R. + #.12 HO2. + #.58 R2O2. + #.37 HCHO + #.12 RCHO + #1.18 MEK + #.1 -C + #1.46 RO2.
8.01E+04	8.01E+04	0.00	-1.00	C8-CELSV + HO. = #.17 RO2-N. + #.71 RO2-R. + #.12 HO2. + #.58 R2O2. + #.37 HCHO + #.12 RCHO + #1.18 MEK + #1.7 -C + #1.46 RO2.
				Various N-Containing
(Phot. Set = CONO)				ME-NITRT + HV = C-O. + NO
1.20E-13	(No T Dependence)			ME-NITRT + HO. = HCHO + NO
1.92E-15	5.50E-14	1.99	0.00	C-O. + O2 = HCHO + HO2.
2.00E-11	(No T Dependence)			C-O. + NO = ME-NITRT
2.00E-11	(No T Dependence)			C-O. + NO2 = CONO2
				Esters and Oxides (Mechanisms for the these compounds are preliminary and undocumented)
2.50E+02	2.50E+02	0.00	-1.00	ME-ACET + HO. = RO2-R. + RCHO + RO2.
2.50E+03	2.50E+03	0.00	-1.00	ET-ACET + HO. = RO2-R. + MEK + #-2 -C + RO2.
6.17E+03	6.17E+03	0.00	-1.00	PR-ACET + HO. = #.076 RO2-N. + #.924 RO2-R. + #.397 R2O2. + #.001 HCHO + #.571 CCHO + #.14 RCHO + #.533 MEK + #.924 -C + #1.397 RO2.
8.66E+02	8.66E+02	0.00	-1.00	ME-IBUAT + HO. = RO2-R. + RCHO + #2 -C + RO2.
4.54E+03	4.54E+03	0.00	-1.00	IPR-ACET + HO. = #.027 RO2-N. + #.973 RO2-R. + #.744 R2O2. + #.744 HCHO + #.744 ACET + #.229 RCHO + #1.202 -C + #1.744 RO2.
6.31E+03	6.31E+03	0.00	-1.00	BU-ACET + HO. = #.12 RO2-N. + #.88 RO2-R. + #.544 R2O2. + #.007 HCHO + #.08 CCHO + #.172 RCHO + #.929 MEK + #1.001 -C + #1.544 RO2.
7.93E+03	7.93E+03	0.00	-1.00	IBU-ACET + HO. = #.122 RO2-N. + #.005 RO2-XN. + #.873 RO2-R. + #.749 R2O2. + #.006 HCHO + #.023 CCHO + #.223 ACET + #.545 RCHO + #.724 MEK + #.137 -C + #1.749 RO2.
2.88E+04	2.88E+04	0.00	-1.00	CSV-ACET + HO. = #.12 RO2-N. + #.88 RO2-R. + #.544 R2O2. + #.007 HCHO + #.08 CCHO + #.172 RCHO + #.929 MEK + #1.001 -C + #1.544 RO2.
9.83E+03	9.83E+03	0.00	-1.00	IBU-IBTR + HO. = #.196 RO2-N. + #.803 RO2-R. + #.858 R2O2. + #.03 HCHO + #.037 CCHO + #.036 ACET + #.118 RCHO + #1.265 MEK + #1.393 -C + #1.858 RO2.
9.91E+03	9.91E+03	0.00	-1.00	IC5IBUAT + HO. = #.188 RO2-N. + #.812 RO2-R. + #1.731 R2O2. + #.422 HCHO + #.518 ACET + #.165 RCHO + #1.008 MEK + #1.563 -C + #2.731 RO2.
9.91E+03	9.91E+03	0.00	-1.00	S-098116 + HO. = #.188 RO2-N. + #.812 RO2-R. + #1.731 R2O2. + #.422 HCHO + #.518 ACET + #.165 RCHO + #1.008 MEK + #4.563 -C + #2.731 RO2.
9.91E+03	9.91E+03	0.00	-1.00	S-098117 + HO. = #.188 RO2-N. + #.812 RO2-R. + #1.731 R2O2. + #.422 HCHO + #.518 ACET + #.165 RCHO + #1.008 MEK + #4.563 -C + #2.731 RO2.
1.03E+02	1.03E+02	0.00	-1.00	ETOX + HO. = RO2-R. + HCHO + -C + RO2.
7.63E+02	7.63E+02	0.00	-1.00	PROX + HO. = RO2-R. + RCHO + RO2.

Table A-4 (continued)

Kinetic Parameters [a]				Reactions [b]
k(300)	A	Ea	B	
9.91E+03	9.91E+03	0.00	-1.00	S-098116 + HO. = #.188 RO2-N. + #.812 RO2-R. + #1.731 R2O2. + #.422 HCHO + #.518 ACET + #.165 RCHO + #1.008 MEK + #4.563 -C + #2.731 RO2.
9.91E+03	9.91E+03	0.00	-1.00	S-098117 + HO. = #.188 RO2-N. + #.812 RO2-R. + #1.731 R2O2. + #.422 HCHO + #.518 ACET + #.165 RCHO + #1.008 MEK + #4.563 -C + #2.731 RO2.
Various N-Containing compounds (Mechanisms for the these compounds are preliminary and undocumented)				
4.05E+04	2.16E+04	-0.38	-1.00	ET-AMINE + HO. = RO2-R. + CCHO + RO2.
7.05E+03	7.05E+03	0.00	-1.00	ACRYLNIT + HO. = RO2-R. + HCHO + #2 -C + RO2.
8.90E+04	3.85E+04	-0.50	-1.00	TM-AMINE + HO. = RO2-R. + #2 HCHO + RO2.
3.08E+02	3.08E+02	0.00	-1.00	NO2-BENZ + HO. = #.236 PHEN + #.207 GLY + #.49 AFG1 + #.764 RO2-R. + #.236 HO2. + #3.19 -C + #.764 RO2.
Halogenated compounds (Mechanisms for the these compounds are preliminary and undocumented)				
6.57E+01	4.62E+02	1.16	1.00	S-043801 + HO. = RO2-R. + CCHO + #-1 -C + RO2.
2.13E+02	1.13E+03	0.99	1.00	S-043802 + HO. = RO2-R. + CCHO + #-1 -C + RO2.
6.02E+01	1.16E+03	1.77	-1.00	S-243819 + HO. = RO2-R. + CCHO + #-1 -C + RO2.
1.55E+02	8.32E+02	1.00	1.00	S-043803 + HO. = RO2-R. + CCHO + #-1 -C + RO2.
2.13E+02	1.13E+03	0.99	1.00	S-043805 + HO. = RO2-R. + CCHO + #-1 -C + RO2.
5.87E+02	5.87E+02	0.00	-1.00	S-043812 + HO. = RO2-R. + CCHO + RO2.
2.64E+03	2.64E+03	0.00	-1.00	S-099018 + HO. = RO2-R. + CCHO + RO2.
3.82E+02	3.82E+02	0.00	-1.00	S-043813 + HO. = RO2-R. + CCHO + RO2.
4.84E+02	2.42E+03	0.96	-1.00	S-043820 + HO. = RO2-R. + CCHO + RO2.
1.81E+01	7.82E+02	2.24	1.00	S-043814 + HO. = RO2-R. + CCHO + RO2.
1.45E+03	1.45E+03	0.00	-1.00	S-099016 + HO. = RO2-R. + CCHO + -C + RO2.
4.51E+03	4.51E+03	0.00	-1.00	S-098104 + HO. = #.076 RO2-N. + #.924 RO2-R. + #.397 R2O2. + #.001 HCHO + #.571 CCHO + #.14 RCHO + #.533 MEK + #-0.076 -C + #1.397 RO2.
1.26E+04	1.26E+04	0.00	-1.00	S-098105 + HO. = #.245 RO2-N. + #.755 RO2-R. + #.867 R2O2. + #.072 CCHO + #.066 RCHO + #1.425 MEK + #.733 -C + #1.867 RO2.
9.66E+03	1.67E+03	-1.04	-1.00	CL-ETHE + HO. = RO2-R. + CCHO + RO2.
1.19E+04	1.19E+04	0.00	-1.00	11CL2ETH + HO. = RO2-R. + CCHO + RO2.
3.38E+03	3.38E+03	0.00	-1.00	S-043815 + HO. = RO2-R. + CCHO + RO2.
3.43E+03	8.26E+02	-0.85	-1.00	CL3-ETHE + HO. = RO2-R. + CCHO + RO2.
2.51E+02	1.42E+04	2.40	-1.00	CL4-ETHE + HO. = RO2-R. + CCHO + RO2.
3.38E+03	3.38E+03	0.00	-1.00	S-099014 + HO. = RO2-R. + CCHO + RO2.
4.64E+04	4.64E+04	0.00	-1.00	CL2IBUTE + HO. = RO2-R. + RO2. + HCHO + ACET
5.72E-04	5.72E-04	0.00	-1.00	CL2IBUTE + O3 = #.1 RO2-R. + #.06 HO2. + #.1 RO2. + #.5 HCHO + #.5 ACET + #.4 MEK + #.22 CO + #.1 MGLY + #-0.12 -C + #.1 HO.
1.47E+00	1.47E+00	0.00	-1.00	CL2IBUTE + NO3 = R2O2. + RO2. + HCHO + ACET + NO2
2.24E+04	2.58E+04	0.09	-1.00	CL2IBUTE + O = #.4 HO2. + #.5 RCHO + #.5 MEK + #.5 -C
1.38E+03	1.38E+03	0.00	-1.00	CL-BEN + HO. = #.236 PHEN + #.207 GLY + #.49 AFG1 + #.764 RO2-R. + #.236 HO2. + #3.19 -C + #.764 RO2.
4.70E+02	4.70E+02	0.00	-1.00	CL2-BEN + HO. = #.236 PHEN + #.207 GLY + #.49 AFG1 + #.764 RO2-R. + #.236 HO2. + #3.19 -C + #.764 RO2.

[a] 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-5.

[b] Format of reaction listing same as used in documentation of the detailed mechanism (Carter 1990).unreactive "TRACE" species, is the kinetic reactivity of the explicit species which it represents.

Table A-4 gives the reactions of the detailed model species for which separate mechanistic parameter assignments are made, i.e., the reactions for all species listed on Table A-2 except for those which are represented explicitly (whose reactions are given on Table A-3), or for those which are represented by other species using the lumped molecule approach. The documentation for the mechanisms are given in the footnotes for the species on Table A-2. These species are represented as shown on Table A-4 if their reactivities are being calculated. If they are part of the base ROG mixture, their parameters are used to determine the parameters for the lumped species which represents them.

Table A-5 gives the absorption coefficients and quantum yields for the photolysis reactions in the SAPRC-90 mechanism. The photolysis rates depend on the actinic fluxes for the scenarios, which are given in Appendix B. The photolysis rates for the actinic fluxes used in these calculations are given for selected zenith angles in Table A-6. Photolysis rates at other zenith angles were computed using non-linear curve fits to these data.

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Table A-5. 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	0.030	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									

Table A-5. (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 = 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									
Photolysis File = HCHOAVGR														
281.0	1.62E-20	0.602	282.0	9.77E-21	0.614	283.0	5.96E-21	0.626	284.0	3.31E-20	0.638	285.0	4.09E-20	0.650
286.0	2.42E-20	0.662	287.0	1.22E-20	0.674	288.0	2.19E-20	0.686	289.0	3.14E-20	0.698	290.0	1.54E-20	0.710
291.0	1.49E-20	0.717	292.0	9.59E-21	0.724	293.0	3.22E-20	0.731	294.0	5.45E-20	0.738	295.0	4.07E-20	0.745
296.0	2.41E-20	0.752	297.0	1.79E-20	0.759	298.0	3.16E-20	0.766	299.0	2.81E-20	0.773	300.0	1.14E-20	0.780
301.0	1.27E-20	0.779	302.0	1.21E-20	0.778	303.0	2.78E-20	0.777	304.0	5.40E-20	0.776	305.0	5.30E-20	0.775
306.0	4.13E-20	0.774	307.0	2.23E-20	0.773	308.0	1.77E-20	0.772	309.0	2.43E-20	0.771	310.0	2.00E-20	0.770
311.0	9.15E-21	0.755	312.0	1.05E-20	0.740	313.0	1.43E-20	0.725	314.0	3.07E-20	0.710	315.0	4.50E-20	0.695
316.0	3.29E-20	0.680	317.0	3.77E-20	0.665	318.0	3.10E-20	0.650	319.0	1.22E-20	0.635	320.0	1.26E-20	0.620
321.0	1.48E-20	0.589	322.0	7.70E-21	0.558	323.0	4.66E-21	0.527	324.0	7.11E-21	0.496	325.0	1.51E-20	0.465
326.0	3.90E-20	0.434	327.0	3.50E-20	0.403	328.0	1.49E-20	0.372	329.0	2.30E-20	0.341	330.0	3.05E-20	0.310
331.0	1.43E-20	0.279	332.0	4.22E-21	0.248	333.0	2.01E-21	0.217	334.0	1.66E-21	0.186	335.0	9.68E-22	0.155
336.0	1.57E-21	0.124	337.0	3.27E-21	0.093	338.0	1.38E-20	0.062	339.0	3.18E-20	0.031	340.0	2.39E-20	0.000
Photolysis File = HCHOAVGM														
281.0	1.62E-20	0.341	282.0	9.77E-21	0.332	283.0	5.96E-21	0.323	284.0	3.31E-20	0.314	285.0	4.09E-20	0.305
286.0	2.42E-20	0.296	287.0	1.22E-20	0.287	288.0	2.19E-20	0.278	289.0	3.14E-20	0.269	290.0	1.54E-20	0.260
291.0	1.49E-20	0.256	292.0	9.59E-21	0.252	293.0	3.22E-20	0.248	294.0	5.45E-20	0.244	295.0	4.07E-20	0.240
296.0	2.41E-20	0.236	297.0	1.79E-20	0.232	298.0	3.16E-20	0.228	299.0	2.81E-20	0.224	300.0	1.14E-20	0.220
301.0	1.27E-20	0.221	302.0	1.21E-20	0.222	303.0	2.78E-20	0.223	304.0	5.40E-20	0.224	305.0	5.30E-20	0.225
306.0	4.13E-20	0.226	307.0	2.23E-20	0.227	308.0	1.77E-20	0.228	309.0	2.43E-20	0.229	310.0	2.00E-20	0.230
311.0	9.15E-21	0.245	312.0	1.05E-20	0.260	313.0	1.43E-20	0.275	314.0	3.07E-20	0.290	315.0	4.50E-20	0.305
316.0	3.29E-20	0.320	317.0	3.77E-20	0.335	318.0	3.10E-20	0.350	319.0	1.22E-20	0.365	320.0	1.26E-20	0.380
321.0	1.48E-20	0.411	322.0	7.70E-21	0.442	323.0	4.66E-21	0.473	324.0	7.11E-21	0.504	325.0	1.51E-20	0.535
326.0	3.90E-20	0.566	327.0	3.50E-20	0.597	328.0	1.49E-20	0.628	329.0	2.30E-20	0.659	330.0	3.05E-20	0.690
331.0	1.43E-20	0.690	332.0	4.22E-21	0.690	333.0	2.01E-21	0.690	334.0	1.66E-21	0.690	335.0	9.68E-22	0.690
336.0	1.57E-21	0.690	337.0	3.27E-21	0.690	338.0	1.38E-20	0.690	339.0	3.18E-20	0.690	340.0	2.39E-20	0.690
341.0	8.91E-21	0.661	342.0	6.91E-21	0.632	343.0	1.40E-20	0.603	344.0	1.13E-20	0.574	345.0	3.94E-21	0.545
346.0	9.93E-22	0.516	347.0	7.18E-22	0.487	348.0	6.70E-22	0.458	349.0	7.21E-22	0.429	350.0	1.87E-22	0.400
351.0	8.57E-22	0.372	352.0	5.46E-21	0.344	353.0	1.39E-20	0.316	354.0	1.39E-20	0.288	355.0	6.64E-21	0.260
356.0	1.97E-21	0.232	357.0	4.27E-22	0.204	358.0	3.22E-22	0.176	359.0	2.57E-22	0.148	360.0	3.73E-22	0.120
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 = ACETONE														
279.8	5.30E-20	0.560	283.7	5.30E-20	0.460	287.8	5.10E-20	0.360	292.0	4.40E-20	0.250	296.3	3.50E-20	0.210
300.5	3.00E-20	0.150	303.0	2.80E-20	0.120	304.0	2.50E-20	0.110	305.0	2.30E-20	0.100	306.0	2.10E-20	0.090
307.0	2.00E-20	0.080	308.0	1.80E-20	0.070	309.0	1.70E-20	0.060	310.0	1.50E-20	0.050	311.0	1.40E-20	0.048
312.0	1.30E-20	0.046	313.0	1.20E-20	0.043	314.0	1.10E-20	0.041	316.0	9.20E-21	0.037	320.0	5.30E-21	0.028
325.0	2.80E-21	0.031	330.0	1.90E-21	0.033	335.0	0.00E+00	0.036						
Photolysis File = KETONE														
210.0	1.10E-21	0.100	220.0	1.20E-21	0.100	230.0	4.60E-21	0.100	240.0	1.30E-20	0.100	250.0	2.68E-20	0.100
260.0	4.21E-20	0.100	270.0	5.54E-20	0.100	280.0	5.92E-20	0.100	290.0	5.16E-20	0.100	300.0	3.44E-20	0.100
310.0	1.53E-20	0.100	320.0	4.60E-21	0.100	330.0	1.10E-21	0.100	340.0	0.00E+00	0.100			
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 = 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

Table A-5. (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 = GLYOXAL2														
355.0	0.00E+00	0.029	360.0	2.29E-21	0.029	365.0	2.87E-21	0.029	370.0	8.03E-21	0.029	375.0	1.00E-20	0.029
380.0	1.72E-20	0.029	382.0	1.58E-20	0.029	384.0	1.49E-20	0.029	386.0	1.49E-20	0.029	388.0	2.87E-20	0.029
390.0	3.15E-20	0.029	391.0	3.24E-20	0.029	392.0	3.04E-20	0.029	393.0	2.23E-20	0.029	394.0	2.63E-20	0.029
395.0	3.04E-20	0.029	396.0	2.63E-20	0.029	397.0	2.43E-20	0.029	398.0	3.24E-20	0.029	399.0	3.04E-20	0.029
400.0	2.84E-20	0.029	401.0	3.24E-20	0.029	402.0	4.46E-20	0.029	403.0	5.27E-20	0.029	404.0	4.26E-20	0.029
405.0	3.04E-20	0.029	406.0	3.04E-20	0.029	407.0	2.84E-20	0.029	408.0	2.43E-20	0.029	409.0	2.84E-20	0.029
410.0	6.08E-20	0.029	411.0	5.07E-20	0.029	411.5	6.08E-20	0.029	412.0	4.86E-20	0.029	413.0	8.31E-20	0.029
413.5	6.48E-20	0.029	414.0	7.50E-20	0.029	414.5	8.11E-20	0.029	415.0	8.11E-20	0.029	415.5	6.89E-20	0.029
416.0	4.26E-20	0.029	417.0	4.86E-20	0.029	418.0	5.88E-20	0.029	419.0	6.69E-20	0.029	420.0	3.85E-20	0.029
421.0	5.67E-20	0.029	421.5	4.46E-20	0.029	422.0	5.27E-20	0.029	422.5	1.05E-19	0.029	423.0	8.51E-20	0.029
424.0	6.08E-20	0.029	425.0	7.29E-20	0.029	426.0	1.18E-19	0.029	426.5	1.30E-19	0.029	427.0	1.07E-19	0.029
428.0	1.66E-19	0.029	429.0	4.05E-20	0.029	430.0	5.07E-20	0.029	431.0	4.86E-20	0.029	432.0	4.05E-20	0.029
433.0	3.65E-20	0.029	434.0	4.05E-20	0.029	434.5	6.08E-20	0.029	435.0	5.07E-20	0.029	436.0	8.11E-20	0.029
436.5	1.13E-19	0.029	437.0	5.27E-20	0.029	438.0	1.01E-19	0.029	438.5	1.38E-19	0.029	439.0	7.70E-20	0.029
440.0	2.47E-19	0.029	441.0	8.11E-20	0.029	442.0	6.08E-20	0.029	443.0	7.50E-20	0.029	444.0	9.32E-20	0.029
445.0	1.13E-19	0.029	446.0	5.27E-20	0.029	447.0	2.43E-20	0.029	448.0	2.84E-20	0.029	449.0	3.85E-20	0.029
450.0	6.08E-20	0.029	451.0	1.09E-19	0.029	451.5	9.32E-20	0.029	452.0	1.22E-19	0.029	453.0	2.39E-19	0.029
454.0	1.70E-19	0.029	455.0	3.40E-19	0.029	455.5	4.05E-19	0.029	456.0	1.01E-19	0.029	457.0	1.62E-20	0.029
458.0	1.22E-20	0.029	458.5	1.42E-20	0.029	459.0	4.05E-21	0.029	460.0	4.05E-21	0.029	460.5	6.08E-21	0.029
461.0	2.03E-21	0.029	462.0	0.00E+00	0.029									
Photolysis File = MEGLYOX														
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	350.0	0.00E+00	0.107
354.0	4.21E-22	0.107	358.0	1.26E-21	0.107	360.0	2.10E-21	0.107	362.0	2.10E-21	0.107	364.0	2.94E-21	0.107
366.0	3.36E-21	0.107	368.0	4.21E-21	0.107	370.0	5.47E-21	0.107	372.0	5.89E-21	0.107	374.0	7.57E-21	0.107
376.0	7.99E-21	0.107	378.0	8.83E-21	0.107	380.0	1.01E-20	0.107	382.0	1.09E-20	0.107	384.0	1.35E-20	0.107
386.0	1.51E-20	0.107	388.0	1.72E-20	0.107	390.0	2.06E-20	0.107	392.0	2.10E-20	0.107	394.0	2.31E-20	0.107
396.0	2.48E-20	0.107	398.0	2.61E-20	0.107	400.0	2.78E-20	0.107	402.0	2.99E-20	0.107	404.0	3.20E-20	0.107
406.0	3.79E-20	0.107	408.0	3.95E-20	0.107	410.0	4.33E-20	0.107	412.0	4.71E-20	0.107	414.0	4.79E-20	0.107
416.0	4.88E-20	0.107	418.0	5.05E-20	0.107	420.0	5.21E-20	0.107	422.0	5.30E-20	0.107	424.0	5.17E-20	0.107
426.0	5.30E-20	0.107	428.0	5.21E-20	0.107	430.0	5.55E-20	0.107	432.0	5.13E-20	0.107	434.0	5.68E-20	0.107
436.0	6.22E-20	0.107	438.0	6.06E-20	0.107	440.0	5.47E-20	0.107	441.0	6.14E-20	0.107	442.0	5.47E-20	0.107
443.0	5.55E-20	0.107	443.5	6.81E-20	0.107	444.0	5.97E-20	0.107	445.0	5.13E-20	0.107	446.0	4.88E-20	0.107
447.0	5.72E-20	0.107	448.0	5.47E-20	0.107	449.0	6.56E-20	0.107	450.0	5.05E-20	0.107	451.0	3.03E-20	0.107
452.0	4.29E-20	0.107	453.0	2.78E-20	0.107	454.0	2.27E-20	0.107	456.0	1.77E-20	0.107	458.0	8.41E-21	0.107
460.0	4.21E-21	0.107	464.0	1.68E-21	0.107	468.0	0.00E+00	0.107						
Photolysis File = BZCHO														
299.0	1.78E-19	0.050	304.0	7.40E-20	0.050	306.0	6.91E-20	0.050	309.0	6.41E-20	0.050	313.0	6.91E-20	0.050
314.0	6.91E-20	0.050	318.0	6.41E-20	0.050	325.0	8.39E-20	0.050	332.0	7.65E-20	0.050	338.0	8.88E-20	0.050
342.0	8.88E-20	0.050	346.0	7.89E-20	0.050	349.0	7.89E-20	0.050	354.0	9.13E-20	0.050	355.0	8.14E-20	0.050
364.0	5.67E-20	0.050	368.0	6.66E-20	0.050	369.0	8.39E-20	0.050	370.0	8.39E-20	0.050	372.0	3.45E-20	0.050
374.0	3.21E-20	0.050	376.0	2.47E-20	0.050	377.0	2.47E-20	0.050	380.0	3.58E-20	0.050	382.0	9.90E-21	0.050
386.0	0.00E+00	0.050												
Photolysis File = AROMUNKN														
200.0	7.90E-20	1.000	350.0	7.90E-20	1.000	360.0	0.00E+00	1.000						
Photolysis File = CONO														
250.0	1.55E-18	1.000	260.0	1.00E-18	1.000	280.0	1.83E-19	1.000	285.0	1.49E-19	1.000	290.0	1.08E-19	1.000
295.0	8.60E-20	1.000	300.0	7.00E-20	1.000	305.0	6.50E-20	1.000	310.0	9.10E-20	1.000	315.0	8.10E-20	1.000
320.0	1.45E-19	1.000	325.0	9.70E-20	1.000	330.0	2.37E-19	1.000	335.0	1.19E-19	1.000	340.0	3.07E-19	1.000
345.0	1.45E-19	1.000	350.0	2.91E-19	1.000	355.0	1.78E-19	1.000	360.0	1.62E-19	1.000	365.0	1.67E-19	1.000
370.0	1.24E-19	1.000	375.0	9.70E-20	1.000	380.0	4.90E-20	1.000	385.0	4.30E-20	1.000	390.0	4.30E-20	1.000
395.0	2.70E-20	1.000	400.0	1.10E-20	1.000	405.0	1.40E-20	1.000	410.0	0.00E+00	1.000			

Table A-6. SAPRC-90 Photolysis rates used in reactivity calculations, given as a function of the solar zenith angle. Calculated for actinic fluxes for 640 meters and summer conditions as given in Table B-2.

Phot File	Photolysis rate constants in units of min^{-1}									
	0	10	20	30	40	50	60	70	78	86
NO2	6.779E-1	6.738E-1	6.587E-1	6.342E-1	5.918E-1	5.244E-1	4.023E-1	2.368E-1	8.709E-2	4.488E-3
NO3NO	1.436E+0	1.436E+0	1.430E+0	1.423E+0	1.403E+0	1.365E+0	1.239E+0	1.017E+0	6.768E-1	3.495E-1
NO3NO2	1.332E+1	1.332E+1	1.324E+1	1.315E+1	1.291E+1	1.248E+1	1.118E+1	8.929E+0	5.662E+0	2.477E+0
O3O3P	3.745E-2	3.737E-2	3.697E-2	3.641E-2	3.536E-2	3.370E-2	2.978E-2	2.379E-2	1.565E-2	8.352E-3
O3O1D	2.647E-3	2.559E-3	2.292E-3	1.884E-3	1.366E-3	8.196E-4	3.399E-4	7.154E-5	6.606E-6	4.392E-8
HONO	1.197E-1	1.188E-1	1.159E-1	1.111E-1	1.029E-1	8.995E-2	6.725E-2	3.746E-2	1.244E-2	4.511E-4
H2O2	5.267E-4	5.189E-4	4.938E-4	4.531E-4	3.921E-4	3.098E-4	1.989E-4	8.736E-5	2.169E-5	6.123E-7
HCHOAVGR	2.126E-3	2.091E-3	1.980E-3	1.799E-3	1.531E-3	1.175E-3	7.177E-4	2.870E-4	6.242E-5	1.561E-6
HCHOAVGM	3.070E-3	3.036E-3	2.923E-3	2.737E-3	2.441E-3	2.011E-3	1.367E-3	6.465E-4	1.721E-4	5.118E-6
CCHOR	4.160E-4	4.062E-4	3.758E-4	3.277E-4	2.615E-4	1.824E-4	9.651E-5	3.088E-5	5.129E-6	9.076E-8
RCHO	1.496E-3	1.465E-3	1.369E-3	1.216E-3	9.991E-4	7.294E-4	4.148E-4	1.502E-4	2.957E-5	6.698E-7
ACETONE	5.727E-5	5.578E-5	5.123E-5	4.415E-5	3.471E-5	2.388E-5	1.263E-5	4.232E-6	7.900E-7	1.738E-8
KETONE	1.106E-4	1.083E-4	1.012E-4	8.985E-5	7.385E-5	5.398E-5	3.080E-5	1.123E-5	2.231E-6	5.113E-8
CO2H	5.178E-4	5.104E-4	4.863E-4	4.472E-4	3.884E-4	3.085E-4	1.998E-4	8.900E-5	2.252E-5	6.406E-7
GLYOXAL1	3.238E-3	3.187E-3	3.023E-3	2.757E-3	2.360E-3	1.830E-3	1.135E-3	4.665E-4	1.055E-4	2.778E-6
GLYOXAL2	5.148E-3	5.134E-3	5.072E-3	4.978E-3	4.794E-3	4.476E-3	3.759E-3	2.630E-3	1.305E-3	2.056E-4
MEGLYOX	1.183E-2	1.178E-2	1.161E-2	1.133E-2	1.083E-2	1.000E-2	8.269E-3	5.651E-3	2.712E-3	3.789E-4
BZCHO	3.108E-3	3.082E-3	2.989E-3	2.838E-3	2.589E-3	2.213E-3	1.599E-3	8.445E-4	2.621E-4	8.678E-6
AROMUNKN	3.725E-2	3.687E-2	3.556E-2	3.342E-2	2.998E-2	2.496E-2	1.727E-2	8.450E-3	2.356E-3	7.098E-5
CONO	1.582E-1	1.570E-1	1.527E-1	1.457E-1	1.338E-1	1.156E-1	8.494E-2	4.609E-2	1.490E-2	5.567E-4

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APPENDIX B. SCENARIO CONDITIONS AND CALCULATION METHODS

This Appendix documents the scenario conditions and related input data used in the reactivity calculations. Discussion is also given on the methods used to compute kinetic reactivities, determine the amounts of test VOCs to add in the reactivity calculations, and to compute the incremental and mechanistic reactivities from the results.

Scenario Conditions

The conditions of the 39 base case EKMA scenarios were taken from the OZIPM4 input files received from Bauges (1991). OZIPM4 is the computer program used by the EPA and others to conduct EKMA model simulations, and a detailed description of its program and input data is given elsewhere (EPA, 1989). It is assumed in the subsequent discussion that the reader is familiar with the capabilities of the OZIPM4 model, the types of input data it requires, and how these are used. The 39 OZIPM4 input files as received by Bauges are given in Table B-1. (Because of its length, it is given at the end of this Appendix.)

The OZIPM4 computer program was not used in this work because it presently is not configured for use with mechanisms with variable parameters as employed by SAPRC90, and because the software developed at SAPRC for this purpose can conduct equivalent calculations on a more automated basis. Therefore, we used a computer program, called OZICONV, to convert the OZIPM4 input files to a format compatible with the SAPRC software. The conditions of the scenarios as implemented in the SAPRC software are given in Table B-1 for the inputs which varied from scenario to scenario, and are summarized below for the inputs which were common to all scenarios. These scenario-varying conditions were used to derive the conditions of the "averaged conditions" scenario, which are given in Table B-2.

As discussed in the OZIPM4 documentation (EPA, 1989), reactants can be either present initially, emitted throughout the day, or present (in constant concentrations) aloft and entrained into the reacting mixture as the inversion height increases. The EKMA documentation makes a distinction between "ground layer background" and controllable NMOCs and NO_x, and in these scenarios the ground level background pollutants are 1.79 ppm methane, varying amounts of CO, and 0.1 ppb each of isoprene (ISOP), α-pinene (APIN), and unknown terpenes (UNKN) which were represented in the model by a species whose parameters were averages of those of α- and β-pinene. The aloft layer contained 30 ppb of a mixture of

Table B-2. Detailed input data for the "averaged conditions" scenario.

Scenario ID	AVGEPA	Averaged Conditions Scenario	
Latitude (deg):	36.22		
Declination (deg):	16.50	Solar - clock time (min):	-75.81
Base ROG Input (mmolC/m2/day)	15.38	Initial Base ROG (% of input)	60.36
NOx Input (mmol/m2/day)	2.34	Initial NOx (% of input)	45.67

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.7802	0.0300	0.0731	0.0683	0.0601	0.0433	0.0313	0.0293	0.0267	0.0230	0.0232	0.0247
NOx	0.0898		0.0929	0.0872	0.0749	0.0585	0.0459	0.0419	0.0404	0.0365	0.0359	0.0361
Ozone		0.0704										
CH4	1.790	1.790										
CO	2.028	0.500	1.5408	1.4238	1.2324	0.8982	0.5115	0.4688	0.4376	0.3868	0.3999	0.4332
ISOP	0.0001		0.0023	0.0047	0.0080	0.0101	0.0120	0.0129	0.0131	0.0134	0.0122	0.0099
APIN	0.0001		0.0010	0.0012	0.0013	0.0014	0.0016	0.0017	0.0018	0.0019	0.0019	0.0018
UNKN	0.0001		0.0008	0.0011	0.0016	0.0019	0.0022	0.0024	0.0029	0.0032	0.0031	0.0028

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	293.	596.	899	1201.	1503.	1610.	1716.	1823.	1823.	1823.	1823.
T (deg K)	295.5	297.7	299.9	301.8	303.3	304.5	305.6	305.8	306.1	305.9	305.0
H2O (10^4 ppm)	1.994	2.040	2.059	2.036	2.029	1.991	1.888	1.854	1.899	1.997	2.033

ROG which is different from the base ROG mixture (these are discussed below), varying amounts of ozone and CO, and 1.79 ppm of methane.

For each scenario, a certain fraction of the base ROG inputs and a certain fraction of the NO_x inputs were present initially, and the rest were emitted throughout the day. The total amounts of ROG and NO_x input into the scenarios are quantified as millimoles meter^{-2} day^{-1}. Note that the total for the base ROG does not count the ROGs present aloft or the biogenic species. The conversion factor used is:

$$ppm = \frac{mmol\ m^{-2}}{Height\ (m)} \cdot 24.6268. \qquad (I)$$

Although this is strictly appropriate only for 300K, it was used regardless of temperature. The fractions present initially varied from scenario to scenario, and are given on Table B-1 or B-2 for each scenario. The concentrations of NMOC (base ROG) and NO_x corresponding to those fractions, which are computed from the above equation using the initial inversion height, for the base case scenarios are also given on the tables.

The emissions rates are given on the tables as mmol m^{-2} hr^{-2}, and are converted to ppm min^{-1} using Equation (I), the appropriate time conversion factor, and the instantaneous inversion height. To be consistent with the treatment of emissions by the OZIPM4 program, the emission rates are assumed to be constant during each hourly interval, changing as indicated on the table after each full hour of simulation. Thus the values given for "Hr-1" are the constant emissions for the time interval from the start of the simulation to the first hour, etc. Although the hourly emissions are constant in mmol m^{-2} hr^{-1} units, they are not constant in ppm min^{-1} units if the inversion height is changing. In general, the hourly emission differ from scenario to scenario.

Note that the NO_x inputs and the initial and emitted NO_x levels given in Tables B-1 and B-2 are for the base case scenarios only. For the adjusted NO_x scenarios, these were all modified by the same factor to achieve the desired reactivity characteristic. These adjustments involve changing the NO_x input, initial NO_x and hourly emitted NO_x values by the same factor. Thus the adjustments do not involve changing the fraction of the NO_x inputs which are initial or the fraction of the total which is emitted during each hour.

The test VOCs in the incremental reactivity calculations are input in exactly the same way as the base ROG, except that the total amount input varies depending on the compound's kinetic reactivity. The methods for determining how much test VOC to add is discussed in the next section. The fraction of the test VOC which is present initially is the same as the fraction of the initially present base ROG, and the hourly emission rates are the same percentage of the total as those for the base ROG.

The NMOC and NO_x inputs are represented by mixtures of model species which were the same for all scenarios. The NO_x composition consisted of 73.5% NO, 24.5% NO_2, and 2.0% HONO when present initially, and 94.9% NO, 5% NO_2 and 0.1% HONO when emitted. (This was implemented by having the fractions change linearly from the initial values to the emitted values during the first 0.1 minutes of the simulation. The SAPRC software does not conveniently allow fractions of pollutants in mixtures to be different initially than emitted, but it does allow compositions to change with time.) Separate mixtures were used to represent the NMOCs aloft and the base ROG mixture, but the composition of the base ROG mixture was the same regardless of whether it was present initially or aloft. Table B-3 gives the detailed composition of the base ROG mixture which was used to represent the initially present and emitted NMOCs, and Table B-4 gives them in terms of model species used in the EKMA calculations and those recommended for general airshed calculations (see Appendix A). Detailed and model species compositions used for the NMOCs aloft are given in Tables B-5 and B-6, respectively.

Table B-3. Detailed composition of the base ROG mixture.

DMSname	Description	ppb/Mix	ppbC/Mix	% C
	Alkanes	**114.36**	**539.51**	**51.5**
ETHANE	Ethane	17.65	35.31	3.4
PROPANE	Propane	14.80	44.41	4.2
N-C4	n-Butane	18.93	75.72	7.2
N-C5	n-Pentane	6.42	32.11	3.1
N-C6	n-Hexane	1.38	8.30	0.8
N-C7	n-Heptane	1.26	8.80	0.8
N-C8	n-Octane	0.78	6.20	0.6
N-C9	n-Nonane	0.78	7.00	0.7
N-C10	n-Decane	1.93	19.30	1.8
N-C11	n-Undecane	0.17	1.90	0.2
N-C12	n-Dodecane	0.34	4.10	0.4
N-C13	n-Tridecane	0.02	0.20	0.0
2-ME-C3	Isobutane	8.25	33.01	3.2
2-ME-C4	Iso-Pentane	15.88	79.42	7.6
2-ME-C5	2-Methyl Pentane	3.72	22.30	2.1
3-ME-C5	3-Methylpentane	2.65	15.90	1.5
22-DM-C4	2,2-Dimethyl Butane	0.48	2.90	0.3
23-DM-C4	2,3-Dimethyl Butane	1.00	6.00	0.6
24-DM-C5	2,4-Dimethyl Pentane	0.63	4.40	0.4
3-ME-C6	3-Methyl Hexane	1.33	9.30	0.9
23-DM-C5	2,3-Dimethyl Pentane	1.17	8.20	0.8
CYCC5	Cyclopentane	0.74	3.70	0.4
ME-CYCC5	Methylcyclopentane	1.68	10.10	1.0
CYCC6	Cyclohexane	0.72	4.30	0.4
ME-CYCC6	Methylcyclohexane	0.71	5.00	0.5
ET-CYCC6	Ethylcyclohexane	0.19	1.50	0.1
BR-C6	Branched C6 Alkanes	0.25	1.50	0.1
BR-C7	Branched C7 Alkanes	2.19	15.30	1.5
BR-C8	Branched C8 Alkanes	4.23	33.81	3.2
BR-C9	Branched C9 Alkanes	1.79	16.10	1.5
BR-C10	Branched C10 Alkanes	1.63	16.30	1.6
BR-C11	Branched C11 alkanes	0.17	1.90	0.2
BR-C12	Branched C12 Alkanes	0.34	4.10	0.4
BR-C13	Branched C13 Alkanes	0.02	0.20	0.0
CYC-C7	C7 Cycloalkanes	0.13	0.90	0.1
	Alkenes	**39.18**	**160.83**	**15.4**
ETHENE	Ethene	14.10	28.21	2.7
PROPENE	Propene	3.33	10.00	1.0
1-BUTENE	1-Butene	1.20	4.80	0.5
C4-OLE1	C4 Terminal Alkanes	0.15	0.60	0.1
3M-1-BUT	3-Methyl-1-Butene	0.34	1.70	0.2
1-PENTEN	1-Pentene	0.84	4.20	0.4
1-HEXENE	1-Hexene	0.35	2.10	0.2
ISOBUTEN	Isobutene	1.20	4.80	0.5
2M-1-BUT	2-Methyl-1-Butene	0.96	4.80	0.5
T-2-BUTE	trans-2-Butene	1.20	4.80	0.5
C-2-BUTE	cis-2-Butene	0.95	3.80	0.4
2M-2-BUT	2-Methyl-2-Butene	0.54	2.70	0.3
13-BUTDE	1,3-Butadiene	0.65	2.60	0.2
ISOPRENE	Isoprene	1.36	6.80	0.6
CYC-HEXE	Cyclohexene	0.18	1.10	0.1
A-PINENE	a-Pinene	0.53	5.30	0.5
3-CARENE	3-Carene	0.20	2.00	0.2
C5-OLE1	C5 Terminal Alkanes	0.46	2.30	0.2
C6-OLE1	C6 Terminal Alkanes	2.33	14.00	1.3
C7-OLE1	C7 Terminal Alkanes	1.24	8.70	0.8

Table B-1 (continued)

DMSname	Description	ppb/Mix	ppbC/Mix	% C
C8-OLE1	C8 Terminal Alkanes	0.25	2.00	0.2
C9-OLE1	C9 Terminal Alkanes	0.54	4.90	0.5
C10-OLE1	C10 Terminal Alkanes	0.10	1.00	0.1
C11-OLE1	C11 Terminal Alkanes	0.20	2.20	0.2
C4-OLE2	C4 Internal Alkenes	0.15	0.60	0.1
C5-OLE2	C5 Internal Alkenes	3.32	16.60	1.6
C6-OLE2	C6 Internal Alkenes	1.05	6.30	0.6
C7-OLE2	C7 Internal Alkenes	0.46	3.20	0.3
C8-OLE2	C8 Internal Alkenes	0.23	1.80	0.2
C9-OLE2	C9 Internal Alkenes	0.26	2.30	0.2
C10-OLE2	C10 Internal Alkenes	0.10	1.00	0.1
C11-OLE2	C11 Internal Alkenes	0.20	2.20	0.2
C7-OL2D	C7 Cyclic or di-olefins	0.20	1.40	0.1
	Aromatic Hydrocarbons	**34.43**	**279.26**	**26.7**
BENZENE	Benzene	3.45	20.70	2.0
TOLUENE	Toluene	9.67	67.71	6.5
C2-BENZ	Ethyl Benzene	1.34	10.70	1.0
N-C3-BEN	n-Propyl Benzene	0.38	3.40	0.3
I-C3-BEN	Isopropyl Benzene	0.20	1.80	0.2
C9-BEN1	C9 Monosub. Benzenes	0.17	1.50	0.1
S-C4-BEN	s-Butyl Benzene	0.24	2.40	0.2
C10-BEN1	C10 Monosub. Benzenes	0.19	1.90	0.2
C11-BEN1	C11 Monosub. Benzenes	0.68	7.50	0.7
C12-BEN1	C12 Monosub. Benzenes	0.03	0.30	0.0
O-XYLENE	o-Xylene	1.91	15.30	1.5
P-XYLENE	p-Xylene	2.29	18.30	1.7
M-XYLENE	m-Xylene	2.29	18.30	1.7
C9-BEN2	C9 Disub. Benzenes	2.59	23.30	2.2
C10-BEN2	C10 Disub. Benzenes	1.61	16.10	1.5
C11-BEN2	C11 Disub. Benzenes	0.10	1.10	0.1
C12-BEN2	C12 Disub. Benzenes	0.09	1.10	0.1
135-TMB	1,3,5-Trimethyl Benzene	0.76	6.80	0.6
123-TMB	1,2,3-Trimethyl Benzene	0.79	7.10	0.7
C9-BEN3	C9 Trisub. Benzenes	2.47	22.20	2.1
C10-BEN3	C10 Trisub. Benzenes	1.68	16.80	1.6
C11-BEN3	C11 Trisub. Benzenes	0.10	1.10	0.1
C12-BEN3	C12 Trisub. Benzenes	0.09	1.10	0.1
C10-BEN4	C10 Tetrasub. Benzenes	0.44	4.40	0.4
C9-STYR	C9 Styrenes	0.50	4.50	0.4
C10-STYR	C10 Styrenes	0.38	3.80	0.4
ACETYLEN	**Acetylene**	**10.20**	**20.40**	**1.9**
	Aldehydes	**16.42**	**33.20**	**3.2**
FORMALD	Formaldehyde	8.30	8.30	0.8
ACETALD	Acetaldehyde	5.00	10.00	1.0
PROPALD	C3 Aldehydes	0.73	2.20	0.2
C4-RCHO	C4 Aldehydes	0.33	1.30	0.1
C5-RCHO	C5 Aldehydes	1.12	5.60	0.5
C6-RCHO	C6 Aldehydes	0.77	4.60	0.4
BENZALD	Benzaldehyde	0.17	1.20	0.1
	Ketones	**4.38**	**14.30**	**1.4**
ACETONE	Acetone	3.23	9.70	0.9
MEK	C4 Ketones	1.15	4.60	0.4

Table B-4. Composition of the base ROG mixture in terms of lumped model species. "EKMA" is the composition used for the EKMA calculations in this work. "AIRSHED" is the composition recommended for grid model calculations

Model Species	Description	ppb/ppmC (EKMA)	ppb/ppmC (AIRSHED)
AAR1	Alkane/Aromatic #1	52.59	
AAR2	Alkane/Aromatic #2	55.54	
AAR3	Alkane/Aromatic #3	21.58	
ALK1	Alkane#1		69.77
ALK2	Alkane#2		22.19
ARO1	Aromatic #1		14.01
ARO2	Aromatic #2		17.20
ETHE	Ethene	14.10	14.10
OLE1	Higher Alkene #1	11.34	11.34
OLE2	Higher Alkene #2	14.61	14.61
HCHO	Formaldehyde	8.30	8.30
CCHO	Acetaldehyde	5.00	5.00
RCHO	Higher Aldehydes	2.95	2.95
BALD	Benzaldehyde	0.17	0.17
ACET	Acetone	3.23	3.23
MEK	Higher Ketones	1.15	1.15
INERT	Inert or ignored Carbon	87.42	79.80

The inversion height, temperature, water concentrations, and the light intensities can vary with time. The treatment of light intensity discussed below. The instantaneous values of the other parameters at the start of the simulation and at each hour afterwards are Tables B-1 and B-2. The values for intermediate times are determined by linear interpolation.

The photolysis rates are assumed to depend only on the solar zenith angle, i.e., clear sky conditions are assumed at all times for all scenarios. The zenith angle (z) is calculated from the latitude (Lat), the solar declination (Dec) (which depends on the time of the year), and the minutes before or after solar noon (t^{sol}) as follows:

$$z = \cos^{-1}[\sin(Lat)\cdot\sin(Dec)-\cos(Lat)\cdot\cos(Dec)\cdot\cos(360\cdot t^{sol}/1440)] \qquad (II)$$

The solar declination was computed from the date, and the difference between solar and clock times was computed from the longitude. These were calculated using the algorithms employed in the OZIPM4 program which was provided by Jeffries (personal communication, 1991). The actinic fluxes, which were calculated by Jeffries (personal communication, 1991) as a function of zenith

Table B-5. Detailed composition of the aloft ROG mixture.

DMSname	Description	ppb/Mix	ppbC/Mix	% C
	Alkanes	**239.32**	**727.94**	**72.8**
ETHANE	Ethane	115.31	230.62	23.1
PROPANE	Propane	50.97	152.92	15.3
N-C4	n-Butane	25.03	100.10	10.0
N-C5	n-Pentane	7.59	37.94	3.8
N-C6	n-Hexane	2.16	12.94	1.3
N-C8	n-Octane	0.38	3.00	0.3
2-ME-C3	Isobutane	13.43	53.71	5.4
2-ME-C4	Iso-Pentane	12.31	61.57	6.2
2-ME-C5	2-Methyl Pentane	2.60	15.59	1.6
3-ME-C5	3-Methylpentane	1.41	8.46	0.8
23-DM-C4	2,3-Dimethyl Butane	0.61	3.65	0.4
CYCC5	Cyclopentane	2.43	12.17	1.2
CYCC6	Cyclohexane	0.48	2.87	0.3
BR-C7	Branched C7 Alkanes	2.74	19.19	1.9
BR-C8	Branched C8 Alkanes	0.96	7.71	0.8
CYC-C6	C6 Cycloalkanes	0.91	5.48	0.5
	Alkenes	**21.88**	**57.37**	**5.7**
ETHENE	Ethene	15.55	31.10	3.1
PROPENE	Propene	2.70	8.09	0.8
ISOPRENE	Isoprene	3.63	18.17	1.8
	Aromatic Hydrocarbons	**14.19**	**99.65**	**10.0**
BENZENE	Benzene	4.34	26.04	2.6
TOLUENE	Toluene	5.20	36.37	3.6
C2-BENZ	Ethyl Benzene	0.94	7.52	0.8
O-XYLENE	o-Xylene	2.17	17.39	1.7
P-XYLENE	p-Xylene	0.77	6.17	0.6
M-XYLENE	m-Xylene	0.77	6.17	0.6
ACETYLEN	**Acetylene**	**9.34**	**18.67**	**1.9**
	Aldehydes	**85.62**	**96.37**	**9.6**
FORMALD	Formaldehyde	74.86	74.86	7.5
ACETALD	Acetaldehyde	10.75	21.51	2.2

Table B-6. Composition of the aloft ROG mixture in terms of lumped model species. "EKMA" is the composition used for the EKMA calculations in this work. "AIRSHED" is the composition recommended for grid model calculations

Model Species	Description	ppb/ppmC (EKMA)	ppb/ppmC (AIRSHED)
AAR1	Alkane/Aromatic #1	122.93	
AAR2	Alkane/Aromatic #2	38.67	
AAR3	Alkane/Aromatic #3	3.60	
ALK1	Alkane#1		122.33
ALK2	Alkane#2		5.47
ARO1	Aromatic #1		7.56
ARO2	Aromatic #2		3.71
ETHE	Ethene	15.55	15.55
OLE1	Higher Alkene #1	2.70	2.70
OLE2	Higher Alkene #2	3.63	3.63
HCHO	Formaldehyde	74.86	74.86
CCHO	Acetaldehyde	10.75	10.75
INERT	Inert or ignored Carbon	176.8	242.0

angle for "normal summer conditions", are given in Table B-7. These were used to calculate the photolysis rates for those zenith angles, which are given in Appendix A. The photolysis rates for these 10 zenith angles were then used as inputs to a non-linear optimization program to derive functions which could predict the photolysis rate for any zenith angle. In the model simulations, the zenith angle was computed using Equation (II) at each time step of the simulation, and these functions were then used to calculate the photolysis rates for that step.

Reactivity Calculation Methods

The principles behind the various measures of reactivity are given in the main body of the report, but certain implementation details may not be evident from the discussion there. In this section, more details are given on the algorithms for determining how much VOC to add when calculating its incremental reactivity, and how kinetic and incremental reactivities are computed from the results.

Table B-3. Actinic fluxes for 640 m and summer conditions.

WL Interval (microns)		Actinic fluxes at selected zenith angles (photons-cm^{-2}-min^{-1})									
		0	10	20	30	40	50	60	70	78	86
0.298	0.300	3.287E+13	3.077E+13	2.490E+13	1.688E+13	8.800E+12	2.994E+12	4.389E+11	1.057E+10	2.048E+07	6.632E+00
0.300	0.302	8.206E+13	7.777E+13	6.542E+13	4.766E+13	2.798E+13	1.157E+13	2.374E+12	1.094E+11	6.288E+08	3.430E+03
0.302	0.304	1.450E+14	1.388E+14	1.204E+14	9.286E+13	5.996E+13	2.897E+13	7.777E+12	6.034E+11	8.208E+09	3.839E+05
0.304	0.306	2.431E+14	2.344E+14	2.084E+14	1.681E+14	1.170E+14	6.392E+13	2.122E+13	2.488E+12	6.692E+10	1.595E+07
0.306	0.308	3.982E+14	3.863E+14	3.500E+14	2.925E+14	2.158E+14	1.298E+14	5.090E+13	8.247E+12	3.793E+11	3.108E+08
0.308	0.310	4.827E+14	4.706E+14	4.326E+14	3.716E+14	2.869E+14	1.860E+14	8.302E+13	1.731E+13	1.210E+12	2.532E+09
0.310	0.312	7.235E+14	7.078E+14	6.582E+14	5.776E+14	4.620E+14	3.174E+14	1.567E+14	3.970E+13	3.838E+12	1.638E+10
0.312	0.314	8.982E+14	8.812E+14	8.268E+14	7.377E+14	6.065E+14	4.359E+14	2.326E+14	6.856E+13	8.512E+12	6.236E+10
0.314	0.316	1.078E+15	1.060E+15	1.002E+15	9.053E+14	7.604E+14	5.660E+14	3.210E+14	1.063E+14	1.600E+13	1.762E+11
0.316	0.318	1.220E+15	1.201E+15	1.141E+15	1.042E+15	8.899E+14	6.809E+14	4.048E+14	1.468E+14	2.560E+13	3.830E+11
0.318	0.320	1.320E+15	1.302E+15	1.242E+15	1.143E+15	9.895E+14	7.737E+14	4.774E+14	1.858E+14	3.627E+13	6.817E+11
0.320	0.322	1.543E+15	1.523E+15	1.458E+15	1.351E+15	1.181E+15	9.394E+14	5.968E+14	2.455E+14	5.229E+13	1.162E+12
0.322	0.324	1.422E+15	1.405E+15	1.349E+15	1.255E+15	1.107E+15	8.926E+14	5.805E+14	2.495E+14	5.683E+13	1.427E+12
0.324	0.326	1.520E+15	1.503E+15	1.446E+15	1.352E+15	1.200E+15	9.784E+14	6.484E+14	2.886E+14	6.927E+13	1.896E+12
0.326	0.328	2.407E+15	2.381E+15	2.295E+15	2.152E+15	1.922E+15	1.581E+15	1.064E+15	4.873E+14	1.219E+14	3.543E+12
0.328	0.330	2.331E+15	2.308E+15	2.228E+15	2.095E+15	1.879E+15	1.558E+15	1.062E+15	4.980E+14	1.287E+14	3.894E+12
0.330	0.332	2.407E+15	2.383E+15	2.304E+15	2.172E+15	1.956E+15	1.632E+15	1.125E+15	5.378E+14	1.428E+14	4.429E+12
0.332	0.334	2.340E+15	2.318E+15	2.243E+15	2.119E+15	1.915E+15	1.607E+15	1.118E+15	5.437E+14	1.476E+14	4.642E+12
0.334	0.336	2.351E+15	2.330E+15	2.257E+15	2.136E+15	1.936E+15	1.632E+15	1.145E+15	5.652E+14	1.564E+14	4.947E+12
0.336	0.338	2.062E+15	2.044E+15	1.982E+15	1.879E+15	1.707E+15	1.446E+15	1.022E+15	5.111E+14	1.438E+14	4.551E+12
0.338	0.340	2.475E+15	2.454E+15	2.381E+15	2.261E+15	2.059E+15	1.751E+15	1.246E+15	6.307E+14	1.802E+14	5.683E+12
0.340	0.342	2.567E+15	2.546E+15	2.472E+15	2.350E+15	2.146E+15	1.831E+15	1.311E+15	6.710E+14	1.945E+14	6.099E+12
0.342	0.344	2.538E+15	2.518E+15	2.446E+15	2.328E+15	2.130E+15	1.824E+15	1.314E+15	6.794E+14	1.995E+14	6.221E+12
0.344	0.346	2.260E+15	2.243E+15	2.180E+15	2.078E+15	1.905E+15	1.636E+15	1.185E+15	6.189E+14	1.841E+14	5.708E+12
0.346	0.348	2.497E+15	2.478E+15	2.411E+15	2.300E+15	2.112E+15	1.820E+15	1.325E+15	6.986E+14	2.105E+14	6.493E+12
0.348	0.350	2.515E+15	2.496E+15	2.430E+15	2.321E+15	2.135E+15	1.845E+15	1.350E+15	7.184E+14	2.192E+14	6.742E+12
0.350	0.352	2.857E+15	2.836E+15	2.762E+15	2.641E+15	2.434E+15	2.109E+15	1.551E+15	8.326E+14	2.571E+14	7.906E+12
0.352	0.354	2.919E+15	2.899E+15	2.825E+15	2.703E+15	2.495E+15	2.169E+15	1.602E+15	8.677E+14	2.714E+14	8.362E+12
0.354	0.356	3.286E+15	3.263E+15	3.182E+15	3.048E+15	2.818E+15	2.456E+15	1.822E+15	9.954E+14	3.152E+14	9.765E+12
0.356	0.358	2.606E+15	2.588E+15	2.524E+15	2.420E+15	2.241E+15	1.958E+15	1.460E+15	8.041E+14	2.578E+14	8.055E+12
0.358	0.360	2.545E+15	2.529E+15	2.468E+15	2.368E+15	2.196E+15	1.924E+15	1.441E+15	8.000E+14	2.598E+14	8.216E+12
0.360	0.362	3.051E+15	3.032E+15	2.960E+15	2.843E+15	2.641E+15	2.319E+15	1.744E+15	9.764E+14	3.212E+14	1.032E+13
0.362	0.364	3.265E+15	3.244E+15	3.169E+15	3.047E+15	2.834E+15	2.494E+15	1.884E+15	1.063E+15	3.542E+14	1.160E+13
0.364	0.366	3.344E+15	3.324E+15	3.248E+15	3.125E+15	2.911E+15	2.568E+15	1.948E+15	1.108E+15	3.739E+14	1.252E+13
0.366	0.368	3.795E+15	3.772E+15	3.688E+15	3.551E+15	3.312E+15	2.929E+15	2.230E+15	1.279E+15	4.371E+14	1.503E+13
0.368	0.370	3.674E+15	3.652E+15	3.572E+15	3.443E+15	3.215E+15	2.850E+15	2.178E+15	1.259E+15	4.359E+14	1.543E+13
0.370	0.372	3.634E+15	3.613E+15	3.536E+15	3.410E+15	3.189E+15	2.833E+15	2.174E+15	1.266E+15	4.440E+14	1.623E+13
0.372	0.374	3.002E+15	2.985E+15	2.922E+15	2.821E+15	2.642E+15	2.351E+15	1.811E+15	1.063E+15	3.776E+14	1.430E+13
0.374	0.376	3.319E+15	3.301E+15	3.233E+15	3.123E+15	2.928E+15	2.612E+15	2.020E+15	1.193E+15	4.295E+14	1.688E+13
0.376	0.378	4.240E+15	4.217E+15	4.132E+15	3.994E+15	3.750E+15	3.352E+15	2.601E+15	1.549E+15	5.646E+14	2.308E+13
0.378	0.380	4.099E+15	4.078E+15	3.997E+15	3.866E+15	3.634E+15	3.255E+15	2.536E+15	1.520E+15	5.614E+14	2.393E+13
0.380	0.382	3.839E+15	3.820E+15	3.745E+15	3.626E+15	3.412E+15	3.062E+15	2.394E+15	1.446E+15	5.406E+14	2.406E+13
0.382	0.384	2.394E+15	2.382E+15	2.336E+15	2.263E+15	2.132E+15	1.918E+15	1.504E+15	9.148E+14	3.464E+14	1.612E+13
0.384	0.386	3.421E+15	3.404E+15	3.341E+15	3.238E+15	3.054E+15	2.752E+15	2.166E+15	1.326E+15	5.085E+14	2.477E+13
0.386	0.388	3.264E+15	3.249E+15	3.189E+15	3.094E+15	2.921E+15	2.637E+15	2.083E+15	1.284E+15	4.983E+14	2.543E+13
0.388	0.390	3.821E+15	3.803E+15	3.735E+15	3.625E+15	3.427E+15	3.099E+15	2.456E+15	1.524E+15	5.988E+14	3.205E+13
0.390	0.392	4.403E+15	4.383E+15	4.306E+15	4.182E+15	3.958E+15	3.586E+15	2.851E+15	1.781E+15	7.081E+14	3.976E+13
0.392	0.394	2.584E+15	2.573E+15	2.528E+15	2.457E+15	2.327E+15	2.113E+15	1.685E+15	1.059E+15	4.262E+14	2.511E+13
0.394	0.396	4.423E+15	4.404E+15	4.329E+15	4.210E+15	3.992E+15	3.630E+15	2.904E+15	1.837E+15	7.481E+14	4.626E+13
0.396	0.398	3.031E+15	3.018E+15	2.968E+15	2.888E+15	2.742E+15	2.497E+15	2.004E+15	1.276E+15	5.255E+14	3.410E+13
0.398	0.400	5.702E+15	5.678E+15	5.585E+15	5.438E+15	5.167E+15	4.714E+15	3.795E+15	2.430E+15	1.013E+15	6.895E+13
0.400	0.402	6.444E+15	6.418E+15	6.315E+15	6.152E+15	5.852E+15	5.347E+15	4.317E+15	2.782E+15	1.172E+15	8.374E+13
0.402	0.404	6.061E+15	6.037E+15	5.942E+15	5.792E+15	5.514E+15	5.047E+15	4.086E+15	2.648E+15	1.128E+15	8.455E+13
0.404	0.406	5.943E+15	5.920E+15	5.829E+15	5.685E+15	5.417E+15	4.966E+15	4.032E+15	2.628E+15	1.132E+15	8.895E+13
0.406	0.408	5.951E+15	5.929E+15	5.839E+15	5.698E+15	5.434E+15	4.989E+15	4.063E+15	2.663E+15	1.160E+15	9.546E+13
0.408	0.410	6.253E+15	6.231E+15	6.138E+15	5.992E+15	5.720E+15	5.260E+15	4.295E+15	2.831E+15	1.246E+15	1.074E+14
0.410	0.412	6.410E+15	6.388E+15	6.294E+15	6.148E+15	5.874E+15	5.410E+15	4.429E+15	2.936E+15	1.305E+15	1.178E+14
0.412	0.414	6.588E+15	6.565E+15	6.470E+15	6.324E+15	6.047E+15	5.577E+15	4.578E+15	3.051E+15	1.371E+15	1.294E+14
0.414	0.416	6.502E+15	6.480E+15	6.389E+15	6.247E+15	5.979E+15	5.522E+15	4.544E+15	3.044E+15	1.382E+15	1.363E+14
0.416	0.418	6.757E+15	6.734E+15	6.641E+15	6.497E+15	6.223E+15	5.756E+15	4.748E+15	3.198E+15	1.466E+15	1.511E+14
0.418	0.420	6.345E+15	6.324E+15	6.239E+15	6.106E+15	5.853E+15	5.421E+15	4.483E+15	3.035E+15	1.404E+15	1.511E+14
0.420	0.430	3.267E+16	3.257E+16	3.215E+16	3.151E+16	3.027E+16	2.814E+16	2.344E+16	1.609E+16	7.658E+15	9.328E+14
0.430	0.440	3.395E+16	3.386E+16	3.346E+16	3.287E+16	3.169E+16	2.965E+16	2.497E+16	1.755E+16	8.736E+15	1.296E+15
0.440	0.450	3.997E+16	3.988E+16	3.945E+16	3.882E+16	3.754E+16	3.530E+16	3.002E+16	2.152E+16	1.112E+16	1.949E+15
0.450	0.460	4.356E+16	4.347E+16	4.305E+16	4.243E+16	4.115E+16	3.888E+16	3.334E+16	2.433E+16	1.301E+16	2.651E+15
0.460	0.470	4.423E+16	4.416E+16	4.376E+16	4.319E+16	4.199E+16	3.984E+16	3.443E+16	2.553E+16	1.408E+16	3.281E+15
0.470	0.480	4.514E+16	4.507E+16	4.470E+16	4.417E+16	4.304E+16	4.099E+16	3.567E+16	2.682E+16	1.520E+16	3.995E+15
0.480	0.490	4.443E+16	4.437E+16	4.402E+16	4.356E+16	4.252E+16	4.062E+16	3.556E+16	2.706E+16	1.570E+16	4.569E+15
0.490	0.500	4.545E+16	4.540E+16	4.507E+16	4.463E+16	4.363E+16	4.179E+16	3.677E+16	2.828E+16	1.673E+16	5.323E+15
0.500	0.510	4.571E+16	4.567E+16	4.535E+16	4.495E+16	4.400E+16	4.225E+16	3.734E+16	2.898E+16	1.745E+16	5.990E+15
0.510	0.520	4.449E+16	4.445E+16	4.416E+16	4.380E+16	4.293E+16	4.131E+16	3.667E+16	2.872E+16	1.757E+16	6.451E+15
0.520	0.530	4.669E+16	4.665E+16	4.637E+16	4.601E+16	4.514E+16	4.351E+16	3.875E+16	3.056E+16	1.892E+16	7.339E+15
0.530	0.540	4.823E+16	4.819E+16	4.791E+16	4.756E+16	4.670E+16	4.508E+16	4.026E+16	3.195E+16	2.000E+16	8.131E+15
0.540	0.550	4.813E+16	4.810E+16	4.783E+16	4.751E+16	4.669E+16	4.514E+16	4.043E+16	3.228E+16	2.043E+16	8.694E+15
0.550	0.560	4.835E+16	4.832E+16	4.806E+16	4.774E+16	4.694E+16	4.542E+16	4.075E+16	3.265E+16	2.079E+16	9.109E+15
0.560	0.580	9.710E+16	9.705E+16	9.654E+16	9.595E+16	9.439E+16	9.145E+16	8.227E+16	6.631E+16	4.262E+16	1.949E+16
0.580	0.600	9.616E+16	9.612E+16	9.563E+16	9.508E+16	9.361E+16	9.083E+16	8.201E+16	6.665E+16	4.350E+16	2.102E+16
0.600	0.620	9.662E+16	9.661E+16	9.619E+16	9.576E+16	9.448E+16	9.204E+16	8.370E+16	6.903E+16	4.623E+16	2.439E+16
0.620	0.640	9.748E+16	9.749E+16	9.718E+16	9.696E+16	9.600E+16	9.407E+16	8.648E+16	7.292E+16	5.079E+16	3.021E+16
0.640	0.660	9.553E+16	9.557E+16	9.535E+16	9.526E+16	9.455E+16	9.305E+16	8.622E+16	7.391E+16	5.305E+16	3.453E+16
0.660	0.680	9.588E+16	9.594E+16	9.578E+16	9.581E+16	9.530E+16	9.414E+16	8.785E+16	7.642E+16	5.631E+16	3.962E+16
0.680	0.700	9.082E+16	9.087E+16	9.069E+16	9.067E+16	9.011E+16	8.894E+16	8.296E+16	7.225E+16	5.346E+16	3.798E+16
0.700	0.720	7.802E+16	7.805E+16	7.784E+16	7.773E+16	7.712E+16	7.594E+16	7.064E+16	6.133E+16	4.526E+16	3.185E+16
0.720	0.740	9.688E+16	9.694E+16	9.674E+16	9.672E+16	9.614E+16	9.497E+16	8.888E+16	7.814E+16	5.891E+16	4.408E+16
0.740	0.760	8.389E+16	8.399E+16	8.399E+16	8.428E+16	8.427E+16	8.402E+16	7.984E+16	7.216E+16	5.686E+16	4.824E+16
0.760	0.800	1.727E+17	1.728E+17	1.727E+17	1.729E+17	1.724E+17	1.712E+17	1.618E+17	1.453E+17	1.136E+17	9.424E+16
0.800	0.840	1.454E+17	1.454E+17	1.450E+17	1.448E+17	1.436E+17	1.415E+17	1.322E+17	1.162E+17	8.771E+16	6.342E+16
0.840	0.880	1.611E+17	1.613E+17	1.615E+17	1.623E+17	1.627E+17	1.632E+17	1.568E+17	1.454E+17	1.195E+17	1.114E+17
0.880	0.920	9.398E+16	9.384E+16	9.306E+16	9.196E+16	8.976E+16	8.633E+16	7.768E+16	6.400E+16	4.326E+16	2.097E+16
0.920	0.960	5.485E+16	5.462E+16	5.372E+16	5.230E+16	4.988E+16	4.637E+16	3.966E+16	3.020E+16	1.844E+16	7.716E+15
0.960	1.000	1.359E+17	1.360E+17	1.356E+17	1.354E+17	1.344E+17	1.327E+17	1.247E+17	1.115E+17	8.649E+16	6.546E+16
1.000	1.040	1.584E+17	1.587E+17	1.590E+17	1.600E+17	1.607E+17	1.618E+17	1.570E+17	1.487E+17	1.266E+17	1.242E+17

Before reactivities can be calculated for any VOC in a scenario, the base case calculation must be carried out. The base case calculation not only determines the levels of ozone and other pollutant in the absence of the added test VOCs, it also does all the computations necessary to determine (or at least estimate) the kinetic reactivities of all the test VOCs. This is done by including in the base case simulations a number of dummy test species, of which 1 mmol m^{-2} day^{-1} are emitted with the same schedule (fraction present initially and hourly fractions of total input) as the test VOCs in the reactivity calculations. There are three types of such dummy species: an inert "TRACE" species which does not react, "Tnn" species with react with OH radicals at varous rate constants but which form no products other than regenerating the OH radicals, and "T_name" species which react or photolyze with exactly the same rate constants as some explicit species in the mechanism, but which form no products other than the species which with they react. The ratio of the final concentration of the reactive species to the TRACE species is used as the kinetic reactivity of the reactive species. The final concentration of the TRACE species is also used as a factor to convert from mmol m^{-2} day^{-1} to final ppm, as discussed below.

The kinetic reactivities of these trace species provide all the information needed to compute or at least estimate the kinetic reactivities of most of the test compounds prior to conducting the calculation with the added compound. If the test compound is an explicitly represented species which reacts with the same rate constants as one of the dummy species, the kinetic reactivity is that of the dummy species. If the test compound is an alkane, aromatic, or alkene other than ethene, it is which is represented in the model using a species with adjustable parameters. In this case, the program knows the compound's OH radial rate constant (kOH) prior to the computation, and can use this to determine the kinetic reactivity from the dependence of kinetic reactivities on kOH. The latter is obtained from functions which are derived by fits of the kinetic reactivities of the "Tnn" dummy species to their OH rate constants. (The use of only kOH to determine the kinetic reactivity is an approximation for the alkenes, but is inconsequential because they tend to have kinetic reactivities close to unity in any case.) If the test compound is explicitly represented in the mechanism but does not have a corresponding "T_" dummy species, a file is read which gives the kOH or method to compute the kinetic reactivities for the compounds for any compound. (In these calculations, the only species where this was done are those which the data in the file indicated should be given kinetic reactivities of unity.)

The test VOC could also be a mixture. In this case, the kinetic reactivity of the mixture is determined by summing up the amounts of each component of the mixture which is estimated to react from its kinetic reactivity and mole fraction, to determine a molar kinetic reactivity for the mixture.

The kinetic reactivities of the test VOCs have to be calculated prior to the reactivity simulation because they are used in part to estimate the appropriate amount of VOC to add to the scenario to calculate its incremental reactivity. The amount added is given by

$$\text{VOC added (mmol m}^{-2}\text{ day}^{-1}) = \frac{\text{MOLRCT}}{\text{KR}\cdot(\text{final TRACE})\cdot\text{nC}} \qquad \text{(III)}$$

where KR is the kinetic reactivity, nC is the number of carbons in the VOC, "final TRACE" serves as the conversion factor from mmol m^{-2} day^{-1} to ppm at the end of the simulation, and "MOLRCT" is the approximate amount of VOC which is desired to have reacted by the end of the scenario, in units of ppmC reacted at the end of the simulation. The value of the MOLRCT parameter is set to provide an appropriate balance between having the effect of the added VOC be sufficiently large to have an effect on the result which is much greater than numerical errors, but which is small enough that the result approximates the true incremental reactivity ($\partial O_3/\partial VOC$). After experimentation with varying values, we found that if 10^{-5} is used as the stepwise relative error tolerance constant, then a MOLRCT of 5×10^{-4} gives the desired results. This was used in the calculations reported here. This yields a change in ozone of ~0.3-1.5% for most VOCs when added to maximum reactivity scenarios, and correspondingly smaller changes when added to lower NO_x scenarios.

When the model simulations are being conducted, the program checks the ozone concentration at each time step in the simulation, and saves the instantaneous maximum ($MaxO_3$). The hourly values of ozone ($[O_3]_{hour\ i}$) and the final integrated ozone ($IntO_3$) are also saved. The incremental reactivities (IR) are then computed as:

$$\text{Ozone yield IR} = \frac{MaxO_3^{test} - MaxO_3^{base}}{(\text{VOC added})\cdot(\text{final TRACE})\cdot\text{nC}}$$

$$IntO_3\ \text{IR} = \frac{(\text{Final IntO3})^{test} - (\text{final IntO3})^{base}}{(\text{VOC added})\cdot\text{nC}}$$

$$IntO_3{>}90\ \text{IR} = \frac{\sum([O_3]_{hour\ i}^{test} - [O_3]_{hour\ i}^{base})\cdot([O_3]_{hour\ i}^{base} \geq 0.09)}{(\text{VOC added})\cdot\text{nC}}$$

where (VOC added) is in units of mmol m^{-2} day^{-1}, nC is the number of carbons in the VOC, $MaxO_3$ and the hourly $[O_3]$'s are in units of ppm, $IntO_3$ is in units of ppm-min, the superscripts "base" and "test" refer to the results of the base case and the added test VOC calculation, respectively, and ($[O_3]_{hour\ i}^{base} \geq 0.09$) has a value of 1 if true and 0 if false. The use of (final TRACE) in the denominator for the ozone yield IR serves to convert the units of (VOC added) to final ppmC units, so both the numerator and denominator have essentially molar units, giving a result which is essentially unitless. No conversion is done for $IntO_3$ and

IntO_3>90 reactivities because the results are only given in terms of relative reactivities, so the units are essentially arbitrary.

Table B-8 give examples of the selected raw calculation results of ozone yield reactivities for all the added VOC calculations conducted for the averaged conditions maximum reactivity and maximum ozone scenarios. This shows the pre-computed kinetic reactivities, amounts of each test VOC added, the percent change in ozone caused by adding the VOC, and the molar ozone yield mechanistic reactivity (Ozone yield IR·nC/KR). In addition to detailed model species, reactivities are calculated for pure mechanism species "R.xx.nn" or "P.xx.nn" which are used to compute reactivities for species which are not calculated explicitly as discussed by Carter and Atkinson (1989) and in Appendix B of Carter (1991), and for the example LEV and TLEV exhaust mixtures. In addition, to show the magnitude of numerical errors, reactivities were calculated for a "NULL-3", a dummy species whose reactions have no effects on any other model species. Their reactivities indicate the minimum magnitude of numerical errors in the calculations.

Note that the way the amount of test VOC is computed is such that the numerical uncertainty is translated into a constant uncertainty in the molar ozone yield mechanistic reactivity. The "NULL-3" mechanistic reactivities in these scenarios have magnitudes of less than 0.003. Based on these and similar results, we conclude that the numerical uncertainty corresponds to uncertainty in mechanistic reactivities of less than 0.005.

If a detailed model species is not listed on Table B-8, it means that either it is represented using the "lumped molecule" approach (which can be determined from the tabulation of detailed model species in Appendix A), or that its reactivities were derived from their kinetic reactivities and the mechanistic reactivities of the "pure mechanism" species, as discussed elsewhere (Carter and Atkinson, 1989; Carter, 1991). This approach, which was only applied to non-aromatic species which react only with OH, involves no chemical approximations and is mathematically valid in the incremental reactivity limit. To demonstrate this, Table B-9 compares the mechanistic reactivities computed this way with the directly calculated values for all the applicable VOCs whose reactivities were directly calculated in the MIR and MOR averaged conditions scenarios. (This approach could be used for aromatics but was not because of the relatively large number of aromatic product parameters compared to the number of aromatic detailed model species.) This derivation approach appears to have a positive bias of ~5-7%.

Table B-8. Kinetic reactivities, amounts added, percent ozone changes, and molecular mechanistic reactivities for the MIR and MOR "averaged conditions" scenario calculations.

Test Species	MIR Scenario K.Rct.	Added	dO3 (%)	M.Rct	MOR Scenario K.Rct.	Added	dO3 (%)	M.Rct
Pure mechanism species [a]								
R.XR.30.	0.9160	4.0E-2	-2.17	-7.2431	0.9531	3.9E-2	-0.49	-2.0367
R.RH.3.0	0.2612	1.4E-1	0.29	0.9632	0.3865	9.6E-2	0.10	0.4162
R.RH.30.	0.9160	4.0E-2	0.32	1.0797	0.9531	3.9E-2	0.12	0.5108
R.NR.3.0	0.2612	1.4E-1	-0.84	-2.8312	0.3865	9.6E-2	-0.38	-1.5910
R.NR.30.	0.9160	4.0E-2	-1.13	-3.7673	0.9531	3.9E-2	-0.37	-1.5418
R.XN.3.0	0.2612	1.4E-1	-0.78	-2.6154	0.3865	9.6E-2	-0.55	-2.2737
R.XN.30.	0.9160	4.0E-2	-1.04	-3.4875	0.9531	3.9E-2	-0.62	-2.5661
R.RR.3.0	0.2612	1.4E-1	0.59	1.9794	0.3865	9.6E-2	0.24	0.9932
R.RR.30.	0.9160	4.0E-2	0.65	2.1882	0.9531	3.9E-2	0.26	1.0864
P.R2.3.0	0.2612	1.4E-1	0.31	1.0285	0.3865	9.6E-2	0.15	0.6015
P.R2.30.	0.9160	4.0E-2	0.33	1.1160	0.9531	3.9E-2	0.14	0.5811
P.A1.3.0	0.2612	1.4E-1	0.61	2.0385	0.3865	9.6E-2	0.13	0.5181
P.A1.30.	0.9160	4.0E-2	0.88	2.9541	0.9531	3.9E-2	0.21	0.8548
P.A2.3.0	0.2612	1.4E-1	0.64	2.1365	0.3865	9.6E-2	0.18	0.7314
P.A2.30.	0.9160	4.0E-2	1.01	3.3703	0.9531	3.9E-2	0.36	1.4657
P.K3.3.0	0.2612	1.4E-1	0.08	0.2516	0.3865	9.6E-2	0.02	0.0838
P.K3.30.	0.9160	4.0E-2	0.12	0.4037	0.9531	3.9E-2	0.04	0.1575
P.A3.3.0	0.2612	1.4E-1	0.93	3.1006	0.3865	9.6E-2	0.22	0.8920
P.A3.30.	0.9160	4.0E-2	1.49	4.9827	0.9531	3.9E-2	0.48	1.9953
P.K4.3.0	0.2612	1.4E-1	0.20	0.6614	0.3865	9.6E-2	0.07	0.3007
P.K4.30.	0.9160	4.0E-2	0.32	1.0700	0.9531	3.9E-2	0.13	0.5558
Detailed model species								
CO	0.0353	1.0E+0	0.27	0.9351	0.0568	6.5E-1	0.09	0.3941
METHANE	0.0013	2.8E+1	1.16	3.8862	0.0021	1.7E+1	0.34	1.4491
ETHANE	0.0401	4.6E-1	0.60	3.9601	0.0645	2.9E-1	0.20	1.6147
PROPANE	0.1594	7.7E-2	0.29	2.8628	0.2454	5.0E-2	0.09	1.1627
N-C4	0.3149	2.9E-2	0.30	4.0758	0.4554	2.0E-2	0.11	1.7700
N-C8	0.7071	6.5E-3	0.08	2.1858	0.8436	5.5E-3	0.03	1.1280
224TM-C5	0.4197	1.1E-2	0.19	5.1708	0.5796	8.0E-3	0.06	2.0803
N-C15	0.8959	2.8E-3	0.03	1.5759	0.9469	2.6E-3	0.02	0.9382
ETHENE	0.6948	2.7E-2	0.98	6.4035	0.8349	2.2E-2	0.27	2.2431
PROPENE	0.9478	1.3E-2	0.90	8.9690	0.9731	1.3E-2	0.28	3.4327
ISOBUTEN	0.9825	9.4E-3	0.49	6.5367	0.9904	9.3E-3	0.14	2.2760
1-BUTENE	0.9636	9.6E-3	0.84	11.1537	0.9820	9.4E-3	0.25	4.2134
T-2-BUTE	0.9809	9.4E-3	0.93	12.3269	0.9863	9.4E-3	0.27	4.5265
13-BUTDE	0.9794	9.4E-3	0.97	12.9546	0.9837	9.4E-3	0.29	4.8007
1-PENTEN	0.9635	7.7E-3	0.59	9.7521	0.9820	7.5E-3	0.18	3.6888
2M-1-BUT	0.9820	7.5E-3	0.45	7.5400	0.9881	7.5E-3	0.14	2.8079
2M-2-BUT	0.9880	7.5E-3	0.60	9.9124	0.9901	7.5E-3	0.17	3.4622
C5-OLE2	0.9796	7.6E-3	0.83	13.6432	0.9840	7.5E-3	0.24	4.9779
CYC-PNTE	0.9790	7.6E-3	0.71	11.6191	0.9832	7.5E-3	0.20	4.1108
ISOPRENE	0.9918	7.5E-3	0.82	13.4651	0.9932	7.5E-3	0.24	4.9417
1-HEXENE	0.9734	6.3E-3	0.41	8.2438	0.9870	6.2E-3	0.12	3.1088
C6-OLE2	0.9796	6.3E-3	0.63	12.4952	0.9840	6.3E-3	0.18	4.5434
CYC-HEXE	0.9787	6.3E-3	0.52	10.3338	0.9826	6.3E-3	0.16	3.8853
C7-OLE1	0.9734	5.4E-3	0.33	7.5798	0.9870	5.4E-3	0.10	2.8695
C7-OLE2	0.9796	5.4E-3	0.52	12.0645	0.9840	5.4E-3	0.15	4.3854
C8-OLE1	0.9734	4.8E-3	0.26	6.7242	0.9870	4.7E-3	0.08	2.5595
C8-OLE2	0.9796	4.7E-3	0.50	13.1893	0.9840	4.7E-3	0.15	4.8432
C9-OLE1	0.9734	4.2E-3	0.21	6.2653	0.9870	4.2E-3	0.06	2.3804
C9-OLE2	0.9796	4.2E-3	0.43	12.9026	0.9840	4.2E-3	0.13	4.7053
C10-OLE1	0.9734	3.8E-3	0.18	5.9842	0.9870	3.7E-3	0.05	2.2560
C10-OLE2	0.9796	3.8E-3	0.38	12.6697	0.9840	3.8E-3	0.11	4.6283
C11-OLE1	0.9734	3.5E-3	0.16	5.7712	0.9870	3.4E-3	0.05	2.1816
C11-OLE2	0.9796	3.4E-3	0.34	12.5000	0.9840	3.4E-3	0.10	4.5755
C12-OLE1	0.9734	3.2E-3	0.14	5.6705	0.9870	3.1E-3	0.04	2.1483

Table B-8 (continued)

Test Species	MIR Scenario Added	K.Rct.	dO3 (%)	M.Rct	MOR Scenario Added	K.Rct.	dO3 (%)	M.Rct
C12-OLE2	0.9796	3.1E-3	0.31	12.4739	0.9840	3.1E-3	0.09	4.5453
C13-OLE1	0.9734	2.9E-3	0.13	5.5490	0.9870	2.9E-3	0.04	2.0949
C13-OLE2	0.9796	2.9E-3	0.29	12.3230	0.9840	2.9E-3	0.08	4.5290
A-PINENE	0.9827	3.8E-3	0.30	9.8717	0.9901	3.7E-3	0.09	3.7016
B-PINENE	0.9846	3.8E-3	0.40	13.1808	0.9871	3.7E-3	0.11	4.8219
BENZENE	0.1739	3.5E-2	0.20	4.0957	0.2662	2.3E-2	0.03	0.8366
TOLUENE	0.5734	9.2E-3	0.40	9.3954	0.7358	7.2E-3	0.05	1.5467
C2-BENZ	0.6373	7.3E-3	0.37	9.6322	0.7913	5.8E-3	0.05	1.6613
N-C3-BEN	0.5789	7.1E-3	0.31	9.3887	0.7409	5.6E-3	0.04	1.5630
I-C3-BEN	0.6069	6.8E-3	0.32	9.4961	0.7658	5.4E-3	0.04	1.6290
S-C4-BEN	0.5789	6.4E-3	0.28	9.4087	0.7409	5.0E-3	0.04	1.5707
O-XYLENE	0.8364	5.5E-3	0.66	17.5705	0.9213	5.0E-3	0.14	4.6168
P-XYLENE	0.8467	5.5E-3	0.67	17.7261	0.9263	5.0E-3	0.14	4.7133
M-XYLENE	0.9366	4.9E-3	0.74	19.8304	0.9663	4.8E-3	0.17	5.5941
135-TMB	0.9825	4.2E-3	0.90	26.6258	0.9891	4.2E-3	0.21	7.7551
123-TMB	0.9671	4.3E-3	0.80	23.5653	0.9838	4.2E-3	0.18	6.7913
124-TMB	0.9667	4.3E-3	0.80	23.5428	0.9836	4.2E-3	0.18	6.7658
TETRALIN	0.9700	3.8E-3	0.09	2.8338	0.9853	3.8E-3	0.01	0.3223
NAPHTHAL	0.9245	4.0E-3	0.11	3.5532	0.9586	3.9E-3	0.00	0.2039
ME-NAPH	0.9826	3.4E-3	0.28	10.2101	0.9903	3.4E-3	0.05	2.2382
23-DMN	0.9840	3.1E-3	0.44	17.5899	0.9865	3.1E-3	0.09	4.4610
STYRENE	0.9826	4.7E-3	0.19	5.1325	0.9892	4.7E-3	-0.02	-0.7659
ACETYLEN	0.1101	1.7E-1	0.39	2.5628	0.1726	1.1E-1	0.13	1.0337
MEOH	0.1309	2.8E-1	0.88	2.9284	0.2037	1.8E-1	0.22	0.9007
ETOH	0.3818	4.8E-2	0.52	3.4666	0.5363	3.5E-2	0.16	1.3075
FORMALD	0.9326	4.0E-2	1.52	4.9881	0.9619	3.8E-2	0.33	1.3642
ACETALD	0.8740	2.1E-2	0.90	6.0176	0.9352	2.0E-2	0.26	2.1696
PROPALD	0.9257	1.3E-2	0.87	8.8823	0.9539	1.3E-2	0.26	3.2236
ACETONE	0.0509	2.4E-1	1.36	13.6136	0.0715	1.7E-1	0.27	3.3742
MEK	0.1872	4.9E-2	0.73	9.7609	0.2693	3.4E-2	0.18	3.0594
GLYOXAL	1.0000	1.9E-2	0.43	2.7810	1.0000	1.9E-2	0.11	0.8614
MEGLYOX	1.0000	1.2E-2	2.27	23.1753	1.0000	1.2E-2	0.54	6.9164
BENZALD	0.9034	5.9E-3	-0.06	-1.3361	1.0000	5.3E-3	-0.10	-2.8478
PHENOL	1.0000	6.2E-3	0.12	2.3031	1.0000	6.2E-3	-0.04	-0.9468
CRESOL	1.0000	5.3E-3	0.23	5.3856	1.0000	5.3E-3	-0.05	-1.4554
Base ROG Mixture and TLEV and LEV Exhausts [b]								
ARBROG	0.1133	3.3E-1	2.61	8.5497	0.1305	2.8E-1	0.65	2.7167
RFA	0.1295	2.9E-1	2.47	8.0766	0.1502	2.5E-1	0.61	2.5013
M85	0.1664	2.2E-1	1.36	4.5534	0.2238	1.7E-1	0.32	1.2715
CNG	0.0421	8.8E-1	1.43	4.7455	0.0563	6.6E-1	0.40	1.6520
LPG	0.1054	3.5E-1	1.62	5.3894	0.1329	2.8E-1	0.44	1.8248
E85	0.2105	1.8E-1	1.43	4.6187	0.2722	1.4E-1	0.40	1.6037
PH2	0.1298	2.9E-1	2.41	7.8584	0.1487	2.5E-1	0.61	2.5088
PH2-L	0.1209	3.1E-1	2.29	7.4786	0.1409	2.6E-1	0.57	2.3904
RFA-L	0.1122	3.3E-1	2.54	8.3911	0.1318	2.8E-1	0.62	2.5884
Dummy species (reacting with kOH = $3 \cdot 10^3$ ppm^{-1} min^{-1})								
NULL-3	0.2612	1.4E-1	0.00	0.0008	0.3865	9.6E-2	0.00	-0.0028

[a] Species names as follows: "R." prefix means that the species mechanism is in the form OH + R.xx.nn = product, while a "P." prefix means that the mechanism is in the form OH + P.xx.nn = OH + product. The "xx" indicates the product and nn indicates the rate constant in units of 10^3 ppm^{-1} min^{-1}. Product codes are as follows: XR = (no product); RH = HO_2; NR = RO2-R·; NR = RO2-N·; XN = RO2-XN·; R2 = R2O2·; A1 = HCHO; A2 = CCHO; A3 = RCHO; K3 = ACET; and K4 = MEK.

[b] "ARBROG is the base ROG mixture. Others are exhausts, where the "-L" suffix means it is a LEV exhaust.

Table B-9 Differences between mechanistic reactivities calculated direcly and those derived using the "pure species" approach.

DMSname	Mechanistic reactivities (per molecule) — MIR Scenario — Direct	Derived	(diff)	— MOR Scenario — Direct	Derived	(diff)
METHANE	3.89	4.02	3%	1.45	1.51	4%
ETHANE	1.98	2.06	4%	0.81	0.86	7%
PROPANE	0.95	0.97	1%	0.39	0.40	2%
N-C4	1.02	1.04	2%	0.44	0.45	3%
N-C8	0.27	0.28	4%	0.14	0.15	8%
N-C15	0.11	0.10	0%	0.06	0.06	2%
224TM-C5	0.65	0.68	5%	0.26	0.28	7%
MEOH	2.93	3.00	3%	0.90	0.93	4%
ETOH	1.73	1.82	5%	0.65	0.70	7%

References.

Bauges, K. (1991): Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC.. Letter to Bart Croes, California Air Resources Board, May 18.

Carter, W. P. L. and R. Atkinson (1989): "A Computer Modeling Study of Incremental Hydrocarbon Reactivity", Environ. Sci. and Technol., 23, 864.

Carter, W. P. L. (1991): "Development of Ozone Reactivity Scales for Volatile Organic Compounds", EPA-600/3-91/050, August.

EPA (1989): "User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms) Volume I," EPA-540/4-89-009a, July.

Jeffries, H. E. (1991): Department of Environmental Science and Engineering, School of Public Health, University of North Carolina, Chapel Hill, NC, private communication.

Table B-1. Detailed input data and OZIPM4 input files for the individual scenarios.

Scenario ID	**ATLGA1**	**ATLANTA, GA**	**6/ 6/88**
Latitude (deg):	33.75	Longtitude (deg):	84.38
Declination (deg):	22.68	Solar - clock time (min):	-96.14
Base ROG Input (mmolC/m2/day)	11.76	Initial Base ROG (% of input)	56.11
NOx Input (mmol/m2/day)	1.62	Initial NOx (% of input)	43.82

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.6502	0.0300	0.0433	0.0439	0.0419	0.0422	0.0433	0.0423	0.0430	0.0438	0.0461	0.0492
NOx	0.0700		0.0572	0.0575	0.0535	0.0536	0.0562	0.0491	0.0550	0.0560	0.0595	0.0643
Ozone		0.0630										
CH4	1.790	1.790										
CO	1.200	0.500	0.526	0.517	0.494	0.503	0.532	0.500	0.527	0.539	0.579	0.637
ISOP	0.0001		0.0045	0.0068	0.0103	0.0134	0.0165	0.0194	0.0220	0.0248	0.0267	0.0214
APIN	0.0001		0.0007	0.0009	0.0011	0.0012	0.0012	0.0013	0.0014	0.0015	0.0015	0.0015
UNKN	0.0001		0.0017	0.0023	0.0026	0.0029	0.0031	0.0033	0.0034	0.0036	0.0039	0.0034

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	625.	1000.	1376.	1750.	1882.	2014.	2146.	2146.	2146.	2146.
T (deg K)	293.0	295.0	296.0	299.0	300.0	301.0	302.0	302.0	304.0	305.0	304.0
H2O (10^4 ppm)	1.351	1.351	1.249	1.303	1.281	1.215	1.022	0.947	0.977	1.034	0.934

OZIPM4 Input File:

```
TITL
ATLANTA, GA    BASE CASE SIMULATION   6/6/88
PLAC              33.75      84.38        4.      1988.        6.        6.
ATLANTA, GA
DILU               250.       2146.       0.         0.        0.
TEMP               11.         293.      295.       296.      299.      300.
      301.         302.        302.      304.       305.      304.      303.
WATE               11.        28.95
       61.          54.         47.       41.        38.       34.       30.
       27.          25.         23.       23.        22.
TRAN                0.         .063       0.        .03        0.       .002
MASS               -10.         .65       .07       250.
      7.48         7.59        7.24      7.29       7.48      7.31      7.44
      7.58         7.97        8.51
      4.30         4.32        4.02      4.03       4.22      3.69      4.13
      4.21         4.47        4.83
BIOG               -10.          3.       250.
ISOP                0.         .0001       0.         0.       .0001      0.
     68.13
       .31          .47         .71       .92       1.13      1.33      1.51
       1.7         1.83        1.47
APIN                1.         .0001       0.         0.       .0001      0.
    136.24
         0.          .75         .75       0.         0.        0.        7.
         0.
        .10          .12         .15       .16        .17       .18       .19
        .21          .21          .2
UNKN                1.         .0001       0.         0.       .0001      0.
    136.24
         0.         .375        .875       0.         0.        0.       7.5
         0.
        .24          .31         .36       .40        .42       .45       .47
        .50          .53         .47
CRED                0.         -10.       250.
CO                  1.2          0.         .5       -20.       0.        .4
     14.85        14.59       13.94     14.18      15.02     14.1      14.86
      15.2        16.33       17.97
SPEC                1.
O3
PLOT                0.          0.         0.         0.        0.        0.
ISOP                0.          0.         1.         0.        1.
       .17
```

Table B-1 (continued)

Scenario ID	**AUSTX1**	**AUSTIN, TX**	**9/ 9/88**
Latitude (deg):	30.28	Longtitude (deg):	97.75
Declination (deg):	5.22	Solar - clock time (min):	-87.79
Base ROG Input (mmolC/m2/day)	11.22	Initial Base ROG (% of input)	83.30
NOx Input (mmol/m2/day)	1.21	Initial NOx (% of input)	61.49

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.9203	0.0300	0.0159	0.0167	0.0158	0.0160	0.0165	0.0161	0.0164	0.0167	0.0178	0.0191
NOx	0.0730		0.0399	0.0392	0.0374	0.0376	0.0387	0.0363	0.0383	0.0387	0.0405	0.0385
Ozone		0.0850										
CH4	1.790	1.790										
CO	1.500	0.500	0.265	0.252	0.233	0.239	0.255	0.245	0.253	0.259	0.282	0.312
ISOP	0.0001		0.0006	0.0007	0.0010	0.0019	0.0031	0.0036	0.0042	0.0048	0.0048	0.0042
APIN	0.0001		0.0006	0.0006	0.0007	0.0007	0.0009	0.0009	0.0010	0.0011	0.0011	0.0010
UNKN	0.0001		0.0001	0.0001	0.0002	0.0002	0.0003	0.0003	0.0004	0.0004	0.0004	0.0004

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	618.	985.	1353.	1720.	1849.	1979.	2108.	2108.	2108.	2108.
T (deg K)	294.0	296.0	298.0	300.0	302.0	304.0	305.0	306.0	307.0	307.0	306.0
H2O (10^4 ppm)	1.880	2.041	2.240	2.214	2.143	2.017	1.499	1.298	1.373	1.373	1.298

OZIPM4 Input File

```
TITL
AUSTIN, TX  BASE CASE SIMULATION  9/9/88
PLAC          30.28      97.75        5.      1988.        9.        9.
AUSTIN, TX
DILU            250.       2108.       0.        0.        0.
TEMP             11.        294.      296.      298.      300.      302.
      304.       305.       306.      307.      307.      306.      306.
WATE             11.      29.26
       79.        76.        74.       65.       56.       47.       40.
       33.        27.        27.       27.       27.
TRAN              0.       .085        0.       .03        0.      .002
MASS            -10.       0.92      .073      250.
     2.62       2.76       2.60      2.63      2.72      2.66      2.70
     2.76       2.93       3.15
     2.23       2.19       2.09      2.10      2.16      2.03      2.14
     2.16       2.26       2.15
BIOG            -10.         3.      250.
ISOP              0.      .0001        0.        0.     .0001        0.
    68.13
      .04        .05        .07       .13       .21       .25       .29
      .33        .33        .29
APIN              1.      .0001        0.        0.     .0001        0.
   136.24
        0.        .75        .75       0.        0.        0.        7.
        0.
      .08        .08         .1        .1       .12       .13       .14
      .15        .15        .14
UNKN              1.      .0001        0.        0.     .0001        0.
   136.24
        0.       .375       .875       0.        0.        0.       7.5
        0.
      .02        .02        .03       .03       .04       .04       .05
      .05        .05        .05
CRED              0.       -10.      250.
CO              1.5          0.        .5      -20.        0.        .4
     7.48       7.11       6.58      6.73      7.20      6.90      7.14
     7.32       7.95       8.79
CALC            0.92       .073        0.        0.        0.
```

Table B-1 (continued)

Scenario ID	**BALMD1**	**BALTIMORE, MD**	7/ 7/88
Latitude (deg):	39.30	Longtitude (deg):	76.59
Declination (deg):	22.57	Solar - clock time (min):	-71.24
Base ROG Input (mmolC/m2/day)	16.79	Initial Base ROG (% of input)	58.05
NOx Input (mmol/m2/day)	3.26	Initial NOx (% of input)	41.73

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.9604	0.0300	0.1566	0.1526	0.0202	0.0203	0.0206	0.0203	0.0069	0.0069	0.0073	0.0078
NOx	0.1341		0.2418	0.2442	0.0169	0.0169	0.0175	0.0163	0.0068	0.0069	0.0073	0.0080
Ozone		0.0840										
CH4	1.790	1.790										
CO	1.900	0.500	3.331	3.262	0.303	0.306	0.319	0.302	0.151	0.155	0.166	0.182
ISOP	0.0001		0.0026	0.0047	0.0127	0.0157	0.0203	0.0227	0.0308	0.0296	0.0287	0.0224
APIN	0.0001		0.0009	0.0011	0.0015	0.0017	0.0020	0.0022	0.0028	0.0028	0.0028	0.0024
UNKN	0.0001		0.0001	0.0001	0.0032	0.0035	0.0042	0.0047	0.0079	0.0079	0.0078	0.0066

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	432.	614.	796.	977.	1041.	1105.	1169.	1169.	1169.	1169.
T (deg K)	299.0	300.0	302.0	304.0	305.0	307.0	309.0	309.0	309.0	309.0	307.0
H2O (10^4 ppm)	2.364	2.368	2.464	2.589	2.415	2.287	2.091	2.091	2.033	2.266	2.235

OZIPM4 Input File

```
TITL
BALTIMORE, MD BASE CASE SIMULATION  7/7/88
PLAC          39.30      76.59       4.      1988.       7.       7.
BALTIMORE, MD
DILU           250.      1169.       0.         0.       0.
TEMP            11.       299.      300.       302.     304.     305.
     307.      309.       309.      309.       309.     307.     306.
WATE            11.      29.91
      72.       68.        63.       59.        52.      44.      37.
      36.       36.        35.       39.        43.
TRAN             0.       .084        0.       .03        0.     .002
MASS           -10.        .96      .134      250.
     38.66     37.68       4.99      5.01       5.09     5.00     1.70
      1.70      1.79       1.93
     36.53     36.88       2.56      2.56       2.64     2.46     1.03
      1.04      1.11       1.21
BIOG           -10.          3.      250.
ISOP             0.       .0001        0.         0.     .0001        0.
     68.13
       .18       .32        .87      1.08       1.39     1.56     2.11
      2.03      1.97       1.54
APIN             1.       .0001        0.         0.     .0001.       0.
    136.24
        0.       .75        .75        0.         0.       0.       7.
        0.
       .13       .15        .21       .23        .27       .3      .38
       .38       .38        .33
UNKN             1.       .0001        0.         0.     .0001        0.
    136.24
        0.       .375       .875       0.         0.       0.       7.5
        0.
       .01       .01        .44       .48        .57      .65     1.09
      1.08      1.07        .91
CRED             0.        -10.      250.
CO             1.9          0.         .5       -20.       0.       .4
     93.97     92.03       8.54      8.63       9.00     8.51     4.25
      4.36      4.68       5.14
```

Table B-1 (continued)

Scenario ID	**BATLA1**	**BATON ROUGE, LA**	**4/26/88**
Latitude (deg):	30.46	Longtitude (deg):	91.19
Declination (deg):	13.60	Solar - clock time (min):	-62.25
Base ROG Input (mmolC/m2/day)	11.13	Initial Base ROG (% of input)	55.65
NOx Input (mmol/m2/day)	1.63	Initial NOx (% of input)	26.80

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.6102	0.0300	0.0447	0.0447	0.0433	0.0432	0.0437	0.0432	0.0437	0.0441	0.0456	0.0472
NOx	0.0430		0.0759	0.0754	0.0730	0.0727	0.0737	0.0711	0.0734	0.0737	0.0758	0.0674
Ozone		0.0620										
CH4	1.790	1.790										
CO	1.500	0.500	0.394	0.385	0.365	0.363	0.377	0.358	0.376	0.387	0.415	0.442
ISOP	0.0001			0.0038	0.0050	0.0074	0.0089	0.0103	0.0114	0.0105	0.0096	0.0083
APIN	0.0001		0.0010	0.0016	0.0018	0.0020	0.0021	0.0023	0.0024	0.0023	0.0023	0.0022
UNKN	0.0001		0.0010	0.0019	0.0021	0.0025	0.0026	0.0028	0.0028	0.0028	0.0027	0.0026

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	392.	534.	676.	818.	868.	918.	968.	968.	968.	968.
T (deg K)	291.0	293.0	296.0	297.0	299.0	300.0	301.0	301.0	302.0	302.0	302.0
H2O (10^4 ppm)	1.570	1.571	1.640	1.567	1.568	1.456	1.359	1.286	1.363	1.324	1.324

OZIPM4 Input File

```
TITL
BATON ROUGE, LA   BASE CASE SIMULATION   4/26/88
PLAC          30.46      91.19        5.      1988.        4.        26.
BATON ROUGE, LA
DILU             250.       968.        0.        0.        0.
TEMP              11.        291.       293.      296.      297.      299.
      300.       301.       301.       302.      302.      302.      301.
WATE              11.       29.77
       78.        69.        60.        54.       48.       42.       39.
       37.        35.        35.        34.       34.
TRAN               0.        .062        0.        .03       0.        .002
MASS             -10.        .61        .043      250.
      7.31       7.32       7.09       7.07      7.15      7.06      7.15
      7.22       7.46       7.73
      5.73       5.69       5.51       5.49      5.56      5.37      5.54
      5.56       5.72       5.09
BIOG             -10.        3.         250.
ISOP               0.        .0001      0.        0.        .0001     0.
     68.13
       0.         .26        .34        .51       .61       .71       .78
       .72        .66        .57
APIN               1.        .0001      0.        0.        .0001     0.
    136.24
       0.         .75        .75        0.        0.        0.        7.
       0.
       .14        .22        .25        .27       .29       .31       .33
       .32        .31        .3
UNKN               1.        .0001      0.        0.        .0001     0.
    136.24
       0.         .375       .875       0.        0.        0.        7.5
       0.
       .14        .26        .29        .34       .36       .38       .39
       .38        .37        .35
CRED               0.       -10.        250.
CO               1.5          0.         .5      -20.        0.        .4
     11.12      10.86      10.31      10.24     10.63     10.11     10.62
     10.93      11.72      12.47
```

Table B-1 (continued)

Scenario ID	**BIRAL1**	**BIRMINGHAM, AL**	**7/31/87**
Latitude (deg):	33.53	Longtitude (deg):	86.81
Declination (deg):	18.45	Solar - clock time (min):	-53.67
Base ROG Input (mmolC/m2/day)	12.83	Initial Base ROG (% of input)	90.74
NOx Input (mmol/m2/day)	1.85	Initial NOx (% of input)	67.34

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.0204	0.0300	0.0162	0.0164	0.0157	0.0159	0.0163	0.0023	0.0023	0.0024	0.0025	0.0027
NOx	0.1090		0.0270	0.0272	0.0264	0.0265	0.0272	0.0388	0.0383	0.0384	0.0387	0.0380
Ozone		0.0810										
CH4	1.790	1.790										
CO	4.400	0.500	0.290	0.278	0.267	0.275	0.291	0.053	0.054	0.055	0.058	0.061
ISOP	0.0001			0.0188	0.0328	0.0386	0.0418	0.0440	0.0468	0.0439	0.0347	0.0176
APIN	0.0001		0.0011	0.0015	0.0018	0.0020	0.0021	0.0021	0.0022	0.0022	0.0020	0.0018
UNKN	0.0001		0.0031	0.0047	0.0058	0.0063	0.0066	0.0074	0.0078	0.0077	0.0067	0.0062

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	281.	576.	870.	1165.	1459.	1563.	1666.	1770.	1770.	1770.	1770.
T (deg K)	299.0	302.0	305.0	306.0	307.0	309.0	310.0	310.0	310.0	310.0	309.0
H2O (10^4 ppm)	2.414	2.492	2.550	2.312	2.089	1.879	1.865	1.805	1.865	1.926	1.936

OZIPM4 Input File

```
TITL
BIRMINGHAM, AL   BASE CASE SIMULATION  7/31/87
PLAC          33.53       86.81          5.       1987.          7.          31.
BIRMINGHAM, AL
DILU                       281.       1770.          0.          0.          0.
TEMP                        11.        299.        302.        305.        306.        307.
      309.                 310.        310.        310.        310.        309.        308.
WATE                        11.       29.32
       75.                  65.         56.         48.         41.         33.         32.
       31.                  30.         31.         32.         34.
TRAN                         0.        .081          0.         .03          0.        .002
MASS                       -10.        1.02        .109        281.
     3.06                  3.09        2.96        2.99        3.08         .43         .44
      .45                   .47         .50
     2.31                  2.33        2.26        2.27        2.33        3.32        3.28
     3.29                  3.31        3.25
BIOG                       -10.          3.        281.
ISOP                         0.       .0001          0.          0.       .0001          0.
    68.13
        0.                  1.29        2.25        2.65        2.87        3.02        3.21
     3.01                  2.38        1.21
APIN                         1.       .0001          0.          0.       .0001          0.
   136.24
        0.                   .75         .75          0.          0.          0.          7.
        0.
      .15                    .21         .25         .27         .29         .29          .3
       .3                    .27         .25
UNKN                         1.       .0001          0.          0.       .0001          0.
   136.24
        0.                  .375        .875          0.          0.          0.         7.5
        0.
      .43                    .64         .79         .86          .9        1.01        1.07
     1.05                    .92         .85
CRED                         0.        -10.        281.
CO                         4.4           0.          .5        -20.          0.          .4
     8.17                  7.84        7.54        7.75        8.22        1.50        1.52
     1.56                  1.65        1.73
```

Table B-1 (continued)

Scenario ID	**BOSMA1**	**BOSTON, MA**	**6/16/88**
Latitude (deg):	42.38	Longtitude (deg):	71.03
Declination (deg):	23.36	Solar - clock time (min):	-44.78
Base ROG Input (mmolC/m2/day)	14.26	Initial Base ROG (% of input)	48.14
NOx Input (mmol/m2/day)	2.19	Initial NOx (% of input)	42.71

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr)									
			Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.5202	0.0300	0.0518	0.0521	0.0500	0.0504	0.0515	0.0507	0.0511	0.0509	0.0534	0.0566
NOx	0.0710		0.0604	0.0585	0.0545	0.0549	0.0571	0.0527	0.0563	0.0556	0.0594	0.0635
Ozone		0.1050										
CH4	1.790	1.790										
CO	1.600	0.500	0.832	0.811	0.783	0.795	0.837	0.803	0.831	0.828	0.889	0.974
ISOP	0.0001		0.0020	0.0035	0.0057	0.0068	0.0068	0.0080	0.0198	0.0172	0.0166	0.0111
APIN	0.0001		0.0007	0.0008	0.0009	0.0010	0.0010	0.0011	0.0022	0.0020	0.0020	0.0017
UNKN	0.0001		0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0041	0.0038	0.0038	0.0032

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	325.	775.	1225.	1674.	2123.	2282.	2440.	2598.	2598.	2598.	2598.
T (deg K)	299.0	300.0	302.0	304.0	305.0	305.0	306.0	305.0	304.0	304.0	302.0
H2O (10^4 ppm)	2.038	1.987	2.075	2.108	2.232	2.185	2.411	2.371	2.328	2.460	2.349

OZIPM4 Input File

```
TITL
BOSTON, MA BASE CASE SIMULATION   6/16/88
PLAC          42.38      71.03       4.    1988.       6.      16.
BOSTON, MA
DILU           325.       2598.       0.       0.       0.
TEMP            11.        299.     300.     302.     304.     305.
      305.      306.       305.     304.     304.     302.     301.
WATE            11.      29.94
       62.       57.        53.      48.      48.      47.      47.
       49.       51.        53.      56.      60.
TRAN            0..        .105      0.      .03       0.      .002
MASS           -10.        .52      .071     325.
     10.86     10.93      10.49    10.56    10.79    10.62    10.72
     10.67     11.19      11.87
      6.14      5.95       5.54     5.58     5.80     5.36     5.72
      5.65      6.04       6.45
BIOG           -10.         3.      325.
ISOP             0.        .0001      0.       0.      .0001     0.
     68.13
       .14       .24        .39      .47      .47      .55      1.36
      1.18      1.14        .76
APIN             1.        .0001      0.       0.      .0001     0.
    136.24
         0.       .75        .75      0.       0.       0.       7.
         0.
        .1        .11        .13      .14      .14      .15      .3
       .28       .28        .23
UNKN             1.        .0001      0.       0.      .0001     0.
    136.24
         0.       .375       .875     0.       0.       0.       7.5
         0.
        .01       .01        .01      .01      .01      .01      .56
       .52       .52        .44
CRED             0.        -10.      325.
CO              1.6          0.        .5     -20.       0.       .4
     23.47     22.88      22.08    22.42    23.62    22.65    23.43
     23.35     25.09      27.47
```

Table B-1 (continued)

Scenario ID	**CHANC1**	**CHARLOTTE, NC**	**6/ 8/88**
Latitude (deg):	35.25	Longtitude (deg):	80.76
Declination (deg):	22.87	Solar - clock time (min):	-82.05
Base ROG Input (mmolC/m2/day)	7.46	Initial Base ROG (% of input)	53.08
NOx Input (mmol/m2/day)	0.96	Initial NOx (% of input)	47.69

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.3901	0.0300	0.0463	0.0470	0.0452	0.0454	0.0465	0.0453	0.0462	0.0470	0.0486	0.0516
NOx	0.0450		0.0523	0.0538	0.0502	0.0502	0.0529	0.0444	0.0516	0.0525	0.0556	0.0595
Ozone		0.0920										
CH4	1.790	1.790										
CO	1.500	0.500	0.326	0.331	0.322	0.326	0.346	0.318	0.341	0.348	0.352	0.388
ISOP	0.0001		0.0055	0.0118	0.0205	0.0235	0.0261	0.0284	0.0283	0.0286	0.0243	0.0195
APIN	0.0001		0.0009	0.0011	0.0014	0.0015	0.0015	0.0017	0.0017	0.0017	0.0017	0.0015
UNKN	0.0001		0.0021	0.0028	0.0036	0.0038	0.0039	0.0042	0.0042	0.0044	0.0041	0.0036

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	803.	1357.	1910.	2462.	2657.	2851.	3046.	3046.	3046.	3046.
T (deg K)	294.0	297.0	300.0	303.0	304.0	305.0	306.0	306.0	306.0	306.0	305.0
H2O (10^4 ppm)	1.599	1.691	1.717	1.683	1.655	1.617	1.521	1.473	1.473	1.806	2.021

OZIPM4 Input File

```
TITL
CHARLOTTE, NC   BASE CASE SIMULATION   6/8/88
PLAC          35.25       80.76          4.       1988.          6.          8.
CHARLOTTE, NC
DILU             250.        3046.         0.          0.          0.
TEMP              11.         294.        297.        300.        303.        304.
      305.        306.        306.        306.        305.        304.
WATE              11.       28.92
       68.         60.         51.         42.         39.         36.         32.
       32.         31.         31.         38.         45.
TRAN               0.        .092          0.        .03           0.        .002
MASS             -10.         .39        .045        250.
      5.08        5.15        4.96        4.98        5.10        4.97        5.07
      5.16        5.33        5.66
      2.32        2.39        2.23        2.23        2.35        1.97        2.29
      2.33        2.47        2.64
BIOG             -10.          3.         250.
ISOP               0.       .0001          0.          0.       .0001          0.
     68.13
       .38         .81        1.41        1.61        1.79        1.95        1.94
      1.96        1.67        1.34
APIN               1.       .0001          0.          0.       .0001          0.
    136.24
         0.         .75         .75          0.          0.          0.          7.
         0.
        .12         .15         .19          .2         .21         .23         .23
        .23         .23          .2
UNKN               1.       .0001          0.          0.       .0001          0.
    136.24
         0.        .375        .875          0.          0.          0.         7.5
         0.
        .29         .39         .49         .52         .54         .57         .57
         .6         .56         .49
CRED               0.         -10.         250.
CO               1.5           0.          .5         -20.          0.          .4
      9.21        9.33        9.08        9.21        9.75        8.98        9.63
      9.81        9.94       10.94
```

Table B-1 (continued)

Scenario ID	**CHIIL1**	**CHICAGO, IL**	**8/11/88**
Latitude (deg):	41.88	Longtitude (deg):	87.63
Declination (deg):	15.20	Solar - clock time (min):	-55.67
Base ROG Input (mmolC/m2/day)	24.97	Initial Base ROG (% of input)	67.10
NOx Input (mmol/m2/day)	2.15	Initial NOx (% of input)	41.14

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.6506	0.0300	0.0688	0.0699	0.0679	0.0684	0.0158	0.0156	0.0057	0.0053	0.0056	0.0059
NOx	0.0870		0.0995	0.0967	0.0915	0.0925	0.0388	0.0374	0.0318	0.0323	0.0336	0.0345
Ozone		0.0400										
CH4	1.790	1.790										
CO	2.300	0.500	1.904	1.825	1.762	1.812	0.474	0.468	0.223	0.229	0.245	0.268
ISOP	0.0001		0.0025	0.0044	0.0055	0.0070	0.0066	0.0074	0.0036	0.0036	0.0036	0.0031
APIN	0.0001		0.0009	0.0011	0.0012	0.0012	0.0015	0.0015	0.0020	0.0020	0.0020	0.0019
UNKN	0.0001		0.0003	0.0003	0.0004	0.0004	0.0020	0.0023	0.0045	0.0045	0.0045	0.0042

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	476.	702.	928.	1154.	1233.	1313.	1392.	1392.	1392.	1392.
T (deg K)	298.0	300.0	302.0	303.0	304.0	305.0	306.0	306.0	306.0	306.0	305.0
H2O (10^4 ppm)	2.732	2.835	2.878	2.886	2.841	2.779	2.748	2.603	2.748	2.893	2.870

OZIPM4 Input File

```
TITL
CHICAGO, IL   BASE CASE SIMULATION   8/11/88
PLAC          41.88      87.63       5.      1988.      8.      11.
CHICAGO, IL
DILU                250.      1392.      0.      0.      0.
TEMP                 11.       298.    300.    302.    303.     304.
      305.          306.       306.    306.    305.     304.
WATE                 11.     29.34
       90.           83.       75.     71.     66.      61.      59.
       57.           54.       57.     60.     63.
TRAN                  0.       .04      0.     .03      0.     .002
MASS                -10.      1.65    .087    250.
     25.27          25.67     24.92   25.11    5.79     5.74     2.08
      1.95           2.05      2.17
      9.90           9.62      9.10    9.20    3.86     3.72     3.16
      3.21           3.34      3.43
BIOG                -10.        3.    250.
ISOP                  0.      .0001      0.      0.    .0001       0.
     68.13
       .17             .3       .38     .48     .45      .51      .25
       .25            .25       .21
APIN                  1.      .0001      0.      0.    .0001.      0.
    136.24
         0.           .75       .75      0.      0.       0.       7.
         0.
       .13            .15       .16     .17      .2      .21      .27
       .27            .27       .26
UNKN                  1.      .0001      0.      0.    .0001       0.
    136.24
         0.          .375      .875      0.      0.       0.      7.5
         0.
       .04            .04       .05     .05     .28      .31      .62
       .62            .62       .57
CRED                  0.       -10.    250.
CO                   2.3         0.      .5     -20.      0.       .4
     53.70         51.49     49.72   51.13    13.37    13.21     6.30
      6.45          6.92      7.57
```

Table B-1 (continued)

Scenario ID	**CINOH1**	**CINCINNATI, OH**	**8/18/88**
Latitude (deg):	39.14	Longtitude (deg):	84.51
Declination (deg):	13.03	Solar - clock time (min):	-101.78
Base ROG Input (mmolC/m2/day)	17.29	Initial Base ROG (% of input)	65.80
NOx Input (mmol/m2/day)	2.71	Initial NOx (% of input)	65.15

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.1204	0.0300	0.0682	0.0683	0.0664	0.0666	0.0115	0.0114	0.0115	0.0118	0.0126	0.0138
NOx	0.1741		0.0632	0.0635	0.0608	0.0613	0.0165	0.0157	0.0163	0.0166	0.0174	0.0172
Ozone		0.0700										
CH4	1.790	1.790										
CO	2.300	0.500	1.035	0.998	0.945	0.965	0.321	0.318	0.320	0.329	0.356	0.392
ISOP	0.0001		0.0026	0.0064	0.0118	0.0138	0.0204	0.0189	0.0149	0.0146	0.0085	0.0071
APIN	0.0001		0.0009	0.0012	0.0015	0.0017	0.0017	0.0018	0.0017	0.0017	0.0015	0.0015
UNKN	0.0001		0.0009	0.0012	0.0016	0.0017	0.0031	0.0032	0.0028	0.0028	0.0026	0.0024

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	758.	1266.	1773.	2280.	2459.	2637.	2816.	2816.	2816.	2816.
T (deg K)	296.0	299.0	302.0	305.0	306.0	308.0	310.0	310.0	309.0	309.0	308.0
H2O (10^4 ppm)	2.317	2.420	2.466	2.433	2.336	2.346	2.322	2.262	2.141	2.310	2.346

OZIPM4 Input File

```
TITL
CINCINNATI, OH   BASE CASE SIMULATION   8/18/88
PLAC          39.14       84.51          4.       1988.          8.         18.
CINCINNATI, OH
DILU             250.       2816.          0.          0.          0.
TEMP              11.        296.        299.        302.        305.        306.
      308.        310.        310.        309.        308.        307.
WATE              11.       29.01
       87.         76.         65.         54.         49.         44.         39.
       39.         38.         38.         41.         44.
TRAN               0.         .07          0.         .03          0.        .002
MASS             -10.        1.12        .174        250.
    17.33       17.35       16.87       16.91        2.92         2.9        2.91
        3.        3.21        3.50
     7.94        7.98        7.64        7.70        2.07        1.97        2.05
     2.08        2.19        2.16
BIOG             -10.          3.        250.
ISOP               0.       .0001          0.          0.       .0001          0.
    68.13
      .18         .44         .81         .95         1.4         1.3        1.02
      1.0         .58         .49
APIN               1.       .0001          0.          0.       .0001          0.
   136.24
        0.         .75         .75          0.          0.          0.          7.
        0.
      .13         .17         .21         .23         .23         .25         .23
      .23         .21         .21
UNKN               1.       .0001          0.          0.       .0001          0.
   136.24
        0.        .375        .875          0.          0.          0.         7.5
        0.
      .12         .17         .22         .24         .42         .44         .38
      .38         .36         .33
CRED               0.        -10.        250.
CO               2.3           0.          .5         -20.          0.          .4
    29.20       28.16       26.66       27.21        9.06        8.96        9.04
     9.28       10.05       11.07
```

Table B-1 (continued)

Scenario ID	**CLEOH1**	**CLEVELAND, OH**	**7/ 5/88**
Latitude (deg):	41.49	Longtitude (deg):	81.68
Declination (deg):	22.77	Solar - clock time (min):	-91.27
Base ROG Input (mmolC/m2/day)	15.68	Initial Base ROG (% of input)	49.22
NOx Input (mmol/m2/day)	2.37	Initial NOx (% of input)	50.17

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.7603	0.0300	0.0706	0.0706	0.0680	0.0686	0.0703	0.0696	0.0701	0.0063	0.0066	0.0071
NOx	0.1170		0.0717	0.0706	0.0661	0.0666	0.0696	0.0639	0.0686	0.0066	0.0070	0.0076
Ozone		0.0890										
CH4	1.790	1.790										
CO	1.500	0.500	1.521	1.474	1.417	1.448	1.535	1.502	1.530	0.137	0.147	0.161
ISOP	0.0001		0.0020	0.0041	0.0080	0.0080	0.0095	0.0095	0.0095	0.0133	0.0127	0.0105
APIN	0.0001		0.0009	0.0010	0.0012	0.0012	0.0014	0.0014	0.0014	0.0021	0.0021	0.0020
UNKN	0.0001		0.0001	0.0002	0.0003	0.0003	0.0003	0.0003	0.0003	0.0044	0.0044	0.0040

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	527.	804.	1081.	1358.	1455.	1553.	1650.	1650.	1650.	1650.
T (deg K)	295.0	297.0	300.0	304.0	304.0	305.0	305.0	305.0	305.0	305.0	304.0
H2O (10^4 ppm)	1.447	1.432	1.437	1.466	1.379	1.369	1.232	1.278	1.278	1.278	1.207

OZIPM4 Input File

```
TITL
CLEVELAND, OH    BASE CASE SIMULATION   7/5/88
PLAC          41.49       81.68          4.       1988.          7.          5.
CLEVELAND, OH
DILU                       250.        1650.          0.          0.          0.
TEMP                        11.         295.        297.        300.        304.        304.
      305.                 305.         305.        305.        305.        304.        303.
WATE                        11.      29.385
       57.                  50.          42.         34.         32.         30.         27.
       27.                  28.          28.         28.         28.
TRAN                         0.        .089          0.        .03           0.        .002
MASS                       -10.         .76        .117        250.
    16.26                16.28       15.67       15.80       16.21       16.04       16.16
     1.45                 1.53        1.63
     7.87                 7.75        7.25        7.31        7.63        7.01        7.52
      .72                  .77         .83
BIOG                       -10.          3.        250.
ISOP                         0.       .0001          0.          0.       .0001          0.
    68.13
      .14                  .28         .55         .55         .65         .65         .65
      .91                  .87         .72
APIN                         1.       .0001          0.          0.       .0001          0.
   136.24
        0.                 .75         .75          0.          0.          0.          7.
        0.
      .12                  .14         .17         .17         .19         .19         .19
      .29                  .29         .27
UNKN                         1.       .0001          0.          0.       .0001          0.
   136.24
        0.                .375        .875          0.          0.          0.         7.5
        0.
      .02                  .03         .04         .04         .04         .04         .04
      .61                   .6         .55
CRED                         0.        -10.        250.
CO                         1.5          0.          .5         -20.          0.          .4
    42.90                41.57       39.98       40.86       43.31       42.38       43.16
     3.86                 4.15        4.53
```

Table B-1 (continued)

Scenario ID	**DALTX1**	**DALLAS, TX**	**9/ 9/87**
Latitude (deg):	32.83	Longtitude (deg):	96.86
Declination (deg):	5.60	Solar - clock time (min):	-84.60
Base ROG Input (mmolC/m2/day)	17.51	Initial Base ROG (% of input)	51.04
NOx Input (mmol/m2/day)	3.70	Initial NOx (% of input)	28.13

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.5502	0.0300	0.0486	0.0491	0.0463	0.0468	0.0483	0.0474	0.0481	0.0485	0.0513	0.0551
NOx	0.0640		0.0738	0.0733	0.0713	0.0716	0.0732	0.0697	0.0726	0.0726	0.0750	0.0656
Ozone		0.0750										
CH4	1.790	1.790										
CO	2.000	0.500	1.156	1.108	1.031	1.056	1.132	1.086	1.125	1.150	1.244	1.371
ISOP	0.0001		0.0009	0.0013	0.0022	0.0038	0.0058	0.0058	0.0067	0.0074	0.0067	0.0067
APIN	0.0001		0.0006	0.0007	0.0009	0.0009	0.0011	0.0011	0.0012	0.0012	0.0012	0.0012
UNKN	0.0001		0.0001	0.0001	0.0001	0.0002	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	400.	766.	1132.	1498.	1864.	1992.	2121.	2250.	2250.	2250.	2250.
T (deg K)	294.0	296.0	299.0	300.0	302.0	305.0	305.0	306.0	307.0	306.0	306.0
H2O (10^4 ppm)	1.955	2.019	2.156	1.980	1.917	1.912	1.457	1.349	1.529	1.542	1.686

OZIPM4 Input File

```
TITL
DALLAS, TX    BASE CASE SIMULATION   9/9/87
PLAC            32.83      96.86        5.      1987.        9.        9.
DALLAS, TX
DILU             400.       2250.       0.         0.        0.
TEMP              11.        294.       296.       299.      300.      302.
      305.       305.        306.       307.       306.      306.      305.
WATE              11.       29.32
       82.        75.         67.        58.        50.       42.       37.
       32.        28.         30.        32.        35.
TRAN               0.        .075        0.        .03        0.       .002
MASS             -10.         .55       .064       400.
     12.51      12.63       11.92      12.04      12.44     12.21     12.38
     12.47      13.19       14.19
     12.63      12.56       12.21      12.26      12.54     11.93     12.43
     12.44      12.84       11.23
BIOG             -10.          3.       400.
ISOP               0.       .0001         0.         0.      .0001        0.
     68.13
       .06        .09         .15        .26         .4        .4        .46
       .51        .46         .46
APIN               1.       .0001         0.         0.      .0001        0.
    136.24
         0.        .75         .75        0.         0.        0.        7.
         0.
       .08         .1         .12        .13        .15       .15       .17
       .17        .17         .17
UNKN               1.       .0001         0.         0.      .0001        0.
    136.24
         0.       .375        .875        0.         0.        0.       7.5
         0.
       .02        .02         .02        .03        .04       .04       .04
       .04        .04         .04
CRED               0.        -10.       400.
CO               2.0          0.          .5        -20.       0.        .4
     32.61      31.27       29.09      29.80      31.94     30.65     31.75
     32.44      35.08       38.68
SPEC               1.
O3
PLOT               0.         0.         0.         0.        0.        0.
ISOP               0.         0.         1.         0.        1.
       .14
```

Table B-1 (continued)

Scenario ID	**DENCO1**	**DENVER, CO**	7/26/88
Latitude (deg):	39.75	Longtitude (deg):	104.99
Declination (deg):	19.37	Solar - clock time (min):	-66.48
Base ROG Input (mmolC/m2/day)	29.33	Initial Base ROG (% of input)	42.60
NOx Input (mmol/m2/day)	4.64	Initial NOx (% of input)	36.14

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr)									
			Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.2305	0.0300	0.1456	0.1402	0.1298	0.1314	0.0043	0.0043	0.0043	0.0044	0.0047	0.0051
NOx	0.1651		0.1643	0.1561	0.1462	0.1471	0.0041	0.0039	0.0041	0.0041	0.0043	0.0044
Ozone		0.0570										
CH4	1.790	1.790										
CO	2.200	0.500	7.650	7.082	6.451	6.578	0.191	0.187	0.190	0.195	0.211	0.232
ISOP	0.0001			0.0015	0.0019	0.0031	0.0006	0.0006	0.0006	0.0006	0.0006	0.0004
APIN	0.0001		0.0007	0.0008	0.0009	0.0010	0.0007	0.0007	0.0007	0.0007	0.0007	0.0007
UNKN	0.0001		0.0001	0.0001	0.0001	0.0001	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	865.	1480.	2095.	2709.	2925.	3142.	3358.	3358.	3358.	3358.
T (deg K)	294.0	296.0	297.0	299.0	301.0	301.0	301.0	301.0	301.0	301.0	301.0
H2O (10^4 ppm)	1.011	1.027	1.018	1.065	1.105	1.074	1.013	1.074	1.136	1.228	1.350

OZIPM4 Input File

```
TITL
DENVER, CO    BASE CASE SIMULATION   7/26/88
PLAC            39.75     104.99        6.      1988.        7.        26.
DENVER, CO
DILU             250.      3358.        0.         0.        0.
TEMP              11.       294.       296.       297.      299.       301.
      301.        301.       301.       301.      301.       300.
WATE              11.     24.87
       50.        45.        42.        39.       36.        35.        34.
       33.        35.        37.        40.       44.
TRAN               0.      .057         0.       .03         0.      .002
MASS             -10.      1.23       .165      250.
    62.76      60.41      55.95      56.62      1.87      1.85      1.86
     1.90       2.02       2.18
    35.28      33.53      31.39      31.59       .88       .84       .87
      .88        .93        .95
BIOG             -10.         3.       250.
ISOP               0.      .0001         0.         0.     .0001         0.
    68.13
       0.         .1        .13        .21       .04       .04       .04
      .04        .04        .03
APIN               1.      .0001         0.         0.     .0001         0.
  136.24
       0.         .75        .75        0.         0.        0.        7.
       0.
       .1         .11        .12        .14        .1        .1        .1
       .1         .1         .1
UNKN               1.      .0001         0.         0.     .0001         0.
  136.24
       0.        .375       .875        0.         0.        0.       7.5
       0.
      .01         .01        .01        .02        .04       .04       .04
      .04        .04        .04
CRED               0.       -10.       250.
CO               2.2          0.         .5       -20.        0.        .4
  215.81     199.80     181.98     185.56      5.39      5.27      5.36
    5.50       5.95       6.55
```

Table B-1 (continued)

Scenario ID	**DETMI1**	**DETROIT, MI**	**8/ 2/88**
Latitude (deg):	42.36	Longtitude (deg):	83.10
Declination (deg):	17.71	Solar - clock time (min):	-98.66
Base ROG Input (mmolC/m2/day)	17.29	Initial Base ROG (% of input)	50.51
NOx Input (mmol/m2/day)	2.54	Initial NOx (% of input)	44.85

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.8603	0.0300	0.0700	0.0696	0.0660	0.0666	0.0683	0.0303	0.0305	0.0300	0.0312	0.0323
NOx	0.1120		0.0874	0.0853	0.0810	0.0816	0.0842	0.0251	0.0264	0.0258	0.0273	0.0272
Ozone		0.0680										
CH4	1.790	1.790										
CO	1.700	0.500	1.728	1.668	1.599	1.634	1.725	0.971	0.984	0.788	0.830	0.723
ISOP	0.0001		0.0039	0.0086	0.0120	0.0134	0.0144	0.0154	0.0153	0.0152	0.0154	0.0133
APIN	0.0001		0.0010	0.0012	0.0015	0.0015	0.0017	0.0021	0.0021	0.0021	0.0023	0.0020
UNKN	0.0001		0.0008	0.0011	0.0013	0.0014	0.0015	0.0039	0.0038	0.0038	0.0041	0.0034

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	565.	881.	1196.	1511.	1622.	1733.	1844.	1844.	1844.	1844.
T (deg K)	299.0	301.0	304.0	306.0	307.0	308.0	309.0	309.0	310.0	310.0	308.0
H2O (10^4 ppm)	2.937	2.903	2.976	2.802	2.810	2.809	2.684	2.627	2.715	3.017	2.971

OZIPM4 Input File

```
TITL
DETROIT, MI    BASE CASE SIMULATION   8/2/88
PLAC             42.36      83.10        4.      1988.        8.        2.
DETROIT, MI
DILU              250.       1844.        0.        0.        0.
TEMP               11.        299.       301.      304.      306.      307.
      308.        309.        309.       310.      310.      308.      306.
WATE               11.       29.40
       91.         80.         69.        58.       55.       52.       48.
       47.         46.         45.        50.       55.
TRAN                0.        .068         0.       .03        0.       .002
MASS              -10.         .86        .112      250.
     17.80       17.70       16.78      16.93     17.35      7.69      7.74
      7.62        7.94        8.22
     10.27       10.02        9.52       9.59      9.89      2.95      3.10
      3.03        3.21        3.20
BIOG              -10.          3.       250.
ISOP                0.       .0001         0.        0.      .0001        0.
     68.13
       .27         .59         .82        .92       .99      1.06      1.05
      1.04        1.06         .91
APIN                1.       .0001         0.        0.      .0001        0.
    136.24
        0.         .75         .75        0.        0.        0.        7.
        0.
       .14         .17         .21        .21       .23       .29       .29
       .29         .31         .27
UNKN                1.       .0001         0.        0.      .0001        0.
    136.24
        0.        .375        .875        0.        0.        0.       7.5
        0.
       .11         .15         .18        .19        .2       .53       .52
       .52         .56         .47
CRED                0.        -10.       250.
CO                  1.7          0.        .5      -20.        0.        .4
     48.76       47.05       45.10      46.11     48.65     27.39     27.76
     22.23       23.41       20.40
```

Table B-1 (continued)

Scenario ID	**ELPTX1**	**EL PASO, TX**	**9/ 7/88**
Latitude (deg):	31.77	Longtitude (deg):	106.50
Declination (deg):	5.96	Solar - clock time (min):	-63.51
Base ROG Input (mmolC/m2/day)	12.27	Initial Base ROG (% of input)	85.24
NOx Input (mmol/m2/day)	1.86	Initial NOx (% of input)	76.94

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.0304	0.0300	0.0154	0.0147	0.0138	0.0139	0.0144	0.0140	0.0143	0.0146	0.0156	0.0168
NOx	0.1411		0.0238	0.0234	0.0227	0.0229	0.0233	0.0223	0.0231	0.0232	0.0240	0.0219
Ozone		0.0650										
CH4	1.790	1.790										
CO	4.400	0.500	0.351	0.326	0.297	0.302	0.322	0.306	0.318	0.328	0.360	0.399
ISOP	0.0001		0.0001	0.0001	0.0003	0.0004	0.0007	0.0009	0.0012	0.0012	0.0012	0.0012
APIN	0.0001		0.0004	0.0004	0.0006	0.0006	0.0007	0.0007	0.0009	0.0009	0.0009	0.0009
UNKN	0.0001		0.0001	0.0001	0.0002	0.0002	0.0003	0.0004	0.0004	0.0004	0.0004	0.0004

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	596.	943.	1289.	1635.	1756.	1878.	2000.	2000.	2000.	2000.
T (deg K)	290.0	293.0	295.0	297.0	300.0	301.0	302.0	304.0	304.0	304.0	304.0
H2O (10^4 ppm)	1.057	1.054	1.056	1.014	0.999	0.963	0.748	0.801	0.801	0.763	1.107

OZIPM4 Input File

```
TITL
EL PASO, TX    BASE CASE SIMULATION    9/7/88
PLAC              31.77      106.50          6.      1988.          9.          7.
EL PASO, TX
DILU                250.       2000.          0.         0.          0.
TEMP                 11.        290.        293.       295.        297.        300.
       301.         302.        304.        304.       304.        304.        301.
WATE                 11.       26.01
        64.          53.         47.         40.        33.         30.         26.
        22.          21.         21.         20.        29.
TRAN                  0.        .065          0.        .03          0.        .002
MASS                -10.        1.03        .141       250.
      2.77         2.66        2.49        2.51       2.60        2.53        2.58
      2.64         2.81        3.03
      2.05         2.02        1.96        1.97       2.01        1.92        1.99
      2.00         2.07        1.89
BIOG                -10.          3.        250.
ISOP                  0.       .0001          0.         0.       .0001          0.
     68.13
       .01          .01         .02         .03        .05         .06         .08
       .08          .08         .08
APIN                  1.       .0001          0.         0.       .0001          0.
    136.24
        0.          .75         .75          0.         0.          0.          7.
        0.
       .06          .06         .08         .08         .1          .1         .12
       .12          .12         .12
UNKN                  1.       .0001          0.         0.       .0001          0.
    136.24
        0.         .375        .875          0.         0.          0.         7.5
        0.
       .02          .02         .03         .03        .04         .05         .05
       .05          .05         .05
CRED                  0.        -10.        250.
CO                  4.4           0.          .5       -20.          0.          .4
      9.91         9.21        8.37        8.52       9.07        8.64        8.96
      9.26        10.15       11.27
```

Table B-1 (continued)

Scenario ID	**HARCT1**	**HARTFORD, CT**	**7/ 8/88**
Latitude (deg):	41.79	Longtitude (deg):	72.63
Declination (deg):	22.45	Solar - clock time (min):	-55.56
Base ROG Input (mmolC/m2/day)	10.71	Initial Base ROG (% of input)	75.50
NOx Input (mmol/m2/day)	1.28	Initial NOx (% of input)	70.03

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.3801	0.0300	0.0329	0.0326	0.0312	0.0314	0.0321	0.0315	0.0319	0.0066	0.0071	0.0077
NOx	0.0420		0.0409	0.0404	0.0369	0.0369	0.0391	0.0338	0.0381	0.0101	0.0112	0.0123
Ozone		0.0780										
CH4	1.790	1.790										
CO	1.500	0.500	0.340	0.333	0.320	0.325	0.343	0.326	0.340	0.091	0.099	0.108
ISOP	0.0001		0.0063	0.0117	0.0156	0.0192	0.0223	0.0208	0.0198	0.0238	0.0179	0.0138
APIN	0.0001		0.0015	0.0018	0.0020	0.0022	0.0025	0.0025	0.0025	0.0030	0.0028	0.0025
UNKN	0.0001		0.0026	0.0032	0.0036	0.0040	0.0044	0.0044	0.0044	0.0066	0.0062	0.0054

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	524.	879.	1234.	1589.	1943.	2068.	2193.	2318.	2318.	2318.	2318.
T (deg K)	297.0	299.0	301.0	302.0	304.0	306.0	307.0	308.0	308.0	308.0	306.0
H2O (10^4 ppm)	2.062	2.126	2.170	2.066	2.142	2.203	2.020	2.081	1.971	2.410	2.595

OZIPM4 Input File

```
TITL
HARTFORD, CT BASE CASE SIMULATION  7/8/88
PLAC          41.79      72.63       4.     1988.       7.       8.
HARTFORD, CT
DILU           524.      2318.       0.       0.       0.
TEMP            11.       297.     299.     301.     302.     304.
      306.     307.       308.     308.     308.     306.     304.
WATE            11.      29.8
       71.       65.       59.      53.      49.      45.      41.
       39.       38.       36.      44.      53.
TRAN            0.        .078      0.       .03      0.       .002
MASS           -10.       .38      .042     524.
      5.18      5.14      4.91     4.94     5.05     4.96     5.03
      1.04      1.12      1.22
      2.42      2.39      2.18     2.18     2.31     2.00     2.25
        .6       .66       .73
BIOG           -10.        3.      524.
ISOP            0.        .0001     0.       0.       .0001    0.
     68.13
       .43       .8       1.07     1.32     1.53     1.43     1.36
      1.63      1.23       .95
APIN            1.        .0001     0.       0.       .0001    0.
    136.24
         0.      .75       .75      0.       0.       0.       7.
         0.
        .2       .25       .27      .3       .34      .34      .34
       .41       .39       .34
UNKN            1.        .0001     0.       0.       .0001    0.
    136.24
         0.      .375      .875     0.       0.       0.       7.5
         0.
       .35       .44       .49      .55      .61      .6       .61
        .9       .85       .74
CRED            0.       -10.      524.
CO             1.5         0.       .5      -20.      0.       .4
      9.59      9.40      9.03     9.17     9.67     9.19     9.58
      2.58      2.79      3.06
```

Table B-1 (continued)

Scenario ID	**HOUTX1**	**HOUSTON, TX**	**8/26/88**
Latitude (deg):	29.77	Longtitude (deg):	95.22
Declination (deg):	10.32	Solar - clock time (min):	-82.44
Base ROG Input (mmolC/m2/day)	25.47	Initial Base ROG (% of input)	68.41
NOx Input (mmol/m2/day)	4.19	Initial NOx (% of input)	44.53

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.4305	0.0300	0.0314	0.0315	0.0303	0.0305	0.0312	0.0307	0.0311	0.0316	0.0329	0.0347
NOx	0.1531		0.0565	0.0563	0.0552	0.0554	0.0564	0.0543	0.0560	0.0561	0.0575	0.0508
Ozone		0.0650										
CH4	1.790	1.790										
CO	1.500	0.500	0.933	0.907	0.858	0.875	0.927	0.887	0.921	0.938	1.001	1.086
ISOP	0.0001		0.0031	0.0068	0.0106	0.0121	0.0137	0.0127	0.0106	0.0073	0.0064	0.0051
APIN	0.0001		0.0009	0.0010	0.0012	0.0013	0.0015	0.0015	0.0015	0.0017	0.0015	0.0014
UNKN	0.0001		0.0010	0.0014	0.0017	0.0018	0.0021	0.0019	0.0018	0.0018	0.0017	0.0016

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	300.	587.	873.	1160.	1446.	1546.	1647.	1748.	1748.	1748.	1748.
T (deg K)	297.0	300.0	302.0	304.0	305.0	307.0	307.0	308.0	309.0	307.0	307.0
H2O (10^4 ppm)	2.668	2.909	2.918	2.793	2.495	2.275	2.275	2.460	2.658	2.482	2.585

OZIPM4 Input File

```
TITL
HOUSTON, TX  BASE CASE SIMULATION   8/26/88
PLAC          29.77     95.22        5.      1988.       8.       26.
HOUSTON, TX
DILU                     300.      1748.       0.         0.       0.
TEMP                      11.       297.     300.       302.     304.     305.
      307.       307.      308.     309.       307.     307.     306.
WATE                      11.     29.75
        92.        84.       75.      64.       54.      44.      44.
        44.        45.       46.      48.       50.
TRAN                       0.      .065        0.       .03       0.      .002
MASS                     -10.      1.43      .153      300.
     11.75      11.80     11.33    11.42     11.68    11.50    11.64
     11.82      12.32     13.01
     10.96      10.92     10.71    10.75     10.94    10.54    10.87
     10.88      11.15      9.85
BIOG                     -10.        3.      300.
ISOP                       0.      .0001       0.         0.    .0001       0.
     68.13
       .21        .47       .73      .83       .94      .87      .73
        .5        .44       .35
APIN                       1.      .0001       0.         0.    .0001       0.
    136.24
         0.        .75       .75      0.        0.       0.       7.
         0.
       .12        .14       .17      .18       .21      .21      .21
       .23        .21       .19
UNKN                       1.      .0001       0.         0.    .0001       0.
    136.24
         0.        .375      .875     0.        0.       0.       7.5
         0.
       .14        .19       .23      .25       .29      .26      .25
       .25        .24       .22
CRED                       0.      -10.      300.
CO                       1.5         0.        .5      -20.       0.       .4
     26.33      25.60     24.21    24.69     26.14    25.03    25.97
     26.45      28.23     30.65
```

Table B-1 (continued)

Scenario ID	**INDIN1**	**INDIANAPOLIS, IN**	**7/28/88**
Latitude (deg):	39.78	Longtitude (deg):	86.15
Declination (deg):	18.94	Solar - clock time (min):	-111.10
Base ROG Input (mmolC/m2/day)	12.06	Initial Base ROG (% of input)	58.95
NOx Input (mmol/m2/day)	1.82	Initial NOx (% of input)	32.45

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.7003	0.0300	0.0656	0.0651	0.0629	0.0632	0.0645	0.0635	0.0060	0.0062	0.0065	0.0069
NOx	0.0580		0.1074	0.1087	0.1055	0.1056	0.1081	0.1003	0.0094	0.0096	0.0101	0.0108
Ozone		0.0520										
CH4	1.790	1.790										
CO	2.300	0.500	0.974	0.955	0.926	0.942	0.990	0.952	0.104	0.107	0.114	0.125
ISOP	0.0001		0.0012	0.0020	0.0038	0.0050	0.0061	0.0076	0.0032	0.0031	0.0034	0.0029
APIN	0.0001		0.0008	0.0010	0.0012	0.0013	0.0014	0.0015	0.0023	0.0023	0.0025	0.0023
UNKN	0.0001		0.0008	0.0011	0.0014	0.0015	0.0017	0.0018	0.0061	0.0061	0.0067	0.0061

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	532.	814.	1096.	1377.	1477.	1576.	1675.	1675.	1675.	1675.
T (deg K)	295.0	298.0	301.0	302.0	303.0	304.0	305.0	305.0	306.0	305.0	305.0
H2O (10^4 ppm)	1.947	1.937	1.841	1.875	1.864	1.845	1.681	1.499	1.730	1.772	1.908

OZIPM4 Input File

```
TITL
INDIANAPOLIS, IN   BASE CASE SIMULATION  7/28/88
PLAC            39.78      86.15         4.      1988.         7.        28.
INDIANAPOLIS, IN
DILU              250.       1675.        0.         0.         0.
TEMP               11.        295.      298.       301.       302.      303.
      304.        305.        305.      306.       305.       305.      304.
WATE               11.     29.255
       77.         64.         51.       49.        46.        43.       40.
       37.         33.         36.       39.        42.
TRAN                0.        .052        0.        .03         0.       .002
MASS              -10.         .70      .058       250.
     11.63       11.54       11.15     11.20      11.44      11.25      1.07
      1.10        1.15        1.23
      9.03        9.14        8.87      8.88       9.09       8.43       .79
       .81         .85         .91
BIOG              -10.          3.      250.
ISOP                0.       .0001        0.         0.       .0001        0.
     68.13
       .08         .14         .26       .34        .42        .52       .22
       .21         .23          .2
APIN                1.       .0001        0.         0.       .0001        0.
    136.24
         0.         .75         .75        0.         0.         0.        7.
         0.
       .11         .14         .17       .18        .19        .21       .32
       .32         .34         .32
UNKN                1.       .0001        0.         0.       .0001        0.
    136.24
         0.        .375        .875        0.         0.         0.       7.5
         0.
       .11         .15         .19       .21        .23        .25       .84
       .84         .92         .84
CRED                0.        -10.      250.
CO                2.3           0.        .5        -20.         0.        .4
     27.48       26.94       26.12     26.57      27.92      26.86      2.94
      3.01        3.23        3.53
```

Table B-1 (continued)

Scenario ID	**JACFL1**	**JACKSONVILLE, FL**	**5/ 7/87**
Latitude (deg):	30.36	Longtitude (deg):	81.64
Declination (deg):	16.60	Solar - clock time (min):	-82.90
Base ROG Input (mmolC/m2/day)	7.73	Initial Base ROG (% of input)	63.07
NOx Input (mmol/m2/day)	1.01	Initial NOx (% of input)	41.07

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.4802	0.0300	0.0370	0.0376	0.0349	0.0349	0.0358	0.0354	0.0359	0.0369	0.0392	0.0418
NOx	0.0410		0.0607	0.0611	0.0569	0.0562	0.0584	0.0524	0.0575	0.0586	0.0620	0.0656
Ozone		0.0400										
CH4	1.790	1.790										
CO	1.500	0.500	0.442	0.422	0.384	0.384	0.405	0.397	0.408	0.422	0.459	0.498
ISOP	0.0001		0.0022	0.0032	0.0057	0.0074	0.0071	0.0076	0.0073	0.0076	0.0071	0.0047
APIN	0.0001		0.0007	0.0009	0.0012	0.0013	0.0013	0.0014	0.0014	0.0014	0.0014	0.0012
UNKN	0.0001		0.0009	0.0013	0.0017	0.0018	0.0018	0.0018	0.0018	0.0018	0.0018	0.0015

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	494.	739.	983.	1227.	1313.	1399.	1485.	1485.	1485.	1485.
T (deg K)	287.0	291.0	295.0	299.0	300.0	300.0	301.0	301.0	301.0	301.0	299.0
H2O (10^4 ppm)	1.418	1.521	1.556	1.482	1.537	1.537	1.592	1.629	1.629	1.777	1.712

OZIPM4 Input File

```
TITL
JACKSONVILLE, FL  BASE CASE SIMULATION   5/7/87
PLAC          30.36      81.64        4.      1987.        5.        7.
JACKSONVILLE, FL
DILU             250.      1485.       0.         0.        0.
TEMP              11.       287.      291.       295.      299.      300.
      300.       301.       301.      301.       301.      299.      297.
WATE              11.     30.000
       90.        75.        60.       45.        44.       44.       43.
       43.        44.        44.       48.        52.
TRAN               0.        .04        0.       .03        0.      .002
MASS             -10.        .48      .041       250.
     4.20       4.27       3.97      3.96       4.07      4.02      4.08
     4.19       4.45       4.75
     2.85       2.87       2.67      2.64       2.74      2.46      2.70
     2.75       2.91       3.08
BIOG             -10.         3.      250.
ISOP               0.      .0001        0.         0.     .0001        0.
    68.13
      .15        .22        .39       .51        .49       .52        .5
      .52        .49        .32
APIN               1.      .0001        0.         0.     .0001.       0.
   136.24
        0.        .75        .75       0.         0.        0.        7.
        0.
       .1         .13        .17       .18        .18       .19       .19
      .19         .19        .16
UNKN               1.      .0001        0.         0.     .0001        0.
   136.24
        0.        .375       .875      0.         0.        0.       7.5
        0.
      .12         .18        .23       .25        .25       .25       .25
      .25         .25        .21
CRED               0.       -10.      250.
CO               1.5          0.        .5        -20.       0.        .4
    12.46      11.91      10.84     10.82      11.43     11.21     11.51
    11.90      12.94      14.05
```

Table B-1 (continued)

Scenario ID	**KANMO1**	**KANSAS CITY, MO**	**8/ 7/87**
Latitude (deg):	39.10	Longtitude (deg):	94.57
Declination (deg):	16.63	Solar - clock time (min):	-84.15
Base ROG Input (mmolC/m2/day)	9.07	Initial Base ROG (% of input)	73.66
NOx Input (mmol/m2/day)	1.28	Initial NOx (% of input)	61.13

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.4702	0.0300	0.0478	0.0480	0.0459	0.0170	0.0172	0.0171	0.0171	0.0173	0.0177	0.0183
NOx	0.0550		0.0986	0.0987	0.0962	0.0135	0.0137	0.0127	0.0135	0.0137	0.0140	0.0142
Ozone		0.0650										
CH4	1.790	1.790										
CO	1.200	0.500	0.581	0.558	0.536	0.102	0.104	0.101	0.104	0.105	0.108	0.113
ISOP	0.0001		0.0006	0.0010	0.0017	0.0016	0.0020	0.0026	0.0028	0.0031	0.0029	0.0029
APIN	0.0001		0.0007	0.0009	0.0010	0.0012	0.0012	0.0014	0.0015	0.0017	0.0016	0.0016
UNKN	0.0001		0.0006	0.0007	0.0009	0.0012	0.0012	0.0015	0.0016	0.0020	0.0018	0.0018

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	350.	716.	1082.	1448.	1814.	1942.	2071.	2200.	2200.	2200.	2200.
T (deg K)	296.0	298.0	300.0	302.0	304.0	305.0	306.0	308.0	310.0	309.0	309.0
H2O (10^4 ppm)	2.119	2.209	2.251	2.340	2.456	2.420	1.992	1.909	2.191	2.130	2.242

OZIPM4 Input File

```
TITL
KANSAS CITY, MO   BASE CASE SIMULATION   8/7/87
PLAC          39.10      94.57         5.      1987.         8.         7.
KANSAS CITY, MO
DILU             350.       2200.        0.         0.         0.
TEMP              11.        296.       298.       300.       302.       304.
      305.        306.       308.       310.       309.       309.       308.
WATE              11.      28.86
       80.         74.        67.        62.        58.        54.        48.
       42.         36.        37.        38.        40.
TRAN               0.        .065         0.        .03         0.        .002
MASS             -10.         .47        .055       350.
     6.38        6.40       6.12       2.27       2.29       2.28       2.28
     2.31        2.36       2.44
     5.84        5.85       5.70        .80        .81        .75        .80
      .81         .83        .84
BIOG             -10.          3.       350.
ISOP               0.       .0001         0.         0.      .0001         0.
    68.13
      .04         .07        .12        .11        .14        .18        .19
      .21          .2         .2
APIN               1.       .0001         0.         0.      .0001         0.
   136.24
        0.         .75        .75         0.         0.         0.         7.
        0.
       .1         .12        .14        .16        .16        .19         .2
      .23         .22        .22
UNKN               1.       .0001         0.         0.      .0001         0.
   136.24
        0.        .375       .875         0.         0.         0.        7.5
        0.
      .08          .1        .12        .16        .17         .2        .22
      .27         .25        .25
CRED               0.        -10.       350.
CO               1.2          0.         .5        -20.         0.         .4
    16.39       15.75      15.13       2.88       2.94       2.86       2.92
     2.96        3.06       3.19
SPEC               1.
O3
PLOT               0.         0.         0.         0.         0.         0.
ISOP               0.         0.         1.         0.         1.
      .13
```

Table B-1 (continued)

Scenario ID	**LAKLA1**	**LAKE CHARLES, LA**	**7/26/88**
Latitude (deg):	30.22	Longtitude (deg):	93.22
Declination (deg):	19.38	Solar - clock time (min):	-79.40
Base ROG Input (mmolC/m2/day)	6.96	Initial Base ROG (% of input)	72.91
NOx Input (mmol/m2/day)	0.94	Initial NOx (% of input)	24.88

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr)									
			Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.5002	0.0300	0.0273	0.0271	0.0268	0.0268	0.0270	0.0268	0.0269	0.0271	0.0275	0.0279
NOx	0.0230		0.0754	0.0754	0.0750	0.0750	0.0754	0.0743	0.0752	0.0752	0.0759	0.0743
Ozone		0.0400										
CH4	1.790	1.790										
CO	1.500	0.500	0.071	0.071	0.069	0.069	0.073	0.068	0.072	0.073	0.078	0.084
ISOP	0.0001		0.0017	0.0028	0.0038	0.0034	0.0041	0.0041	0.0041	0.0041	0.0052	0.0057
APIN	0.0001		0.0010	0.0011	0.0012	0.0012	0.0013	0.0013	0.0013	0.0013	0.0014	0.0014
UNKN	0.0001		0.0012	0.0014	0.0016	0.0015	0.0017	0.0017	0.0017	0.0017	0.0018	0.0019

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	291.	332.	373.	414.	428.	443.	457.	457.	457.	457.
T (deg K)	297.0	298.0	299.0	300.0	301.0	302.0	302.0	302.0	302.0	302.0	302.0
H2O (10^4 ppm)	2.695	2.705	2.705	2.763	2.818	2.830	2.908	2.947	2.908	2.830	2.751

OZIPM4 Input File

```
TITL
LAKE CHARLES, LA   BASE CASE SIMULATION   7/26/88
PLAC          30.22      93.22         5.      1988.         7.        26.
LAKE CHARLES, LA
DILU                   250.       457.         0.         0.         0.
TEMP                    11.       297.       298.       299.       300.       301.
      302.       302.       302.       302.       302.       303.
WATE                    11.     30.05
       92.        87.        82.        79.        76.        72.        73.
       74.        75.        74.        72.        70.
TRAN                     0.       .04         0.       .03         0.       .002
MASS                   -10.       .50       .023       250.
      2.79       2.77       2.74       2.74       2.76       2.74       2.75
      2.77       2.81       2.86
      3.28       3.28       3.26       3.26       3.28       3.23       3.27
      3.27       3.30       3.23
BIOG                   -10.         3.       250.
ISOP                     0.      .0001         0.         0.      .0001         0.
     68.13
       .12        .19        .26        .23        .28        .28        .28
       .28        .36        .39
APIN                     1.      .0001         0.         0.      .0001         0.
    136.24
         0.        .75        .75         0.         0.         0.         7.
         0.
       .14        .15        .16        .17        .18        .18        .18
       .18        .19        .19
UNKN                     1.      .0001         0.         0.      .0001         0.
    136.24
         0.       .375       .875         0.         0.         0.       7.5
         0.
       .17        .19        .22        .21        .23        .23        .23
       .23        .25        .26
CRED                     0.       -10.       250.
CO                     1.5         0.         .5       -20.         0.         .4
      2.01       2.00       1.94       1.96       2.05       1.93       2.03
      2.07       2.20       2.36
```

Table B-1 (continued)

Scenario ID	**LOSCA1**	**LOS ANGELES**	**9/ 3/88**
Latitude (deg):	34.04	Longtitude (deg):	118.24
Declination (deg):	7.43	Solar - clock time (min):	-51.88
Base ROG Input (mmolC/m2/day)	23.05	Initial Base ROG (% of input)	71.03
NOx Input (mmol/m2/day)	3.04	Initial NOx (% of input)	70.14

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr)									
			Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.3305	0.0300	0.0291	0.0295	0.0282	0.0283	0.0290	0.0284	0.0285	0.0280	0.0294	0.0313
NOx	0.1731		0.0314	0.0306	0.0284	0.0284	0.0295	0.0271	0.0290	0.0295	0.0314	0.0333
Ozone		0.1000										
CH4	1.790	1.790										
CO	4.000	0.500	0.794	0.756	0.716	0.729	0.770	0.750	0.765	0.782	0.844	0.926
ISOP	0.0001		0.0026	0.0045	0.0085	0.0093	0.0112	0.0120	0.0114	0.0096	0.0079	0.0061
APIN	0.0001		0.0008	0.0009	0.0012	0.0013	0.0016	0.0017	0.0017	0.0015	0.0014	0.0012
UNKN	0.0001		0.0007	0.0009	0.0012	0.0013	0.0015	0.0017	0.0016	0.0014	0.0012	0.0011

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	303.	343.	382.	422.	461.	475.	489.	503.	503.	503.	503.
T (deg K)	298.0	301.0	305.0	306.0	309.0	311.0	310.0	308.0	307.0	306.0	305.0
H2O (10^4 ppm)	2.427	2.455	2.536	2.146	2.307	2.317	2.011	1.855	1.806	1.805	1.752

OZIPM4 Input File

```
TITL
LOS ANGELES, CA   BASE CASE SIMULATION   9/3/88
PLAC          34.04     118.24        7.     1988.        9.        3.
LOS ANGELES
DILU           303.       503.       0.        0.        0.
TEMP            11.        298.      301.      305.      306.      309.
      311.      310.       308.      307.      306.      305.      304.
WATE            11.      29.69
       79.       67.        55.       44.       40.       36.       32.
       33.       34.        35.       37.       38.
TRAN            0.         .10       0.        .03       0.        .002
MASS           -10.       1.46      .190      303.
     10.82     10.97      10.47     10.53     10.77     10.55     10.60
     10.42     10.95      11.64
      4.85      4.72       4.38      4.38      4.56      4.19      4.48
      4.56      4.85       5.14
BIOG           -10.         3.      303.
ISOP            0.         .0001      0.        0.        .0001     0.
     68.13
       .18       .31        .58       .64       .77       .82       .78
       .66       .54        .42
APIN            1.         .0001      0.        0.        .0001     0.
    136.24
        0.       .75        .75       0.        0.        0.        7.
        0.
       .11       .13        .17       .18       .22       .24       .23
       .20       .19        .17
UNKN            1.         .0001      0.        0.        .0001     0.
    136.24
        0.       .375       .875      0.        0.        0.        7.5
        0.
       .10       .13        .17       .18       .21       .24       .22
       .19       .17        .15
CRED            0.        -10.       303.
CO             4.0         0.         .5       -20.       0.        .4
     22.41     21.33      20.20     20.56     21.72     21.16     21.58
     22.06     23.82      26.13
CALC           1.33        .173      0.        0.        0.
```

Table B-1 (continued)

Scenario ID	**LOUKY1**	**LOUISVILLE, KY**	**6/13/88**
Latitude (deg):	38.14	Longtitude (deg):	85.69
Declination (deg):	23.23	Solar - clock time (min):	-102.78
Base ROG Input (mmolC/m2/day)	13.74	Initial Base ROG (% of input)	59.86
NOx Input (mmol/m2/day)	2.48	Initial NOx (% of input)	22.49

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.8103	0.0300	0.0507	0.0497	0.0471	0.0470	0.0480	0.0476	0.0480	0.0488	0.0077	0.0069
NOx	0.0550		0.0978	0.0972	0.0940	0.0936	0.0948	0.0915	0.0938	0.0941	0.0089	0.0094
Ozone		0.0750										
CH4	1.790	1.790										
CO	2.000	0.500	0.777	0.732	0.674	0.673	0.713	0.697	0.715	0.744	0.120	0.132
ISOP	0.0001		0.0017	0.0029	0.0048	0.0061	0.0086	0.0109	0.0109	0.0251	0.0239	0.0208
APIN	0.0001		0.0006	0.0008	0.0010	0.0010	0.0012	0.0014	0.0014	0.0021	0.0020	0.0019
UNKN	0.0001		0.0007	0.0009	0.0012	0.0013	0.0015	0.0017	0.0017	0.0058	0.0058	0.0053

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	699.	1148.	1597.	2044.	2202.	2360.	2518.	2518.	2518.	2518.
T (deg K)	290.0	293.0	296.0	300.0	301.0	303.0	305.0	305.0	306.0	306.0	305.0
H2O (10^4 ppm)	1.527	1.612	1.662	1.762	1.685	1.645	1.521	1.521	1.561	1.609	1.567

OZIPM4 Input File

```
TITL
LOUISVILLE, KY  BASE CASE SIMULATION  6/13/88
PLAC          38.14       85.69          4.       1988.          6.          13.
LOUISVILLE, KY
DILU                250.        2518.          0.          0.          0.
TEMP                 11.         290.         293.         296.        300.        301.
      303.          305.         305.         306.         306.        305.        305.
WATE                 11.       29.68
       81.           71.          61.          51.          46.         40.         34.
       33.           33.          32.          33.          34.
TRAN                  0.         .075           0.         .03          0.         .002
MASS                -10.          .81         .055         250.
     10.25         10.03         9.51         9.49         9.70        9.61        9.70
      9.85          1.55         1.39
     11.25         11.18        10.81        10.77        10.90       10.53       10.79
     10.83          1.02         1.08
BIOG                -10.           3.         250.
ISOP                  0.        .0001           0.          0.        .0001          0.
     68.13
       .12            .2          .33          .42          .59         .75         .75
      1.72          1.64         1.43
APIN                  1.        .0001           0.          0.        .0001          0.
    136.24
         0.          .75          .75           0.          0.          0.          7.
         0.
       .08           .11          .14          .14          .17         .19         .19
       .29           .28          .26
UNKN                  1.        .0001           0.          0.        .0001          0.
    136.24
         0.          .375         .875          0.          0.          0.         7.5
         0.
       .09           .13          .17          .18          .21         .24         .24
        .8           .79          .73
CRED                  0.         -10.         250.
CO                  2.0            0.          .5         -20.          0.          .4
     21.92         20.66        19.02        18.99        20.11       19.66       20.18
     20.98          3.39         3.71
```

Table B-1 (continued)

Scenario ID	**MEMTN1**	**MEMPHIS, TN**	**6/24/87**
Latitude (deg):	35.13	Longtitude (deg):	90.04
Declination (deg):	23.43	Solar - clock time (min):	-62.35
Base ROG Input (mmolC/m2/day)	14.90	Initial Base ROG (% of input)	76.05
NOx Input (mmol/m2/day)	2.20	Initial NOx (% of input)	55.47

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr)									
			Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.9303	0.0300	0.0241	0.0242	0.0232	0.0232	0.0236	0.0231	0.0234	0.0237	0.0248	0.0262
NOx	0.1000		0.0461	0.0459	0.0435	0.0429	0.0441	0.0411	0.0436	0.0442	0.0460	0.0479
Ozone		0.0580										
CH4	1.790	1.790										
CO	2.700	0.500	0.447	0.432	0.407	0.406	0.421	0.397	0.414	0.413	0.445	0.481
ISOP	0.0001		0.0044	0.0061	0.0067	0.0074	0.0083	0.0082	0.0079	0.0073	0.0063	0.0047
APIN	0.0001		0.0018	0.0021	0.0022	0.0023	0.0023	0.0023	0.0023	0.0023	0.0021	0.0019
UNKN	0.0001		0.0015	0.0019	0.0019	0.0020	0.0020	0.0020	0.0020	0.0019	0.0017	0.0016

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	300.	587.	874.	1161.	1447.	1548.	1649.	1750.	1750.	1750.	1750.
T (deg K)	297.0	300.0	302.0	302.0	304.0	305.0	305.0	305.0	305.0	304.0	303.0
H2O (10^4 ppm)	2.425	2.552	2.440	2.324	2.477	2.484	2.576	2.622	2.576	2.433	2.257

OZIPM4 Input File

```
TITL
MEMPHIS, TN    BASE CASE SIMULATION   6/24/87
PLAC             35.13      90.04        5.      1987.        6.        24.
MEMPHIS, TN
DILU              300.       1750.        0.         0.        0.
TEMP               11.        297.       300.       302.      302.       304.
      305.        305.        305.       305.       304.      303.       302.
WATE               11.       29.62
       84.         74.         63.        60.        57.       54.        55.
       56.         57.         56.        56.        55.
TRAN                0.        .058         0.        .03        0.        .002
MASS              -10.         .93        .100       300.
      5.27        5.30        5.09       5.08       5.17      5.05       5.13
      5.20        5.43        5.74
      4.69        4.67        4.43       4.37       4.49      4.18       4.44
      4.50        4.68        4.87
BIOG              -10.          3.        300.
ISOP                0.       .0001         0.         0.      .0001         0.
     68.13
        .3         .42         .46        .51        .57       .56        .54
        .5         .43         .32
APIN                1.       .0001         0.         0.      .0001         0.
    136.24
         0.         .75         .75        0.         0.        0.         7.
         0.
        .25         .29          .3        .31        .32       .32        .32
        .31         .29         .26
UNKN                1.       .0001         0.         0.      .0001         0.
    136.24
         0.        .375        .875        0.         0.        0.         7.5
         0.
        .21         .26         .26        .27        .28       .28        .27
        .26         .24         .22
CRED                0.        -10.        300.
CO                2.7           0.          .5       -20.        0.         .4
     12.62       12.18       11.48      11.45      11.87     11.20      11.67
     11.66       12.55       13.57
```

Table B-1 (continued)

Scenario ID	**MIAFL1**	**MIAMI, FL**	**4/22/87**
Latitude (deg):	25.74	Longtitude (deg):	80.16
Declination (deg):	11.94	Solar - clock time (min):	-79.06
Base ROG Input (mmolC/m2/day)	9.47	Initial Base ROG (% of input)	75.06
NOx Input (mmol/m2/day)	0.98	Initial NOx (% of input)	61.94

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.7003	0.0300	0.0249	0.0251	0.0234	0.0233	0.0241	0.0237	0.0242	0.0249	0.0268	0.0289
NOx	0.0600		0.0402	0.0388	0.0358	0.0356	0.0369	0.0340	0.0367	0.0377	0.0410	0.0439
Ozone		0.0570										
CH4	1.790	1.790										
CO	3.200	0.500	0.339	0.321	0.294	0.294	0.313	0.302	0.316	0.329	0.364	0.402
ISOP	0.0001		0.0013	0.0025	0.0036	0.0061	0.0074	0.0099	0.0085	0.0070	0.0054	0.0042
APIN	0.0001		0.0021	0.0029	0.0034	0.0039	0.0042	0.0046	0.0043	0.0040	0.0037	0.0034
UNKN	0.0001		0.0015	0.0020	0.0023	0.0028	0.0029	0.0033	0.0031	0.0028	0.0026	0.0024

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	739.	1228.	1716.	2204.	2376.	2548.	2720.	2720.	2720.	2720.
T (deg K)	293.0	295.0	297.0	300.0	301.0	303.0	305.0	304.0	303.0	302.0	301.0
H2O (10^4 ppm)	1.925	1.890	1.811	1.779	1.627	1.536	1.628	1.758	1.909	1.959	2.034

OZIPM4 Input File

```
TITL
MIAMI, FL   BASE CASE SIMULATION   4/22/87
PLAC          25.74     80.16        4.      1987.       4.       22.
MIAMI, FL
DILU                   250.     2720.        0.        0.        0.
TEMP                    11.      293.      295.      297.      300.      301.
       303.      305.      304.      303.      302.      301.      300.
WATE                    11.    29.96
         84.       73.       62.       51.       44.       37.       30.
         35.       40.       46.       50.       55.
TRAN                     0.     .057        0.      .03        0.      .002
MASS                   -10.      .70      .060      250.
       3.47      3.49      3.26      3.25      3.35      3.30      3.37
       3.47      3.73      4.02
       1.83      1.77      1.63      1.62      1.68      1.55      1.67
       1.72      1.87      2.00
BIOG                   -10.        3.      250.
ISOP                     0.     .0001        0.        0.     .0001        0.
      68.13
        .09       .17       .25       .42       .51       .68       .58
        .48       .37       .29
APIN                     1.     .0001        0.        0.     .0001        0.
     136.24
          0.       .75       .75        0.        0.        0.        7.
          0.
        .29        .4       .46       .53       .57       .63       .59
        .55       .51       .47
UNKN                     1.     .0001        0.        0.     .0001        0.
     136.24
          0.      .375      .875        0.        0.        0.       7.5
          0.
         .2       .28       .32       .38        .4       .45       .42
        .39       .36       .33
CRED                     0.      -10.      250.
CO                      3.2        0.        .5      -20.        0.        .4
        9.56      9.06      8.28      8.28      8.83      8.52      8.91
        9.28     10.28     11.35
```

Table B-1 (continued)

Scenario ID	**NASTN1**	**NASHVILLE, TN**	**6/22/86**
Latitude (deg):	36.15	Longtitude (deg):	86.81
Declination (deg):	23.44	Solar - clock time (min):	-48.99
Base ROG Input (mmolC/m2/day)	7.36	Initial Base ROG (% of input)	77.22
NOx Input (mmol/m2/day)	0.91	Initial NOx (% of input)	36.63

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.5602	0.0300	0.0529	0.0539	0.0515	0.0102	0.0110	0.0100	0.0102	0.0090	0.0094	0.0099
NOx	0.0330		0.0784	0.0812	0.0748	0.0562	0.0566	0.0557	0.0566	0.0571	0.0581	0.0590
Ozone		0.0500										
CH4	1.790	1.790										
CO	1.800	0.500	0.341	0.345	0.335	0.074	0.077	0.073	0.076	0.078	0.084	0.091
ISOP	0.0001		0.0074	0.0118	0.0168	0.0187	0.0198	0.0198	0.0191	0.0185	0.0168	0.0154
APIN	0.0001		0.0018	0.0020	0.0023	0.0015	0.0016	0.0016	0.0015	0.0015	0.0015	0.0015
UNKN	0.0001		0.0023	0.0027	0.0031	0.0034	0.0036	0.0036	0.0036	0.0035	0.0033	0.0032

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	519.	787.	1056.	1324.	1419.	1513.	1608.	1608.	1608.	1608.
T (deg K)	297.0	300.0	302.0	304.0	306.0	307.0	307.0	307.0	307.0	306.0	306.0
H2O (10^4 ppm)	2.410	2.433	2.272	2.203	2.128	1.893	1.791	1.688	1.842	1.887	2.032

OZIPM4 Input File

```
TITL
NASHVILLE, TN   BASE CASE SIMULATION   6/22/86
PLAC          36.15      86.81        5.      1986.        6.       22.
NASHVILLE, TN
DILU            250.      1608.        0.         0.        0.
TEMP             11.       297.      300.       302.      304.      306.
      307.       307.       307.      307.       306.      306.      305.
WATE             11.     29.44
       84.        71.        59.       51.        44.       37.       36.
       35.        33.        36.       39.        42.
TRAN              0.        .05        0.        .03        0.      .002
MASS            -10.        .56      .033       250.
      5.73       5.83       5.57      1.10       1.19      1.08      1.10
       .97       1.02       1.07
      3.32       3.44       3.17      2.38       2.40      2.36      2.40
      2.42       2.46       2.50
BIOG            -10.         3.       250.
ISOP              0.      .0001         0.         0.      .0001        0.
     68.13
       .51        .81       1.15      1.28       1.36      1.36      1.31
      1.27       1.15       1.06
APIN              1.      .0001         0.         0.      .0001.       0.
    136.24
         0.        .75        .75        0.         0.        0.        7.
         0.
       .25        .28        .32       .21        .22       .22       .21
       .21         .2         .2
UNKN              1.      .0001         0.         0.      .0001        0.
    136.24
         0.       .375       .875        0.         0.        0.       7.5
         0.
       .31        .37        .42       .47         .5        .5       .49
       .48        .45        .44
CRED              0.       -10.       250.
CO              1.8          0.         .5       -20.        0.        .4
      9.61       9.74       9.45      2.08       2.16      2.05      2.13
      2.19       2.36       2.56
```

Table B-1 (continued)

Scenario ID	**NEWNY1**	**NEW YORK, NY**	**6/22/88**
Latitude (deg):	40.74	Longtitude (deg):	73.99
Declination (deg):	23.44	Solar - clock time (min):	-57.92
Base ROG Input (mmolC/m2/day)	39.19	Initial Base ROG (% of input)	51.83
NOx Input (mmol/m2/day)	4.85	Initial NOx (% of input)	49.66

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	2.0007	0.0300	0.3021	0.0930	0.0127	0.0128	0.0098	0.0097	0.0098	0.0100	0.0106	0.0113
NOx	0.2371		0.2922	0.0920	0.0143	0.0144	0.0146	0.0134	0.0143	0.0148	0.0160	0.0174
Ozone		0.1030										
CH4	1.790	1.790										
CO	2.900	0.500	6.228	3.075	0.448	0.455	0.430	0.411	0.426	0.436	0.468	0.510
ISOP	0.0001		0.0025	0.0032	0.0017	0.0022	0.0090	0.0047	0.0039	0.0032	0.0028	0.0026
APIN	0.0001		0.0009	0.0009	0.0009	0.0009	0.0015	0.0014	0.0013	0.0012	0.0012	0.0012
UNKN	0.0001		0.0002	0.0001	0.0002	0.0003	0.0023	0.0019	0.0018	0.0017	0.0015	0.0015

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	500.	749.	999.	1249.	1336.	1424.	1512.	1512.	1512.	1512.
T (deg K)	300.0	300.0	301.0	301.0	302.0	302.0	302.0	301.0	300.0	299.0	299.0
H2O (10^4 ppm)	2.185	2.219	2.353	2.390	2.493	2.493	2.571	2.573	2.566	2.452	2.518

OZIPM4 Input File

```
TITL
NEW YORK, NY    BASE CASE SIMULATION    6/22/88
PLAC            40.74       73.99       4.      1988.       6.      22.
NEW YORK, NY
DILU             250.       1512.       0.        0.        0.
TEMP              11.        300.       300.      301.      301.     302.
      302.       302.        301.       300.      299.      299.     298.
WATE              11.       29.79
       63.        64.         64.       65.       64.       64.      63.
       66.        70.         74.       75.       77.
TRAN               0.        .103        0.        .03       0.      .002
MASS             -10.        2.00       .237      250.
     174.01      53.58        7.33       7.38      5.65      5.57     5.62
       5.75       6.08        6.50
      65.59      20.66        3.20       3.23      3.28      3.01     3.22
       3.32       3.60        3.91
BIOG             -10.          3.        250.
ISOP               0.        .0001        0.        0.      .0001      0.
      68.13
        .17        .22         .12        .15       .62       .32      .27
        .22        .19         .18
APIN               1.        .0001        0.        0.      .0001      0.
     136.24
          0.       .75         .75        0.        0.        0.       7.
          0.
        .12        .12         .12        .12       .21       .19      .18
        .17        .16         .16
UNKN               1.        .0001        0.        0.      .0001      0.
     136.24
          0.       .375        .875       0.        0.        0.      7.5
          0.
       .022        .011         .03       .04       .31       .26      .25
        .23        .21          .21
CRED               0.         -10.       250.
CO                2.9           0.         .5      -20.        0.       .4
     175.69      86.75        12.63      12.83     12.12     11.60    12.01
      12.31      13.20        14.40
```

Table B-1 (continued)

Scenario ID	**PHIPA1**	**PHILADELPHIA, PA**	**7/29/88**
Latitude (deg):	39.96	Longtitude (deg):	75.17
Declination (deg):	18.70	Solar - clock time (min):	-67.15
Base ROG Input (mmolC/m2/day)	19.01	Initial Base ROG (% of input)	25.12
NOx Input (mmol/m2/day)	3.07	Initial NOx (% of input)	24.13

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.4702	0.0300	0.1580	0.1649	0.1613	0.0579	0.0589	0.0586	0.0213	0.0216	0.0226	0.0238
NOx	0.0730		0.1512	0.1496	0.1418	0.0627	0.0644	0.0617	0.0306	0.0307	0.0323	0.0336
Ozone		0.0530										
CH4	1.790	1.790										
CO	1.300	0.500	2.816	2.813	2.828	0.974	1.037	1.021	0.508	0.521	0.563	0.618
ISOP	0.0001		0.0017	0.0022	0.0038	0.0048	0.0060	0.0086	0.0101	0.0099	0.0095	0.0079
APIN	0.0001		0.0009	0.0009	0.0010	0.0011	0.0012	0.0014	0.0018	0.0018	0.0018	0.0018
UNKN	0.0001		0.0001	0.0001	0.0001	0.0006	0.0007	0.0007	0.0041	0.0041	0.0040	0.0036

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	557.	863.	1170.	1476.	1584.	1692.	1800.	1800.	1800.	1800.
T (deg K)	297.0	299.0	300.0	302.0	303.0	304.0	306.0	306.0	306.0	306.0	305.0
H2O (10^4 ppm)	2.933	3.039	2.943	2.952	2.918	2.870	2.967	2.967	2.967	2.967	2.851

OZIPM4 Input File

```
TITL
PHILADELPHIA, PA   BASE CASE SIMULATION   7/29/88
PLAC          39.96       75.17          4.       1988.          7.          29.
PHILADELPHIA, PA
DILU            250.       1800.          0.          0.          0.
TEMP             11.        297.        299.        300.        302.        303.
      304.        306.        306.        306.        305.        305.
WATE             11.     30.095
      100.         92.         84.         75.         70.         65.         60.
       60.         60.         60.         60.         61.
TRAN              0.        .053          0.        .03           0.        .002
MASS            -10.         .47        .073        250.
     44.14       46.05       45.05       16.17       16.46       16.37        5.94
      6.04        6.30        6.66
     21.52       21.29       20.18        8.92        9.16        8.78        4.36
      4.37        4.59        4.78
BIOG            -10.          3.         250.
ISOP              0.       .0001          0.          0.       .0001          0.
     68.13
       .12         .15         .26         .33         .41         .59         .69
       .68         .65         .54
APIN              1.       .0001          0.          0.       .0001          0.
    136.24
         0.         .75         .75          0.          0.          0.          7.
         0.
       .12         .12         .14         .15         .17         .19         .25
       .25         .25         .25
UNKN              1.       .0001          0.          0.       .0001          0.
    136.24
         0.        .375        .875          0.          0.          0.         7.5
         0.
       .01         .02         .02         .08         .09          .1         .56
       .56         .55          .5
CRED              0.        -10.         250.
CO              1.3           0.          .5         -20.          0.          .4
     79.43       79.36       79.78       27.49       29.26       28.81       14.32
     14.69       15.88       17.43
SPEC              1.
O3
PLOT              0.          0.          0.          0.          0.          0.
ISOP              0.          0.          1.          0.          1.
       .18
```

Table B-1 (continued)

Scenario ID	**PHOAZ1**	**PHOENIX, AZ**	**9/ 9/88**
Latitude (deg):	33.48	Longtitude (deg):	112.14
Declination (deg):	5.20	Solar - clock time (min):	-85.33
Base ROG Input (mmolC/m2/day)	39.87	Initial Base ROG (% of input)	98.48
NOx Input (mmol/m2/day)	5.26	Initial NOx (% of input)	97.06

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.6306	0.0300	0.0015	0.0015	0.0014	0.0015	0.0015	0.0015	0.0015	0.0015	0.0016	0.0017
NOx	0.2121		0.0030	0.0030	0.0028	0.0029	0.0030	0.0028	0.0030	0.0030	0.0031	0.0030
Ozone		0.0600										
CH4	1.790	1.790										
CO	2.600	0.500	0.064	0.063	0.063	0.064	0.067	0.065	0.067	0.068	0.073	0.079
ISOP	0.0001		0.0017	0.0042	0.0061	0.0080	0.0086	0.0092	0.0096	0.0095	0.0092	0.0087
APIN	0.0001		0.0007	0.0009	0.0009	0.0012	0.0012	0.0014	0.0017	0.0017	0.0017	0.0017
UNKN	0.0001		0.0008	0.0009	0.0012	0.0015	0.0016	0.0018	0.0020	0.0020	0.0020	0.0020

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	593.	1119.	1645.	2170.	2695.	2880.	3065.	3250.	3250.	3250.	3250.
T (deg K)	301.0	302.0	304.0	306.0	309.0	310.0	312.0	314.0	314.0	314.0	314.0
H2O (10^4 ppm)	1.234	1.196	1.216	1.221	1.277	1.173	1.047	1.166	1.093	1.093	1.166

OZIPM4 Input File

```
TITL
PHOENIX, AZ  BASE CASE SIMULATION  9/9/88
PLAC              33.48     112.14        6.      1988.        9.        9.
PHOENIX, AZ
DILU               593.      3250.        0.         0.        0.
TEMP                11.       301.       302.       304.      306.      309.
      310.         312.       314.       314.       314.      314.      313.
WATE                11.      28.58
       35.          32.       29.        26.        23.       20.       18.
       16.          16.       15.        15.        16.
TRAN                 0.        .06        0.        .03        0.      .002
MASS                -10.       1.63      .212       593.
       .88          .87        .83        .85        .87       .86       .87
       .89          .94       1.02
       .73          .72        .69        .70        .72       .68       .72
       .72          .76        .72
BIOG                -10.         3.       593.
ISOP                  0.      .0001         0.         0.      .0001        0.
     68.13
       .12          .29        .42        .55        .59       .63       .66
       .65          .63         .6
APIN                  1.      .0001         0.         0.      .0001        0.
    136.24
         0.          .75        .75        0.         0.        0.        7.
         0.
        .1           .12        .13        .16        .17       .19       .23
       .23           .23        .23
UNKN                  1.      .0001         0.         0.      .0001        0.
    136.24
         0.         .375       .875        0.         0.        0.       7.5
         0.
       .11           .13        .16        .2         .22       .25       .28
       .27           .27        .27
CRED                  0.       -10.       593.
CO                   2.6         0.        .5        -20.        0.        .4
      1.81         1.79       1.77       1.81       1.90      1.83      1.89
      1.93         2.05       2.22
```

Table B-1 (continued)

Scenario ID	**PORORI**	**PORTLAND, OR**	**6/29/87**
Latitude (deg):	45.50	Longtitude (deg):	122.60
Declination (deg):	23.27	Solar - clock time (min):	-73.65
Base ROG Input (mmolC/m2/day)	6.23	Initial Base ROG (% of input)	47.33
NOx Input (mmol/m2/day)	0.96	Initial NOx (% of input)	34.10

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.2601	0.0300	0.0729	0.0740	0.0712	0.0716	0.0731	0.0718	0.0723	0.0062	0.0066	0.0070
NOx	0.0290		0.0932	0.0932	0.0887	0.0887	0.0921	0.0838	0.0903	0.0092	0.0096	0.0103
Ozone		0.0660										
CH4	1.790	1.790										
CO	1.500	0.500	0.558	0.564	0.566	0.568	0.587	0.562	0.576	0.048	0.050	0.054
ISOP	0.0001		0.0009	0.0012	0.0017	0.0026	0.0032	0.0045	0.0047	0.0070	0.0063	0.0042
APIN	0.0001		0.0023	0.0028	0.0033	0.0037	0.0040	0.0044	0.0045	0.0073	0.0086	0.0076
UNKN	0.0001		0.0015	0.0018	0.0022	0.0025	0.0027	0.0030	0.0031	0.0063	0.0062	0.0054

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	279.	535.	792.	1048.	1304.	1395.	1485.	1575.	1575.	1575.	1575.
T (deg K)	291.0	294.0	296.0	298.0	300.0	301.0	303.0	304.0	305.0	307.0	306.0
H2O (10^4 ppm)	1.630	1.791	1.831	1.848	1.906	1.837	1.773	1.791	1.849	2.121	2.103

OZIPM4 Input File

```
TITL
PORTLAND, OR  BASE CASE SIMULATION   6/29/87
PLAC            45.50     122.60        7.      1987.        6.       29.
PORTLAND, OR
DILU             279.      1575.        0.        0.        0.
TEMP              11.       291.       294.      296.      298.      300.
      301.       303.       304.       305.      307.      306.      305.
WATE              11.      29.77
       81.        74.        67.        60.       55.       50.       45.
       43.        41.        40.        41.       43.
TRAN               0.       .066         0.       .03        0.      .002
MASS             -10.        .26       .029      279.
     6.67       6.77       6.52       6.55      6.69      6.57      6.62
      .57        .60        .64
     4.16       4.16       3.96       3.96      4.11      3.74      4.03
      .41        .43        .46
BIOG             -10.         3.       279.
ISOP               0.      .0001         0.        0.     .0001        0.
    68.13
      .06        .08        .12        .18       .22       .31       .32
      .48        .43        .29
APIN               1.      .0001         0.        0.     .0001        0.
   136.24
        0.        .75        .75         0.        0.        0.        7.
        0.
      .31        .38        .45        .51       .55       .61       .62
       1.       1.18       1.04
UNKN               1.      .0001         0.        0.     .0001        0.
   136.24
        0.       .375       .875         0.        0.        0.       7.5
        0.
      .21        .25         .3        .34       .37       .41       .42
      .86        .85        .74
CRED               0.       -10.       279.
CO               1.5          0.         .5       -20.        0.        .4
    15.73      15.90      15.96      16.03     16.55     15.86     16.26
     1.35       1.42       1.52
```

Table B-1 (continued)

Scenario ID	**RICVA1**	**RICHMOND, VA**	**7/10/88**
Latitude (deg):	37.56	Longtitude (deg):	77.47
Declination (deg):	22.21	Solar - clock time (min):	-75.21
Base ROG Input (mmolC/m2/day)	16.36	Initial Base ROG (% of input)	22.35
NOx Input (mmol/m2/day)	2.65	Initial NOx (% of input)	16.11

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.3601	0.0300	0.2493	0.2529	0.2414	0.0095	0.0096	0.0026	0.0027	0.0026	0.0028	0.0032
NOx	0.0420		0.2707	0.2768	0.2573	0.0074	0.0077	0.0033	0.0036	0.0038	0.0040	0.0043
Ozone		0.0640										
CH4	1.790	1.790										
CO	1.500	0.500	5.827	5.700	5.282	0.117	0.121	0.057	0.060	0.061	0.067	0.074
ISOP	0.0001		0.0017	0.0026	0.0047	0.0281	0.0353	0.0436	0.0428	0.0414	0.0398	0.0356
APIN	0.0001		0.0008	0.0009	0.0011	0.0016	0.0018	0.0023	0.0022	0.0021	0.0021	0.0020
UNKN	0.0001		0.0001	0.0001	0.0001	0.0048	0.0056	0.0078	0.0076	0.0074	0.0073	0.0069

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	583.	916.	1249.	1581.	1698.	1815.	1932.	1932.	1932.	1932.
T (deg K)	296.0	298.0	300.0	302.0	304.0	306.0	308.0	308.0	308.0	308.0	306.0
H2O (10^4 ppm)	2.321	2.400	2.493	2.528	2.530	2.492	2.405	2.405	2.405	2.897	2.981

OZIPM4 Input File

```
TITL
RICHMOND, VA  BASE CASE SIMULATION  7/10/88
PLAC          37.56      77.47       4.      1988.       7.       10.
RICHMOND, VA
DILU           250.      1932.       0.        0.        0.
TEMP            11.       296.      298.      300.      302.      304.
      306.      308.       308.      308.      308.      306.      305.
WATE            11.     29.74
       85.       78.       72.       65.       58.       51.       44.
       44.       44.       44.       53.       61.
TRAN            0.       .064        0.       .03        0.       .002
MASS           -10.       .36       .042      250.
     59.95     60.81     58.04      2.29      2.31       .63       .64
       .62       .68       .76
     33.19     33.94     31.55       .91       .94       .41       .44
       .46       .49       .53
BIOG           -10.        3.       250.
ISOP            0.       .0001       0.        0.      .0001       0.
     68.13
       .12       .18       .32      1.93      2.42      2.99      2.94
      2.84      2.73      2.44
APIN            1.       .0001       0.        0.      .0001       0.
    136.24
        0.       .75       .75       0.        0.        0.        7.
        0.
       .11       .13       .15       .22       .25       .31       .3
       .29       .29       .27
UNKN            1.       .0001       0.        0.      .0001       0.
    136.24
        0.      .375      .875       0.        0.        0.       7.5
        0.
       .01       .01       .01       .66       .77      1.07      1.04
      1.02        1.       .94
CRED            0.       -10.      250.
CO             1.5         0.        .5       -20.       0.        .4
    164.39    160.81    149.02      3.31      3.40      1.60      1.68
      1.73      1.88      2.08
```

Table B-1 (continued)

Scenario ID	**SACCA1**	**SACRAMENTO, CA**	**7/23/88**
Latitude (deg):	38.48	Longtitude (deg):	121.47
Declination (deg):	20.01	Solar - clock time (min):	-72.36
Base ROG Input (mmolC/m2/day)	7.40	Initial Base ROG (% of input)	63.88
NOx Input (mmol/m2/day)	1.12	Initial NOx (% of input)	55.47

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.2201	0.0300	0.0369	0.0368	0.0343	0.0347	0.0359	0.0351	0.0356	0.0347	0.0370	0.0403
NOx	0.0290		0.0469	0.0454	0.0417	0.0419	0.0438	0.0404	0.0430	0.0442	0.0471	0.0509
Ozone		0.0600										
CH4	1.790	1.790										
CO	1.500	0.500	0.371	0.358	0.336	0.342	0.363	0.346	0.359	0.368	0.397	0.437
ISOP	0.0001		0.0013	0.0029	0.0055	0.0058	0.0071	0.0080	0.0086	0.0095	0.0096	0.0087
APIN	0.0001		0.0007	0.0009	0.0012	0.0013	0.0015	0.0017	0.0018	0.0021	0.0023	0.0020
UNKN	0.0001		0.0011	0.0015	0.0020	0.0021	0.0025	0.0028	0.0031	0.0036	0.0039	0.0034

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	529.	643.	756.	870.	983.	1023.	1063.	1103.	1103.	1103.	1103.
T (deg K)	292.0	295.0	298.0	301.0	303.0	305.0	307.0	308.0	310.0	311.0	309.0
H2O (10^4 ppm)	1.416	1.495	1.574	1.583	1.570	1.575	1.348	1.261	1.224	1.487	1.448

OZIPM4 Input File

```
TITL
SACRAMENTO, CA  BASE CASE SIMULATION   7/23/88
PLAC          38.48     121.47        7.      1988.        7.       23.
SACRAMENTO, CA
DILU            529.     1103.        0.         0.        0.
TEMP             11.      292.      295.       298.      301.      303.
      305.      307.      308.      310.       311.      309.      306.
WATE             11.    29.83
        66.       58.       51.       43.        38.       34.       30.
        26.       23.       20.       23.        25.
TRAN              0.      .060        0.       .03         0.      .002
MASS            -10.       .22      .029       529.
      4.01      4.00      3.73      3.77       3.90      3.82      3.87
      3.78      4.03      4.38
      2.44      2.36      2.17      2.18       2.28      2.10      2.24
      2.30      2.45      2.65
BIOG            -10.        3.      529.
ISOP              0.     .0001        0.         0.     .0001         0.
     68.13
       .09        .2        .38       .4        .49       .55       .59
       .65       .66         .6
APIN              1.     .0001        0.         0.     .0001         0.
    136.24
         0.       .75       .75        0.        0.         0.        7.
         0.
        .1        .12       .16       .18        .21       .23       .25
       .29       .31       .27
UNKN              1.     .0001        0.         0.     .0001         0.
    136.24
         0.      .375      .875        0.        0.         0.       7.5
         0.
       .15         .2       .27       .29        .34       .39       .43
        .5       .54       .46
CRED              0.      -10.      529.
CO              1.5          0.        .5       -20.        0.        .4
     10.48     10.11      9.49      9.65      10.23      9.77     10.14
     10.38     11.19     12.32
```

Table B-1 (continued)

Scenario ID	**SAIMO1**	**SAINT LOUIS, MO**	**7/ 8/88**
Latitude (deg):	38.63	Longtitude (deg):	90.20
Declination (deg):	22.45	Solar - clock time (min):	-65.84
Base ROG Input (mmolC/m2/day)	25.63	Initial Base ROG (% of input)	19.42
NOx Input (mmol/m2/day)	4.21	Initial NOx (% of input)	14.22

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.4902	0.0300	0.1738	0.1705	0.1626	0.1643	0.0220	0.0218	0.0220	0.0221	0.0229	0.0239
NOx	0.0590		0.2018	0.1911	0.1773	0.1794	0.0182	0.0161	0.0178	0.0180	0.0188	0.0193
Ozone		0.0820										
CH4	1.790	1.790										
CO	2.300	0.500	5.254	4.936	4.665	4.763	0.359	0.345	0.356	0.362	0.383	0.410
ISOP	0.0001		0.0035	0.0074	0.0074	0.0111	0.0114	0.0131	0.0131	0.0143	0.0121	0.0111
APIN	0.0001		0.0010	0.0012	0.0012	0.0012	0.0014	0.0014	0.0014	0.0015	0.0014	0.0014
UNKN	0.0001		0.0001	0.0001	0.0001	0.0015	0.0016	0.0017	0.0017	0.0019	0.0017	0.0016

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	522.	794.	1066.	1338.	1434.	1529.	1625.	1625.	1625.	1625.
T (deg K)	299.0	301.0	304.0	305.0	305.0	306.0	307.0	307.0	308.0	307.0	307.0
H2O (10^4 ppm)	1.977	1.894	1.862	1.925	1.879	1.940	1.847	1.744	1.899	1.847	1.898

OZIPM4 Input File

```
TITL
ST LOUIS, MO   BASE CASE SIMULATION   7/8/88
PLAC              38.63       90.20          5.       1988.          7.          8.
SAINT LOUIS, MO
DILU                250.        1625.          0.          0.          0.
TEMP                 11.         299.        301.        304.        305.        305.
      306.         307.         307.        308.        307.        307.        306.
WATE                 11.       29.52
       61.          52.          43.         42.         41.         40.         38.
       36.          34.          35.         36.         37.
TRAN                  0.        .082          0.        .03           0.        .002
MASS                -10.         .49        .059        250.
     65.46        64.21        61.25       61.89        8.30        8.21        8.27
      8.34         8.61         9.00
     39.39        37.30        34.61       35.02        3.55        3.15        3.48
      3.52         3.67         3.77
BIOG                -10.           3.        250.
ISOP                  0.       .0001          0.          0.       .0001          0.
     68.13
       .24          .51          .51         .76         .78          .9          .9
       .98          .83          .76
APIN                  1.       .0001          0.          0.       .0001          0.
    136.24
         0.          .75          .75         0.          0.          0.          7.
         0.
       .14          .17          .17         .17         .19         .19         .19
       .21          .19          .19
UNKN                  1.       .0001          0.          0.       .0001          0.
    136.24
         0.         .375         .875         0.          0.          0.         7.5
         0.
       .01          .01          .01         .21         .22         .24         .24
       .26          .23          .22
CRED                  0.         -10.        250.
CO                  2.3            0.          .5         -20.          0.          .4
     148.22       139.24       131.59      134.37       10.12        9.72       10.04
      10.22        10.80        11.56
```

Table B-1 (continued)

Scenario ID	**SALUT1**	**SALT LAKE CITY, UT**	**7/22/88**
Latitude (deg):	40.76	Longtitude (deg):	111.89
Declination (deg):	20.22	Solar - clock time (min):	-94.01
Base ROG Input (mmolC/m2/day)	10.69	Initial Base ROG (% of input)	77.87
NOx Input (mmol/m2/day)	1.26	Initial NOx (% of input)	68.41

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.8203	0.0300	0.0327	0.0324	0.0184	0.0186	0.0193	0.0192	0.0192	0.0192	0.0204	0.0219
NOx	0.0850		0.0498	0.0494	0.0260	0.0262	0.0270	0.0258	0.0269	0.0272	0.0286	0.0289
Ozone		0.0850										
CH4	1.790	1.790										
CO	2.000	0.500	0.686	0.649	0.386	0.397	0.420	0.415	0.419	0.430	0.466	0.514
ISOP	0.0001		0.0029	0.0061	0.0080	0.0112	0.0122	0.0133	0.0138	0.0137	0.0127	0.0117
APIN	0.0001		0.0009	0.0011	0.0006	0.0007	0.0008	0.0008	0.0009	0.0009	0.0009	0.0009
UNKN	0.0001		0.0012	0.0016	0.0015	0.0019	0.0020	0.0021	0.0023	0.0023	0.0023	0.0022

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	626.	1002.	1378.	1753.	1886.	2018.	2150.	2150.	2150.	2150.
T (deg K)	297.0	299.0	301.0	304.0	307.0	307.0	309.0	310.0	310.0	310.0	310.0
H2O (10^4 ppm)	0.779	0.821	0.795	0.794	0.806	0.851	1.052	1.111	1.111	1.111	1.111

OZIPM4 Input File

```
TITL
SALT LAKE CITY, UT   BASE CASE SIMULATION   7/22/88
PLAC            40.76     111.89        6.     1988.        7.       22.
SALT LAKE CITY, UT
DILU              250.     2150.        0.        0.        0.
TEMP               11.      297.      299.      301.      304.      307.
      307.      309.      310.      310.      310.      308.
WATE               11.    25.78
       31.       29.       25.       21.       18.       19.       20.
       21.       21.       21.       21.       21.
TRAN                0.     .085        0.      .03        0.      .002
MASS              -10.      .82      .085      250.
     5.14      5.10      2.89      2.93      3.03      3.01      3.02
     3.02      3.20      3.44
     2.91      2.89      1.52      1.53      1.58      1.51      1.57
     1.59      1.67      1.69
BIOG              -10.        3.      250.
ISOP                0.     .0001        0.        0.     .0001        0.
    68.13
       .2       .42       .55       .77       .84       .91       .95
      .94       .87        .8
APIN                1.     .0001        0.        0.     .0001        0.
   136.24
        0.       .75       .75        0.        0.        0.        7.
        0.
       .12       .15       .08        .1       .11       .11       .12
       .12       .12       .12
UNKN                1.     .0001        0.        0.     .0001        0.
   136.24
        0.      .375      .875        0.        0.        0.       7.5
        0.
       .17       .22       .21       .26       .27       .29       .31
       .31       .31        .3
CRED                0.      -10.      250.
CO                2.0        0.        .5      -20.        0.        .4
     19.35     18.32     10.90     11.19     11.86     11.72     11.83
     12.14     13.16     14.49
```

Table B-1 (continued)

Scenario ID	**SANTX1**	**SAN ANTONIO, TX**	**9/26/88**
Latitude (deg):	29.50	Longtitude (deg):	98.54
Declination (deg):	-1.34	Solar - clock time (min):	-84.69
Base ROG Input (mmolC/m2/day)	6.00	Initial Base ROG (% of input)	54.12
NOx Input (mmol/m2/day)	1.53	Initial NOx (% of input)	39.79

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.3201	0.0300	0.0477	0.0472	0.0432	0.0432	0.0445	0.0435	0.0446	0.0446	0.0480	0.0521
NOx	0.0600		0.0634	0.0630	0.0588	0.0585	0.0598	0.0565	0.0595	0.0596	0.0622	0.0606
Ozone		0.0600										
CH4	1.790	1.790										
CO	1.600	0.500	0.436	0.419	0.379	0.379	0.401	0.382	0.403	0.399	0.438	0.482
ISOP	0.0001		0.0004	0.0006	0.0010	0.0013	0.0022	0.0022	0.0026	0.0029	0.0029	0.0029
APIN	0.0001		0.0006	0.0007	0.0007	0.0009	0.0009	0.0009	0.0010	0.0011	0.0011	0.0011
UNKN	0.0001		0.0003	0.0004	0.0004	0.0004	0.0005	0.0005	0.0006	0.0007	0.0007	0.0007

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	657.	1065.	1472.	1878.	2022.	2165.	2308.	2308.	2308.	2308.
T (deg K)	295.0	297.0	299.0	300.0	302.0	304.0	304.0	305.0	306.0	306.0	306.0
H2O (10^4 ppm)	1.692	1.595	1.443	1.531	1.758	1.972	1.500	1.316	1.392	1.344	1.344

OZIPM4 Input File

```
TITL
SAN ANTONIO, TX   BASE CASE SIMULATION   9/26/88
PLAC          29.50      98.54        5.      1988.        9.        26.
SAN ANTONIO, TX
DILU             250.      2308.        0.         0.        0.
TEMP              11.       295.      297.       299.      300.      302.
      304.       304.       305.      306.       306.      306.      306.
WATE              11.      29.22
       67.        56.        45.       45.        46.       46.       40.
       35.        29.        29.       28.        28.
TRAN               0.        .06        0.        .03        0.       .002
MASS             -10.        .32      .060       250.
     4.21       4.17       3.81      3.81       3.93      3.84      3.94
     3.94       4.24       4.60
     4.50       4.47       4.17      4.15       4.24      4.01      4.22
     4.23       4.41       4.30
BIOG             -10.         3.      250.
ISOP               0.      .0001        0.         0.     .0001        0.
    68.13
      .03        .04        .07       .09        .15       .15       .18
       .2         .2         .2
APIN               1.      .0001        0.         0.     .0001        0.
   136.24
       0.        .75        .75        0.         0.        0.        7.
       0.
      .08         .1         .1       .12        .13       .13       .14
      .15        .15        .15
UNKN               1.      .0001        0.         0.     .0001        0.
   136.24
       0.        .375       .875       0.         0.        0.       7.5
       0.
      .04        .05        .05       .06        .07       .07       .08
      .09        .09        .09
CRED               0.       -10.      250.
CO               1.6          0.        .5        -20.       0.        .4
     12.30      11.82      10.68     10.70      11.31     10.78     11.37
     11.27      12.37      13.60
```

Table B-1 (continued)

Scenario ID	**SDOCA1**	**SAN DIEGO, CA**	**10/ 3/88**
Latitude (deg):	32.73	Longtitude (deg):	117.15
Declination (deg):	-4.10	Solar - clock time (min):	-36.80
Base ROG Input (mmolC/m2/day)	7.67	Initial Base ROG (% of input)	66.72
NOx Input (mmol/m2/day)	1.08	Initial NOx (% of input)	63.08

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.3601	0.0300	0.0338	0.0341	0.0312	0.0312	0.0320	0.0318	0.0321	0.0331	0.0354	0.0380
NOx	0.0480		0.0405	0.0384	0.0342	0.0339	0.0353	0.0335	0.0353	0.0363	0.0395	0.0423
Ozone		0.0900										
CH4	1.790	1.790										
CO	1.600	0.500	0.318	0.302	0.270	0.271	0.284	0.279	0.286	0.297	0.325	0.355
ISOP	0.0001		0.0010	0.0013	0.0015	0.0028	0.0043	0.0043	0.0043	0.0038	0.0031	0.0008
APIN	0.0001		0.0010	0.0011	0.0011	0.0013	0.0014	0.0014	0.0014	0.0014	0.0014	0.0013
UNKN	0.0001		0.0006	0.0008	0.0008	0.0009	0.0010	0.0010	0.0010	0.0009	0.0009	0.0008

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	350.	449.	548.	647.	746.	780.	815.	850.	850.	850.	850.
T (deg K)	299.0	300.0	300.0	301.0	302.0	302.0	302.0	302.0	302.0	301.0	301.0
H2O (10^4 ppm)	3.181	3.270	3.130	3.208	3.204	3.048	2.931	3.009	3.087	3.061	3.171

OZIPM4 Input File

```
TITL
SAN DIEGO, CA BASE CASE SIMULATION  10/3/88
PLAC          32.73     117.15        7.      1988.       10.        3.
SAN DIEGO, CA
DILU           350.       850.        0.         0.        0.
TEMP            11.        299.       300.       300.      301.       302.
      302.      302.       302.       302.       301.      301.       300.
WATE            11.      29.88
       97.       94.        90.        87.        82.       78.        73.
       75.       77.        79.        83.        86.
TRAN             0.       .090         0.        .03        0.       .002
MASS           -10.        .36       .048       200.
      2.18      2.20       2.01       2.01       2.06      2.05       2.07
      2.13      2.28       2.45
      1.16      1.10        .98        .97       1.01       .96       1.01
      1.04      1.13       1.21
BIOG           -10.         3.       200.
ISOP             0.       .0001        0.         0.      .0001        0.
     68.13
       .04       .05        .06        .11        .17       .17        .17
       .15       .12        .03
APIN             1.       .0001        0.         0.      .0001        0.
    136.24
        0.       .75        .75        0.         0.        0.         7.
        0.
       .08       .09        .09        .10        .11       .11        .11
       .11       .11        .10
UNKN             1.       .0001        0.         0.      .0001        0.
    136.24
        0.      .375       .875        0.         0.        0.        7.5
        0.
       .05       .06        .06        .07        .08       .08        .08
       .07       .07        .06
CRED             0.        -10.       200.
CO             1.6          0.         .5        -20.       0.         .4
      5.12      4.87       4.35       4.37       4.58      4.49       4.61
      4.78      5.24       5.72
CALC            .36        .048        0.         0.        0.
```

Table B-1 (continued)

Scenario ID	**SFOCA1**	**SAN FRANCISCO, CA**	**5/20/88**
Latitude (deg):	37.76	Longtitude (deg):	122.39
Declination (deg):	20.05	Solar - clock time (min):	-65.93
Base ROG Input (mmolC/m2/day)	25.01	Initial Base ROG (% of input)	22.74
NOx Input (mmol/m2/day)	5.24	Initial NOx (% of input)	14.93

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.4001	0.0300	0.1600	0.1621	0.1538	0.1530	0.0230	0.0227	0.0230	0.0234	0.0250	0.0266
NOx	0.0550		0.1913	0.1887	0.1730	0.1718	0.0206	0.0192	0.0203	0.0207	0.0221	0.0231
Ozone		0.0700										
CH4	1.790	1.790										
CO	1.700	0.500	4.658	4.582	4.365	4.339	0.692	0.674	0.693	0.722	0.797	0.871
ISOP	0.0001		0.0009	0.0010	0.0010	0.0015	0.0042	0.0071	0.0070	0.0079	0.0086	0.0063
APIN	0.0001		0.0004	0.0006	0.0006	0.0007	0.0009	0.0010	0.0010	0.0011	0.0012	0.0011
UNKN	0.0001				0.0001	0.0001	0.0008	0.0009	0.0009	0.0010	0.0011	0.0009

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	350.	409.	469.	528.	587.	608.	629.	650.	650.	650.	650.
T (deg K)	291.0	292.0	294.0	295.0	297.0	300.0	304.0	304.0	305.0	306.0	304.0
H2O (10^4 ppm)	1.314	1.334	1.459	1.473	1.370	1.288	1.097	0.965	0.882	0.983	0.921

OZIPM4 Input File

```
TITL
SAN FRANCISCO, CA   BASE CASE SIMULATION   5/20/88
PLAC          37.76     122.39        7.     1988.        5.        20.
SAN FRANCISCO, CA
DILU            350.        650.        0.        0.        0.
TEMP             11.        291.       292.      294.      295.      297.
      300.       304.        304.       305.      306.      304.      302.
WATE             11.      29.91
       65.        62.         60.        57.       47.       37.       28.
       25.        22.         19.        20.       21.
TRAN              0.         .07         0.        .03       0.        .002
MASS            -10.         .40        .055      350.
     58.80      59.59       56.53      56.25      8.46      8.35      8.46
      8.59       9.18        9.79
     46.41      45.78       41.98      41.68      5.00      4.66      4.92
      5.02       5.35        5.60
BIOG            -10.          3.        350.
ISOP              0.         .0001       0.        0.        .0001     0.
     68.13
       .06        .07         .07        .1        .29       .49       .48
       .54        .59         .43
APIN              1.         .0001       0.        0.        .0001     0.
    136.24
         0.        .75         .75        0.        0.        0.        7.
         0.
       .06        .08         .08        .1        .12       .14       .14
       .15        .16         .15
UNKN              1.         .0001       0.        0.        .0001     0.
    136.24
         0.       .375         .875       0.        0.        0.        7.5
         0.
         0.        0.          .01        .01       .11       .13       .13
       .14        .15         .13
CRED              0.        -10.        350.
CO              1.7           0.          .5      -20.        0.        .4
    131.40     129.26      123.14     122.41     19.51     19.00     19.54
     20.36      22.47       24.58
SPEC              1.
O3
PLOT              0.          0.         0.        0.        0.        0.
ISOP              0.          0.         1.        0.        1.
       .14
```

Table B-1 (continued)

Scenario ID	**TAMFL1**	**TAMPA, FL**	**4/23/87**
Latitude (deg):	27.93	Longtitude (deg):	82.53
Declination (deg):	12.27	Solar - clock time (min):	-88.34
Base ROG Input (mmolC/m2/day)	7.90	Initial Base ROG (% of input)	70.68
NOx Input (mmol/m2/day)	1.81	Initial NOx (% of input)	33.05

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.5502	0.0300	0.0288	0.0299	0.0276	0.0275	0.0284	0.0282	0.0285	0.0294	0.0313	0.0336
NOx	0.0590		0.0675	0.0687	0.0669	0.0667	0.0667	0.0651	0.0656	0.0653	0.0678	0.0691
Ozone		0.0680										
CH4	1.790	1.790										
CO	2.100	0.500	0.349	0.330	0.298	0.298	0.317	0.312	0.320	0.332	0.365	0.399
ISOP	0.0001		0.0025	0.0032	0.0035	0.0057	0.0103	0.0128	0.0122	0.0112	0.0105	0.0076
APIN	0.0001		0.0009	0.0011	0.0012	0.0014	0.0017	0.0018	0.0018	0.0018	0.0017	0.0015
UNKN	0.0001		0.0016	0.0020	0.0021	0.0025	0.0031	0.0034	0.0033	0.0032	0.0031	0.0028

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	397.	543.	690.	836.	888.	939.	991.	991.	991.	991.
T (deg K)	292.0	294.0	296.0	298.0	299.0	300.0	302.0	302.0	302.0	302.0	300.0
H2O (10^4 ppm)	2.089	2.143	2.172	2.200	2.136	2.057	1.958	1.880	1.801	2.271	2.475

OZIPM4 Input File

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TITL
TAMPA, FL  BASE CASE SIMULATION   4/23/87
PLAC            27.93      82.53        4.      1987.        4.        23.
TAMPA, FL
DILU             250.        991.        0.        0.        0.
TEMP              11.        292.       294.      296.      298.       299.
      300.       302.        302.       302.      300.       298.
WATE              11.      29.945
       97.        88.         79.        71.       65.        59.        53.
       50.        48.         46.        58.       71.
TRAN               0.        .068         0.       .03         0.       .002
MASS             -10.         .55        .059      250.
     3.35       3.47        3.21       3.20      3.30       3.27       3.31
     3.41       3.64        3.90
     5.67       5.77        5.62       5.60      5.60       5.47       5.51
     5.48       5.69        5.80
BIOG             -10.          3.       250.
ISOP               0.       .0001         0.        0.      .0001         0.
    68.13
      .17        .22         .24        .39       .71        .88        .84
      .77        .72         .52
APIN               1.       .0001         0.        0.      .0001         0.
   136.24
        0.        .75         .75        0.        0.         0.         7.
        0.
      .12        .15         .17        .19       .23        .25        .25
      .25        .23         .21
UNKN               1.       .0001         0.        0.      .0001         0.
   136.24
        0.       .375        .875        0.        0.         0.        7.5
        0.
      .22        .27         .29        .34       .43        .46        .45
      .44        .43         .38
CRED               0.        -10.       250.
CO               2.1           0.         .5       -20.        0.         .4
     9.85       9.31        8.42       8.41      8.93       8.81       9.02
     9.36      10.30       11.26
```

Table B-1 (continued)

Scenario ID	**TULOK1**	**TULSA, OK**	**7/22/86**
Latitude (deg):	36.14	Longtitude (deg):	101.98
Declination (deg):	20.43	Solar - clock time (min):	-114.32
Base ROG Input (mmolC/m2/day)	14.86	Initial Base ROG (% of input)	71.09
NOx Input (mmol/m2/day)	2.80	Initial NOx (% of input)	57.67

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr)									
			Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	1.0404	0.0300	0.0287	0.0285	0.0273	0.0277	0.0285	0.0283	0.0284	0.0289	0.0304	0.0324
NOx	0.1591		0.0432	0.0426	0.0419	0.0422	0.0430	0.0416	0.0427	0.0429	0.0443	0.0389
Ozone		0.0700										
CH4	1.790	1.790										
CO	1.500	0.500	0.573	0.546	0.518	0.534	0.569	0.560	0.568	0.581	0.627	0.688
ISOP	0.0001		0.0007	0.0013	0.0017	0.0028	0.0038	0.0038	0.0038	0.0038	0.0028	0.0012
APIN	0.0001		0.0007	0.0009	0.0009	0.0010	0.0012	0.0012	0.0012	0.0012	0.0010	0.0009
UNKN	0.0001		0.0002	0.0003	0.0003	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0003

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	250.	563.	875.	1188.	1500.	1610.	1720.	1830.	1830.	1830.	1830.
T (deg K)	296.0	299.0	301.0	302.0	304.0	306.0	306.0	306.0	306.0	304.0	302.0
H2O (10^4 ppm)	2.131	2.290	2.285	2.229	2.371	2.511	2.463	2.415	3.042	3.234	3.382

OZIPM4 Input File

```
TITL
TULSA, OK    BASE CASE SIMULATION   7/22/86
PLAC              36.14     101.98        5.      1986.        7.        22.
TULSA, OK
DILU             250.      1830.          0.         0.        0.
TEMP              11.       296.        299.       301.      302.      304.
      306.       306.       306.        306.       304.      302.      299.
WATE              11.     29.39
       79.        71.        63.         58.        55.       52.       51.
       51.        50.        63.         75.        88.
TRAN               0.        .07          0.        .03        0.      .002
MASS             -10.       1.04        .159       250.
     6.26       6.23       5.97        6.05       6.22      6.17      6.20
     6.31       6.64       7.08
     5.60       5.53       5.43        5.47       5.58      5.40      5.54
     5.56       5.74       5.04
BIOG             -10.         3.        250.
ISOP               0.      .0001          0.         0.      .0001        0.
    68.13
      .05        .09        .12         .19        .26       .26       .26
      .26        .19        .08
APIN               1.      .0001          0.         0.      .0001        0.
  136.24
        0.        .75        .75          0.         0.        0.        7.
        0.
       .1        .12        .12         .14        .16       .16       .16
      .16        .14        .12
UNKN               1.      .0001          0.         0.      .0001        0.
  136.24
        0.       .375       .875          0.         0.        0.       7.5
        0.
      .03        .04        .04         .05        .06       .06       .06
      .06        .05        .04
CRED               0.       -10.        250.
CO               1.5          0.          .5        -20.        0.        .4
    16.17      15.39      14.61       15.07      16.04     15.80     16.02
    16.38      17.70      19.41
```

Table B-1 (continued)

Scenario ID	**WASDC1**	**WASHINGTON, DC**	**7/30/88**
Latitude (deg):	38.90	Longtitude (deg):	77.05
Declination (deg):	18.46	Solar - clock time (min):	-74.63
Base ROG Input (mmolC/m2/day)	13.48	Initial Base ROG (% of input)	34.08
NOx Input (mmol/m2/day)	2.54	Initial NOx (% of input)	18.58

Reactants Input

Reactants	Init. (ppm)	Aloft (ppm)	Emitted (mmol/m2/hr) Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
NMOCs	0.3901	0.0300	0.1561	0.1623	0.1615	0.0239	0.0248	0.0239	0.0245	0.0253	0.0272	0.0297
NOx	0.0400		0.1651	0.1631	0.1577	0.0445	0.0466	0.0439	0.0460	0.0470	0.0491	0.0512
Ozone		0.0990										
CH4	1.790	1.790										
CO	1.800	0.500	3.073	3.235	3.547	0.481	0.512	0.477	0.505	0.519	0.563	0.624
ISOP	0.0001		0.0047	0.0093	0.0299	0.0312	0.0344	0.0347	0.0338	0.0328	0.0309	0.0261
APIN	0.0001		0.0011	0.0014	0.0019	0.0019	0.0020	0.0020	0.0020	0.0020	0.0020	0.0018
UNKN	0.0001		0.0001	0.0001	0.0047	0.0048	0.0052	0.0053	0.0052	0.0051	0.0050	0.0045

Scenario Conditions

Parameter	Hr-0	Hr-1	Hr-2	Hr-3	Hr-4	Hr-5	Hr-6	Hr-7	Hr-8	Hr-9	Hr-10
Height (M)	290.	514.	738.	961.	1185.	1264.	1342.	1421.	1421.	1421.	1421.
T (deg K)	300.0	302.0	305.0	307.0	307.0	307.0	308.0	308.0	308.0	308.0	306.0
H2O (10^4 ppm)	2.583	2.549	2.654	2.554	2.606	2.658	2.700	2.480	2.204	2.700	2.858

OZIPM4 Input File

```
TITL
WASHINGTON, DC   BASE CASE SIMULATION   7/30/88
PLAC          38.90       77.05          4.       1988.          7.         30.
WASHINGTON, DC
DILU             290.       1421.          0.          0.          0.
TEMP              11.        300.        302.        305.        307.       307.
      307.        308.        308.        308.        306.        305.
WATE              11.       29.99
       74.         65.         57.         49.         50.         51.        53.
       49.         45.         40.         49.         58.
TRAN               0.        .099          0.         .03          0.        .002
MASS             -10.         .39        .040        290.
     30.93       32.15       32.00        4.74        4.91        4.74       4.86
      5.01        5.38        5.88
     19.40       19.16       18.53        5.23        5.48        5.16       5.40
      5.52        5.77        6.01
BIOG             -10.          3.        290.
ISOP               0.       .0001          0.          0.       .0001         0.
     68.13
       .32         .64        2.05        2.14        2.36        2.38       2.32
      2.25        2.12        1.79
APIN               1.       .0001          0.          0.       .0001         0.
    136.24
         0.         .75         .75          0.          0.          0.        7.
         0.
       .15         .19         .26         .26         .28         .28       .28
       .27         .27         .25
UNKN               1.       .0001          0.          0.       .0001         0.
    136.24
         0.        .375        .875          0.          0.          0.       7.5
         0.
       .01         .02         .65         .66         .72         .73       .71
        .7         .68         .62
CRED               0.        -10.        290.
CO               1.8           0.          .5         -20.          0.        .4
     86.69       91.27      100.07       13.58       14.43       13.46      14.24
     14.63       15.88       17.60
```

APPENDIX C. TEST CALCULATIONS AND REACTIVITY SCALE COMPARISONS

In this Appendix, we give results of selected reactivity scale comparisons and test calculations which were not presented in the main body of the report. These include more detailed comparisons of reactivity scales discussed in the main report, calculations using modified procedures for deriving the scale, and calculations using other chemical mechanisms. Because most of the tabulations take several pages, they are all given at the end of this Appendix.

Comparisons of Scales in this Report with Those Submitted to the ARB in 1991.

The observant reader might notice that there are slight differences in some of the MIR and MOIR reactivity values given in Table 4 compared to those which were submitted to the ARB in 1991 and adopted in their regulation. This apparently arose due to some changes in data files or software implementing the mechanism or reactivity calculation procedures which were made as part of our ongoing research between then and now. Table C-1 gives a comparison of the current and 1991 MIR and MOIR values for all the species listed on Table 4 where the difference exceeded 0.5%. The changes are insignificant and can be attributed to the numerical uncertainty associated with these simulation solvers.

Tabulation of $Int O_3$>90 Reactivities and comparison with MIR.

In the discussion of appropriate reactivity scales for regulatory applications, we concluded that scales based on integrated ozone over the standard under base case conditions may have some advantages over MIR. These scales can be derived either using the average ratio (AR) method, the least squares error method based on substitutions of the base ROG for the VOC (L1), or the least squares error method based on substitutions of the VOC for the base ROG (L2). Table C-2 gives a comparison of MIR RAFs and relative reactivities with those in the Base Case $Int O_3$>90 scales. The various methods for deriving the $Int O_3$>90 scales give similar results, except for low mechanistic reactivity VOCs where the L2 method fails. The $Int O_3$>90 scales give RAFs which differ by up to 15% from the MIR values, and often larger differences (usually 30% or less) for relative reactivities of a number of VOCs. However, figure 11 shows that the reactivities in these two scales are highly correlated, and the differences between these two types of scales can be considered to reflect the level of uncertainty associated with the reactivity assessment methodology.

Use of a single "Averaged Conditions" scenario to approximate full MIR or MOIR calculations.

Full MIR, MOIR, EBIR reactivity scale calculation requires simulations of 39 adjusted NO_x scenarios, and then averaging the results to yield the desired scale. However, for most of the sensitivity calculations, a single adjusted NO_x "averaged conditions" scenario was used to approximate each scale. Table C-3 shows the comparisons of the full MIR or MOIR calculations with the corresponding scale calculated using a single averaged conditions scenario. The differences with the RAFs are 1% or less, and the differencess in relative reactivities are less than 2% for all species except for those with very low or negative mechanistic reactivities. The MOIR incremental reactivities also agree within this approximate range, but the single-scenario MIR incremental reactivities are consistently ~4% higher than those derived from all the 39 scenarios. Since RAFs or relative reactivities are the quantities of greatest interest, this suggests that use of an appropriate single scenario would give substantially the same results as averaging a multitude of scenarios when deriving an adjusted NO_x scale. However, this approach gives no indication of the magnitude of uncertainties due to variabilities of other scenario conditions.

Effect of More Detailed Lumping in Simulating the Reactions of the Base ROG Mixture

As shown in Tables A-1 and B-6, only three model species were used to represent the reactions of all the alkanes and aromatics in the base ROG mixture, and only two were used for the C_{3+} alkenes. Some have questioned whether this approximation may introduce errors in the reactivity simulations. To assess this, the MIR and MOIR scales were re-calculated using a larger number of model species for these compounds. In particular, a total of 8 model species, with kOH divisions of 1, 5, 7.5, 10, 15, 20, and 40 x 10^3 ppm^{-1} min^{-1}, were used for the alkanes and aromatics, and 3 model species, with kOH divisions of 6 and $8x10^4$ ppm^{-1} min^{-1} were used for the alkenes. A comparison of the MIR and MOIR scale calculated with the standard lumping and this more detailed lumping is shown on Table C-4. The difference can be seen to be insignificant. Clearly, the lumping used in the standard model does not introduce significant errors in the reactivity assessment.

Effect of SAPRC-90 Mechanism Updates

For reasons discussed in the main body of the report, a slightly out-of-date mechanism was used in the reactivity scale calculation. This is unavoidable because it takes a certain amount of time to implement and evaluate a mechanism,

while research in atmospheric chemistry continues. As discussed in the main body of the report, a preliminary updated SAPRC mechanism (designated SAPRC-91) was developed but was not used because it performed slightly worse than SAPRC-90 in simulating chamber experiments when the methodology of Carter and Lurmann (1991) is employed. Table C-5 gives a complete tabulation of the effect of this update on RAFs and relative and incremental reactivities. The RAFs change by only 6% or less and the relative reactivities for most VOCs change by on the order of 10% for MIR and 15% for MOIR, with the relative reactivities of the alkanes generally increasing and those for the aromatics decreasing. (The large change for β-pinene is due to a change in parameters for that compound because of unpublished results from our laboratories.) The updated mechanism gives consistently higher incremental reactivities for all VOCs.

One problem with both the SAPRC-90 and the SAPRC-91 mechanisms is that recently it was found that the NO_x data in some of the chamber runs used to adjust the mechanism for the xylenes and (to a lesser extent) toluene and the trialkylbenzenes need some corrections. These corrections, which are on the order of 15% in the worst case (a m-xylene run) have now been made to the chamber data, and will be taken into account when the mechanism is re-evaluated in our upcoming ARB program. However, they were not implemented when the SAPRC-90 or SAPRC-91 mechanisms were developed. To see what effect these corrections would have on SAPRC-90 reactivity calculations, we re-optimized the aromatics parameters in the SAPRC-90 mechanism using the corrected NO_x data for the relevant aromatic runs, and used the corrected mechanism to recalculate the MIR and MOIR scales. The results are shown on Table C-6. The calculation was conducted only for MIR conditions, since these are the conditions most affected by the type of adjustments involved. The results show that the adjustment causes a 1% or less change in the RAFs, and no more than a 3% change in the relative and incremental reactivities of most VOCs, including the xylenes. Thus, though this correction obviously needs to be taken into account, it is not a significant problem with the reactivity scales calculated in this work.

Effect of Using an Alternative Aromatics Mechanism

One of the tasks in this program was to develop an alternative aromatics mechanism which takes into account results of Atkinson et al. (1989) that indicate that assumptions incorporated in current aromatics mechanism may be incorrect. An alternative approach to represent aromatics may be also be incorrect, but comparisons of calculations using different approaches would be useful to assess effects of these uncertainties on model predictions. These effects may not necessarily be large, because aromatic mechanisms, though highly uncertain, are adjusted to fit environmental chamber data. The uncertainty in applications of aromatics mechanisms comes not from their lack of ability to fit

environmental chamber data but from the possibility that they may not be extrapolating correctly when going from environmental chamber to atmospheric conditions.

Although a considerable amount of effort was spent for this program to develop an alternative aromatics mechanism, and several versions of it were developed which fit the chamber data as well or slightly better than current mechanisms. However, because of the larger-than-expected effort on development of reactivity scales, this program ran out of time and funds before we had a chance to complete this effort and write up these results. Work in this area is continuing, but we are now waiting on results of ongoing ARB-funded experiments being conducted by Atkinson and co-workers, and on results of analysis of ongoing environmental chamber experiments in our laboratories, before finalizing a mechanism (or mechanisms) and writing up the results. However, in this section we will give a brief description of the current version of an alternative aromatics mechanism which best fits the chamber data, and show the effect of using it on calculated MIR or MOIR reactivities.

All state-of-the art aromatics mechanisms currently used in airshed models are based on the assumption that the OH-aromatic adducts react with O_2, forming either HO_2 and phenolic compounds, or forming OH-aromatic-O_2 adducts which eventually, after NO to NO_2 conversions, form photoreactive fragmentation products (Atkinson, 1989, 1990; Gery et al., 1988; Carter, 1990; Stockwell et al., 1990). However, product data of Atkinson et al. (1989) are difficult to explain in terms of this mechanism, but suggest that the OH-aromatic adduct may react primarily with NO_2 rather than O_2. Kinetic data on OH-aromatic adduct reactions indicate that they react rapidly with NO_2, negligibly with NO, and relatively slowly with O_2 (e.g., Knispel et al. 1990). The O_2 and NO_2 rate constants of Knispel et al. (1990) indicate that the NO_2 reaction becomes important in air if the NO_2 concentration exceeds ~0.1 ppm. However, these rate constant determinations are difficult and are not without uncertainties, and the data of Atkinson et al. (1989) suggest (albeit indirectly) that the NO_2 reaction may be important at even lower NO_x levels. Thus the possibility that the O_2 reaction is negligible under atmospheric conditions cannot be ruled out.

Note that there are no data concerning how rapidly the OH-aromatic adducts react with ozone, which is usually present in polluted atmospheres in concentrations comparable to or greater than that of NO_2. Alkyl radicals react rapidly with ozone (e.g., Paltenghi et al., 1984), so it is unreasonable to assume that OH-aromatic adducts do not. For example, the ozone + isopropyl rate constant has been measured to be $(5\pm1) \times 10^{-11}$ cm^3 $molec^{-1}$ sec^{-1}, which is comparable to the OH-aromatic + NO_2 rate constant of 3.6×10^{-11} cm^3 $molec^{-1}$ sec^{-1} measured by Knispel et al. (1990). Thus it would be unreasonable to assume that this reaction could not compete with the NO_2 reaction if the O_2 reaction is unimportant.

The alternative aromatics mechanisms we developed are based on the assumption that the OH-aromatic adduct does not react with O_2, but instead reacts only with NO_2 or O_3. Although the reality may be that the O_2 reaction may be competitive under sufficiently low NO_x and O_3 conditions, the number of unknown parameters in such cases becomes large, and we have not fully explored the possibilities for the types of mechanisms which would result. However, examining the possibility based on assuming the O_2 reaction is unimportant would be useful at least as a sensitivity analysis.

To satisfactorily fit the chamber data, the NO_2 reaction must regenerate radicals. The possibility of it reacting to form HONO was considered, but if this is assumed to occur to a significant extent, the model predicts a delay in the initial rate of NO oxidation in aromatics chamber runs which is not observed. The best fits are obtained with the following type of overall reaction, which regenerates OH radicals after the same number of NO to NO_2 conversions as in the current aromatics mechanisms:

$$\text{OH-Aro}\cdot + NO_2 \longrightarrow \text{OH-Aro-O}\cdot + NO \qquad (1)$$

$$\text{OH-Aro-O}\cdot \longrightarrow \text{Phenols} + OH \qquad (2)$$

$$\text{OH-Aro-O}\cdot \xrightarrow[NO_2]{NO} \xrightarrow[NO_2]{NO} \text{Fragmentation Products} + HO_2 \qquad (3)$$

A speculative reaction sequence for the fragmentation process can be written which can rationalize the formation of the expected type of products and gives the number of NO to NO_2 conversion shown.

The ozone + OH-aromatic adduct reaction mechanism is obviously at least as uncertain as that for the NO_2 reaction. One possibility is to assume that the initial process is

$$\text{OH-Aro}\cdot + O_3 \longrightarrow \text{OH-Aro-O}\cdot + O_2 \qquad (4)$$

with the OH-Aro-O· reacting as shown above. Satisfactory fits to the chamber data can be obtained with this mechanism, with the result not being particularly sensitive to the k_4/k_1 rate constant ratio because the NO_2 and the ozone reactions have largely the same net effect on ozone formation. The fits are qualitatively like the standard mechanism — no better and no worse. Like the standard mechanism, it underpredicts the initial rate of reaction of high ROG/NO_x experiments if the mechanism is adjusted to fit moderate ROG/NO_x experiments.

A slightly better fit to the chamber data can be obtained if it is assumed that phenols (reaction 2) are not formed from the ozone reaction. The fit is not dramatically better (the problem with the high ROG/NO_x runs remains, though to a slightly reduced extent), but the improvement is probably statistically

significant. This mechanism might be rationalized by the possibility that a higher energy radical is formed in the O_3 reaction, which might react differently than the radical formed from NO_2. With this mechanism, the model simulations of the chamber experiments are more sensitive to the k_4/k_1 rate constant ratio, and the best fit is obtained if the ozone reaction is assumed to occur with a rate constant approximately half that of the NO_2 reaction. This is not unreasonable based on the laboratory data for the NO_2 + aromatic adduct and the O_3 + alkyl radical data discussed above.

Based on this type of mechanism, the mechanisms for benzene, toluene, m-xylene, and 1,3,5-trimethylbenzene were re-optimized using the same chamber data as used to optimize the SAPRC-91 mechanism. (For consistency with the SAPRC-91 mechanism for this comparison, the chamber data with uncorrected NO_x levels were used.) The other aspects in the mechanisms, including the reactions of the aromatic products, were the same as in the SAPRC-91 mechanism. (No analogous alternative mechanisms were developed for naphthalenes. The product parameters of benzene were used when representing naphthalenes in mixtures. No mixtures used in this work contained naphthalenes in significant amounts.) The modified aromatics SAPRC-91 mechanism were then used to calculate reactivities for the "averaged conditions" MIR and MOR scenarios. The results for selected species are shown on Table C-7, where they are compared with those calculated with the standard SAPRC-91 mechanism.

Table C-7 shows that using this alternative aromatics mechanism causes the relative reactivities of the aromatics to increase by varying amounts, while the relative reactivities of most other species decrease. This causes all the RAFs except for Phase 2 gasoline decrease by ~10%. This must be regarded a minimum level of uncertainty in these reactivity scales caused by uncertainties in the aromatics photooxidation mechanisms.

Reactivity Scales Calculated Using Other Chemical Mechanisms

Until recently the SAPRC-90 mechanism has not been implemented in grid models, and the grid model tests of the reactivity scale conducted thus far have utilized either the LCC mechanism of Lurmann et al. (1987), or the Carbon Bond 4 mechanism of Gery et al. (1988). The LCC mechanism is a condensed version of an earlier SAPRC mechanism (Carter et al., 1986), and the Carbon Bond 4 (CB4) mechanism is a condensed mechanism which uses significantly different approaches than the SAPRC mechanisms to represent alkanes, aromatics, and internal alkenes. To permit more unambiguous comparisons of the reactivity scales developed in this work with results of airshed model calculations using these mechanisms, we used them to calculate MIR and MOIR reactivity scales. The results are shown on Figure C-8 and C-9 for the LCC and the CB4 mechanisms, respectively. Since these

calculations were conducted back in 1991, the 1991 version of the SAPRC-90 reactivity scale is shown for comparison. Although large differences can be seen for some species (especially in the case of CB4), the MIR and MOIR RAFs agree to within 7% and 11%, respectively.

The version of the Carbon Bond mechanism used was supplied to us by Jeffries (personal communication, 1991), and was represented as being the version currently being used in the UAM. The LCC mechanism documentation (Lurmann et al., 1987) had a typographical error in the MEK mechanism which unfortunately was implemented in the CMU airshed model. Since this error has now been fixed, the LCC calculations here have the corrected MEK mechanism.

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Table C-1. Differences in SAPRC-90 RAFs and reactivities in this Report compared to the values provided to the ARB in September, 1991. Only cases where the differences are greater than 0.5% are shown.

DMS or Mix	MIR Scale			MOIR Scale		
	Current	9/91	(diff)	Current	9/91	(diff)
LEV and TLEV Exhaust RAFs — All differences < 0.5%						
Relative Reactivities (gram basis)						
CO	0.017	0.017	1%	0.031	0.031	
N-C7	0.26	0.26	1%	0.44	0.44	
N-C8	0.19	0.19	2%	0.34	0.34	
N-C9	0.17	0.17	1%	0.29	0.30	
N-C10	0.147	0.148	1%	0.25	0.26	1%
N-C11	0.132	0.134	1%	0.23	0.23	1%
N-C12	0.119	0.120	1%	0.21	0.21	1%
N-C13	0.110	0.111	1%	0.19	0.19	1%
N-C14	0.101	0.102	1%	0.18	0.18	
ETHENE	2.3	2.3	-1%	2.6	2.6	-1%
TETRALIN	0.30	0.30	1%	0.106	0.106	
NAPHTHAL	0.37	0.37	1%	0.077	0.075	-3%
STYRENE	0.70	0.70	1%	-0.24	-0.24	
I-C3-OH	0.17	0.17	1%	0.26	0.26	
BENZALD	-0.18	-0.18	-2%	-1.02	-1.02	
PHENOL	0.35	0.36	1%	-0.39	-0.39	
Incremental Reactivities (gm O3/gm VOC)						
N-C8	0.60	0.61	2%	0.41	0.41	
N-C9	0.54	0.54	1%	0.36	0.36	
N-C10	0.46	0.47	1%	0.31	0.31	
N-C11	0.42	0.42	1%	0.28	0.28	
N-C12	0.38	0.38	1%	0.25	0.25	
N-C13	0.35	0.35	1%	0.23	0.24	
N-C14	0.32	0.32	1%	0.22	0.22	
ETHENE	7.4	7.3	-2%	3.2	3.2	-1%
TETRALIN	0.94	0.95	1%	0.129	0.129	
NAPHTHAL	1.17	1.18	1%	0.093	0.091	-3%
MEGLYOX	14.8	14.8	-1%	4.5	4.5	-1%
BENZALD	-0.57	-0.55	-2%	-1.24	-1.23	
PHENOL	1.12	1.13	1%	-0.47	-0.47	

Table C-2. Comparison of RAFs and relative reactivities from the MIR scale with those from the Base Case IntO_3>90 scales.

DMS or Mix	MIR	IntO_3>90 AR	(diff)	L1	(diff)	L2	(diff)
LEV and TLEV Exhaust RAFs [a]							
M85-TLEV	0.37	0.40	9%			0.40	9%
CNG-TLEV	0.18	0.20	15%			0.19	10%
LPG-TLEV	0.50	0.58	12%			0.55	7%
E85-TLEV	0.63	0.64	2%			0.61	-3%
PH2-TLEV	0.96	0.99	3%			1.00	4%
PH2-LEV	0.94	0.96	2%			0.95	1%
Relative Reactivities (gram basis)							
CO	0.017	0.028	60%	0.024	38%	0.028	60%
METHANE	0.0047	0.0065	37%	0.0057	21%	0.0065	37%
ETHANE	0.078	0.096	23%	0.081	3%	0.096	23%
PROPANE	0.15	0.19	26%	0.16	7%	0.19	26%
N-C4	0.32	0.39	19%	0.33	2%	0.39	19%
N-C5	0.33	0.43	31%	0.36	10%	0.43	31%
N-C6	0.31	0.39	26%	0.33	8%	0.39	26%
N-C7	0.26	0.27	7%	0.25	-4%	0.27	7%
N-C8	0.19	0.18	-7%	0.17	-12%	0.18	-7%
N-C9	0.17	0.120	-29%	0.112	-34%	0.120	-29%
N-C10	0.147	0.083	-44%	0.080	-45%	0.083	-44%
N-C11	0.132	0.062	-53%	0.061	-54%	0.062	-53%
N-C12	0.119	0.047	-60%	0.048	-60%	0.047	-60%
N-C13	0.110	0.038	-66%	0.038	-66%	0.038	-66%
N-C14	0.101	0.031	-70%	0.032	-69%	0.031	-70%
2-ME-C3	0.38	0.51	34%	0.45	17%	0.51	34%
22-DM-C3	0.116	0.118	2%	0.104	-10%	0.118	2%
2-ME-C4	0.44	0.55	27%	0.48	10%	0.55	27%
22-DM-C4	0.26	0.29	13%	0.26	2%	0.29	13%
23-DM-C4	0.34	0.48	42%	0.41	22%	0.48	42%
2-ME-C5	0.48	0.55	13%	0.48	-1%	0.55	13%
3-ME-C5	0.48	0.59	24%	0.51	6%	0.59	24%
223TM-C4	0.42	0.56	34%	0.49	18%	0.56	34%
23-DM-C6	0.42	0.49	18%	0.42	2%	0.49	18%
24-DM-C6	0.47	0.53	12%	0.46	-2%	0.53	12%
33-DM-C5	0.22	0.24	9%	0.22	-3%	0.24	9%
2-ME-C6	0.34	0.41	21%	0.35	4%	0.41	21%
3-ME-C6	0.44	0.49	11%	0.43	-2%	0.49	11%
224TM-C5	0.29	0.30	4%	0.28	-6%	0.30	4%
234TM-C5	0.51	0.61	20%	0.53	5%	0.61	20%
23-DM-C6	0.42	0.49	18%	0.42	2%	0.49	18%
24-DM-C6	0.47	0.53	12%	0.46	-2%	0.53	12%
25-DM-C6	0.51	0.65	26%	0.57	11%	0.65	26%
2-ME-C7	0.30	0.32	7%	0.29	-6%	0.32	7%
3-ME-C7	0.31	0.35	13%	0.31	-2%	0.35	13%
4-ME-C7	0.38	0.38	1%	0.34	-12%	0.38	1%
24-DM-C7	0.42	0.43	3%	0.39	-9%	0.43	3%
225TM-C6	0.31	0.31	3%	0.29	-6%	0.31	3%
4-ET-C7	0.36	0.33	-7%	0.31	-14%	0.33	-7%
4-PR-C7	0.32	0.28	-13%	0.26	-19%	0.28	-13%
24-DM-C7	0.42	0.43	3%	0.39	-9%	0.43	3%
36-DE-C8	0.39	0.40	4%	0.36	-8%	0.40	4%
CYCC5	0.75	0.90	20%	0.78	4%	0.90	20%
ME-CYCC5	0.89	1.06	19%	0.93	5%	1.06	19%

Table C-2 (continued)

DMS or Mix	MIR	IntO$_3$>90					
		AR	(diff)	L1	(diff)	L2	(diff)
CYCC6	0.40	0.41	1%	0.37	-8%	0.41	1%
13DMCYC5	0.80	0.98	22%	0.87	9%	0.98	22%
ME-CYCC6	0.58	0.59	1%	0.53	-9%	0.59	1%
ET-CYCC5	0.73	0.82	12%	0.72	-1%	0.82	12%
ET-CYCC6	0.61	0.61	-1%	0.55	-10%	0.61	-1%
1E4MCYC6	0.73	0.76	5%	0.68	-6%	0.76	5%
13DECYC6	0.56	0.59	5%	0.53	-6%	0.59	5%
13E5MCC6	0.60	0.66	9%	0.59	-2%	0.66	9%
135ECYC6	0.53	0.57	7%	0.51	-4%	0.57	7%
ETHENE	2.3	2.6	11%	2.5	7%	2.6	11%
PROPENE	3.0	3.1	4%	3.0	1%	3.1	4%
1-BUTENE	2.8	2.8	-1%	2.7	-4%	2.8	-1%
1-PENTEN	2.0	1.8	-9%	1.8	-8%	1.8	-9%
3M-1-BUT	2.0	1.8	-9%	1.8	-8%	1.8	-9%
1-HEXENE	1.40	1.18	-16%	1.17	-16%	1.18	-16%
1-C7-OLE	1.10	0.88	-20%	0.88	-20%	0.88	-20%
1-C8-OLE	0.85	0.62	-27%	0.62	-27%	0.62	-27%
1-C9-OLE	0.70	0.48	-32%	0.49	-30%	0.48	-32%
ISOBUTEN	1.7	2.0	19%	1.9	14%	2.0	19%
2M-1-BUT	1.5	1.8	16%	1.7	10%	1.8	16%
T-2-BUTE	3.1	3.4	8%	3.3	5%	3.4	8%
C-2-BUTE	3.1	3.4	8%	3.3	5%	3.4	8%
2-C5-OLE	2.8	2.8	0%	2.7	-3%	2.8	0%
2M-2-BUT	2.0	2.3	13%	2.2	9%	2.3	13%
2-C6-OLE	2.1	2.1	-1%	2.0	-5%	2.1	-1%
2-C7-OLE	1.7	1.7	-3%	1.6	-8%	1.7	-3%
3-C8-OLE	1.7	1.50	-10%	1.47	-12%	1.50	-10%
3-C9-OLE	1.45	1.30	-10%	1.26	-13%	1.30	-10%
13-BUTDE	3.4	3.5	2%	3.4	0%	3.5	2%
ISOPRENE	2.9	2.9	0%	2.9	1%	2.9	0%
CYC-PNTE	2.4	2.6	6%	2.6	6%	2.6	6%
CYC-HEXE	1.8	1.8	3%	1.7	-2%	1.8	3%
A-PINENE	1.04	1.05	1%	1.01	-2%	1.05	1%
B-PINENE	1.39	1.41	1%	1.39	0%	1.41	1%
ACETYLEN	0.16	0.23	42%	0.19	22%	0.23	42%
ME-ACTYL	1.30	1.36	5%	1.21	-6%	1.36	5%
BENZENE	0.134	0.111	-17%	0.106	-21%	0.111	-17%
TOLUENE	0.86	0.60	-31%	0.67	-22%	0.60	-31%
C2-BENZ	0.85	0.59	-31%	0.68	-20%	0.59	-31%
N-C3-BEN	0.67	0.46	-31%	0.53	-21%	0.46	-31%
I-C3-BEN	0.71	0.49	-30%	0.56	-21%	0.49	-30%
S-C4-BEN	0.60	0.41	-32%	0.47	-21%	0.41	-32%
O-XYLENE	2.0	1.8	-12%	1.9	-7%	1.8	-12%
P-XYLENE	2.1	1.9	-9%	2.0	-3%	1.9	-9%
M-XYLENE	2.6	2.4	-6%	2.7	3%	2.4	-6%
135-TMB	3.2	3.4	5%	3.6	12%	3.4	5%
123-TMB	2.8	2.7	-3%	3.0	6%	2.7	-3%
124-TMB	2.8	2.7	-2%	3.0	6%	2.7	-2%
TETRALIN	0.30	0.15	-49%	0.19	-36%	0.15	-49%
NAPHTHAL	0.37	0.117	-68%	0.20	-46%	0.117	-68%
ME-NAPH	1.03	0.77	-25%	0.89	-13%	0.77	-25%
23-DMN	1.6	1.40	-14%	1.6	-3%	1.40	-14%
STYRENE	0.70	-0.063	-109%	0.29	-58%	-0.063	-109%

Table C-2 (continued)

DMS or Mix	MIR	$IntO_3$>90 AR	(diff)	L1	(diff)	L2	(diff)
MEOH	0.18	0.20	13%	0.19	6%	0.20	13%
ETOH	0.42	0.42	-1%	0.37	-12%	0.42	-1%
N-C3-OH	0.71	0.68	-5%	0.63	-12%	0.68	-5%
I-C3-OH	0.17	0.25	49%	0.22	29%	0.25	49%
N-C4-OH	0.85	0.82	-3%	0.76	-10%	0.82	-3%
I-C4-OH	0.61	0.63	5%	0.58	-5%	0.63	5%
T-C4-OH	0.132	0.18	38%	0.16	21%	0.18	38%
ME-O-ME	0.24	0.43	77%	0.35	45%	0.43	77%
MTBE	0.20	0.30	54%	0.26	31%	0.30	54%
ETBE	0.63	0.85	35%	0.76	21%	0.85	35%
FORMALD	2.3	2.5	9%	2.7	18%	2.5	9%
ACETALD	1.7	1.7	-5%	1.6	-8%	1.7	-5%
PROPALD	2.1	1.8	-13%	1.8	-12%	1.8	-13%
GLYOXAL	0.70	0.77	10%	0.83	18%	0.77	10%
MEGLYOX	4.7	5.5	18%	6.0	28%	5.5	18%
ACETONE	0.18	0.145	-18%	0.15	-14%	0.145	-18%
MEK	0.37	0.34	-8%	0.32	-14%	0.34	-8%
BENZALD	-0.18	-1.18	560%	-0.83	362%	-1.18	560%
PHENOL	0.35	-0.28	-178%	-0.068	-119%	-0.28	-178%
CRESOL	0.73	-0.34	-147%	0.16	-79%	-0.34	-147%

[a] L2 RAFs calculated by minimizing the error in substituting the alternative fuel exhaust for standard exhaust, not by summing up $IntO_3$>90 Base(L2) reactivities for the individual compounds. The L1 method is not applicable to RAFs.

Table C-3. Differences in MIR and MOIR RAFs and reactivities derived using all the 39 scenarios, compared to the values from a single "averaged conditions" scenario.

DMS or Mix	MIR Scale			MOIR Scale		
	All 39	Avg Cond	(diff)	All 39	Avg Cond	(diff)
LEV and TLEV Exhaust RAFs						
M85-TLEV	0.37	0.37		0.38	0.38	
CNG-TLEV	0.18	0.18		0.22	0.22	1%
LPG-TLEV	0.50	0.50		0.59	0.59	
E85-TLEV	0.63	0.63		0.77	0.78	1%
PH2-TLEV	0.98	0.97		0.99	0.99	
PH2-LEV	0.94	0.94		0.97	0.97	
Relative Reactivities (gram basis)						
CO	0.017	0.017	1%	0.031	0.032	
METHANE	0.0047	0.0046	-2%	0.0076	0.0076	-1%
ETHANE	0.078	0.078		0.136	0.137	1%
PROPANE	0.15	0.15		0.26	0.26	-1%
N-C4	0.32	0.32		0.55	0.55	1%
N-C5	0.33	0.33	1%	0.56	0.56	1%
N-C6	0.31	0.31	1%	0.53	0.54	1%
N-C7	0.26	0.26	1%	0.44	0.44	1%
N-C8	0.19	0.20	4%	0.34	0.33	-2%
N-C9	0.17	0.17	2%	0.29	0.29	
N-C10	0.147	0.150	2%	0.25	0.26	
N-C11	0.132	0.135	2%	0.23	0.23	
N-C12	0.119	0.122	3%	0.21	0.21	
N-C13	0.110	0.113	2%	0.19	0.19	
N-C14	0.101	0.104	3%	0.18	0.18	
2-ME-C3	0.38	0.38		0.60	0.60	
22-DM-C3	0.116	0.116		0.18	0.18	-1%
2-ME-C4	0.44	0.44		0.71	0.72	1%
22-DM-C4	0.26	0.26		0.42	0.42	
23-DM-C4	0.34	0.34	1%	0.55	0.56	
2-ME-C5	0.48	0.48		0.74	0.74	
3-ME-C5	0.48	0.48		0.78	0.78	1%
223TM-C4	0.42	0.42		0.65	0.65	
23-DM-C6	0.42	0.42	1%	0.64	0.64	
24-DM-C6	0.47	0.48		0.71	0.71	
33-DM-C5	0.22	0.22		0.38	0.38	
2-ME-C6	0.34	0.34	1%	0.56	0.56	
3-ME-C6	0.44	0.44	1%	0.68	0.69	1%
224TM-C5	0.29	0.28	-5%	0.45	0.42	-6%
234TM-C5	0.51	0.51	1%	0.76	0.76	
23-DM-C6	0.42	0.42	1%	0.64	0.64	
24-DM-C6	0.47	0.48		0.71	0.71	
25-DM-C6	0.51	0.52		0.76	0.76	
2-ME-C7	0.30	0.31	1%	0.49	0.49	
3-ME-C7	0.31	0.32	1%	0.51	0.51	
4-ME-C7	0.38	0.38	1%	0.57	0.58	
24-DM-C7	0.42	0.42		0.62	0.62	
225TM-C6	0.31	0.31	1%	0.48	0.48	
4-ET-C7	0.36	0.36	1%	0.53	0.53	
4-PR-C7	0.32	0.32	1%	0.46	0.46	
24-DM-C7	0.42	0.42		0.62	0.62	
36-DE-C8	0.39	0.39		0.57	0.57	
CYCC5	0.75	0.75		1.16	1.17	1%

Table C-3 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	All 39	Avg Cond	(diff)	All 39	Avg Cond	(diff)
ME-CYCC5	0.89	0.89		1.28	1.28	
CYCC6	0.40	0.41	1%	0.61	0.61	1%
13DMCYC5	0.80	0.81		1.14	1.14	
ME-CYCC6	0.58	0.59		0.82	0.82	
ET-CYCC5	0.73	0.73	1%	1.07	1.08	1%
ET-CYCC6	0.61	0.62	1%	0.84	0.84	
1E4MCYC6	0.73	0.73		0.97	0.97	
13DECYC6	0.56	0.57		0.77	0.77	
13E5MCC6	0.60	0.60		0.82	0.82	
135ECYC6	0.53	0.53		0.72	0.72	
ETHENE	2.3	2.3	-1%	2.6	2.6	
PROPENE	3.0	3.0		3.1	3.1	
1-BUTENE	2.8	2.8		2.9	2.9	
1-PENTEN	2.0	2.0		2.0	2.0	1%
3M-1-BUT	2.0	2.0		2.0	2.0	1%
1-HEXENE	1.40	1.40		1.44	1.44	
1-C7-OLE	1.10	1.10		1.13	1.14	
1-C8-OLE	0.85	0.86	1%	0.88	0.89	1%
1-C9-OLE	0.70	0.71	1%	0.73	0.73	1%
ISOBUTEN	1.7	1.7		1.6	1.6	-1%
2M-1-BUT	1.5	1.5		1.6	1.6	-1%
T-2-BUTE	3.1	3.2		3.1	3.2	2%
C-2-BUTE	3.1	3.2		3.1	3.2	2%
2-C5-OLE	2.8	2.8		2.7	2.8	1%
2M-2-BUT	2.0	2.1	1%	1.9	1.9	1%
2-C6-OLE	2.1	2.1	1%	2.1	2.1	1%
2-C7-OLE	1.7	1.8	1%	1.7	1.7	1%
3-C8-OLE	1.7	1.7	1%	1.6	1.7	2%
3-C9-OLE	1.45	1.47	1%	1.43	1.45	2%
13-BUTDE	3.4	3.4		3.4	3.4	
ISOPRENE	2.9	2.9		2.8	2.8	1%
CYC-PNTE	2.4	2.5	1%	2.3	2.3	2%
CYC-HEXE	1.8	1.8	1%	1.8	1.8	1%
A-PINENE	1.04	1.05	1%	1.06	1.06	
B-PINENE	1.39	1.40	1%	1.37	1.38	1%
ACETYLEN	0.16	0.16		0.27	0.27	
ME-ACTYL	1.30	1.30		1.8	1.8	
BENZENE	0.134	0.134		0.113	0.113	-1%
TOLUENE	0.86	0.86	-1%	0.52	0.49	-6%
C2-BENZ	0.85	0.85		0.52	0.49	-6%
N-C3-BEN	0.67	0.66	-1%	0.40	0.38	-5%
I-C3-BEN	0.71	0.70		0.43	0.41	-4%
S-C4-BEN	0.60	0.60		0.36	0.34	-6%
O-XYLENE	2.0	2.0		1.6	1.6	-2%
P-XYLENE	2.1	2.1		1.6	1.6	-1%
M-XYLENE	2.6	2.6	-1%	2.0	2.0	-1%
135-TMB	3.2	3.2		2.5	2.5	
123-TMB	2.8	2.8	-1%	2.2	2.2	-1%
124-TMB	2.8	2.8		2.2	2.2	-1%
TETRALIN	0.30	0.31	3%	0.106	0.095	-11%
NAPHTHAL	0.37	0.38	2%	0.077	0.060	-22%
ME-NAPH	1.03	1.04		0.63	0.61	-3%
23-DMN	1.6	1.6		1.12	1.11	-1%

Table C-3 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	All 39	Avg Cond	(diff)	All 39	Avg Cond	(diff)
STYRENE	0.70	0.71	2%	-0.24	-0.29	18%
MEOH	0.18	0.18	-1%	0.23	0.23	-1%
ETOH	0.42	0.42		0.60	0.60	1%
N-C3-OH	0.71	0.71		0.93	0.93	
I-C3-OH	0.17	0.17	1%	0.26	0.26	
N-C4-OH	0.85	0.85		1.07	1.07	
I-C4-OH	0.61	0.61		0.78	0.78	
T-C4-OH	0.132	0.131	-1%	0.20	0.20	
ME-O-ME	0.24	0.24		0.46	0.47	1%
MTBE	0.20	0.20		0.33	0.34	
ETBE	0.63	0.63		0.85	0.85	
FORMALD	2.3	2.3		1.7	1.7	
ACETALD	1.7	1.8		1.8	1.8	1%
PROPALD	2.1	2.1	1%	2.1	2.1	1%
GLYOXAL	0.70	0.70		0.58	0.59	1%
MEGLYOX	4.7	4.7	1%	3.7	3.8	2%
ACETONE	0.18	0.18	-1%	0.17	0.16	-2%
MEK	0.37	0.37		0.45	0.45	
BENZALD	-0.18	-0.17	-7%	-1.02	-1.06	4%
PHENOL	0.35	0.36	2%	-0.39	-0.40	3%
CRESOL	0.73	0.73		-0.47	-0.53	12%
Incremental Reactivities (gm O3/gm VOC)						
CO	0.054	0.057	4%	0.038	0.038	
METHANE	0.0150	0.015	1%	0.0093	0.0092	-1%
ETHANE	0.25	0.25	3%	0.17	0.17	1%
PROPANE	0.48	0.50	3%	0.31	0.31	
N-C4	1.02	1.06	4%	0.66	0.67	1%
N-C5	1.04	1.07	4%	0.68	0.69	1%
N-C6	0.98	1.02	4%	0.65	0.65	1%
N-C7	0.81	0.84	4%	0.53	0.54	1%
N-C8	0.60	0.65	7%	0.41	0.40	-2%
N-C9	0.54	0.57	5%	0.36	0.36	
N-C10	0.46	0.49	5%	0.31	0.31	
N-C11	0.42	0.44	6%	0.28	0.28	
N-C12	0.38	0.40	6%	0.25	0.25	
N-C13	0.35	0.37	6%	0.23	0.24	
N-C14	0.32	0.34	6%	0.22	0.22	
2-ME-C3	1.21	1.24	3%	0.73	0.73	
22-DM-C3	0.37	0.38	3%	0.22	0.22	-1%
2-ME-C4	1.38	1.43	4%	0.87	0.88	1%
22-DM-C4	0.82	0.85	3%	0.51	0.51	
23-DM-C4	1.07	1.11	4%	0.67	0.68	1%
2-ME-C5	1.5	1.6	3%	0.90	0.90	1%
3-ME-C5	1.5	1.6	4%	0.94	0.95	1%
223TM-C4	1.32	1.36	4%	0.79	0.79	
23-DM-C6	1.31	1.36	4%	0.78	0.78	
24-DM-C6	1.5	1.6	4%	0.86	0.86	
33-DM-C5	0.71	0.73	4%	0.46	0.46	1%
2-ME-C6	1.08	1.12	4%	0.68	0.68	1%
3-ME-C6	1.40	1.45	4%	0.83	0.83	1%
224TM-C5	0.93	0.91	-2%	0.54	0.51	-6%
234TM-C5	1.6	1.7	4%	0.92	0.92	

Table C-3 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	All 39	Avg Cond	(diff)	All 39	Avg Cond	(diff)
23-DM-C6	1.31	1.36	4%	0.78	0.78	
24-DM-C6	1.5	1.6	4%	0.86	0.86	
25-DM-C6	1.6	1.7	4%	0.93	0.93	
2-ME-C7	0.96	1.00	4%	0.59	0.60	1%
3-ME-C7	0.99	1.03	4%	0.62	0.62	
4-ME-C7	1.20	1.25	4%	0.70	0.70	
24-DM-C7	1.33	1.38	4%	0.75	0.75	
225TM-C6	0.97	1.01	4%	0.58	0.58	
4-ET-C7	1.13	1.18	4%	0.64	0.64	
4-PR-C7	1.01	1.05	4%	0.56	0.56	
24-DM-C7	1.33	1.38	4%	0.75	0.75	
36-DE-C8	1.23	1.27	4%	0.69	0.69	
CYCC5	2.4	2.5	4%	1.41	1.42	1%
ME-CYCC5	2.8	2.9	4%	1.6	1.6	
CYCC6	1.28	1.33	4%	0.74	0.75	1%
13DMCYC5	2.5	2.6	4%	1.38	1.39	
ME-CYCC6	1.8	1.9	4%	1.00	1.00	
ET-CYCC5	2.3	2.4	4%	1.30	1.31	1%
ET-CYCC6	1.9	2.0	4%	1.02	1.02	1%
1E4MCYC6	2.3	2.4	4%	1.18	1.18	
13DECYC6	1.8	1.8	4%	0.93	0.93	
13E5MCC6	1.9	2.0	3%	1.00	1.00	
135ECYC6	1.7	1.7	4%	0.87	0.87	
ETHENE	7.4	7.6	3%	3.2	3.2	
PROPENE	9.4	9.7	3%	3.8	3.8	1%
1-BUTENE	8.9	9.2	3%	3.5	3.5	
1-PENTEN	6.2	6.4	3%	2.5	2.5	1%
3M-1-BUT	6.2	6.4	3%	2.5	2.5	1%
1-HEXENE	4.4	4.6	4%	1.7	1.7	
1-C7-OLE	3.5	3.6	3%	1.38	1.39	1%
1-C8-OLE	2.7	2.8	4%	1.07	1.08	1%
1-C9-OLE	2.2	2.3	4%	0.89	0.89	1%
ISOBUTEN	5.3	5.5	4%	1.9	1.9	
2M-1-BUT	4.9	5.1	3%	1.9	1.9	
T-2-BUTE	10.0	10.3	4%	3.8	3.8	2%
C-2-BUTE	10.0	10.3	4%	3.8	3.8	2%
2-C5-OLE	8.8	9.1	4%	3.3	3.4	1%
2M-2-BUT	6.4	6.7	4%	2.3	2.3	2%
2-C6-OLE	6.7	7.0	4%	2.5	2.5	2%
2-C7-OLE	5.5	5.8	4%	2.1	2.1	2%
3-C8-OLE	5.3	5.5	5%	2.0	2.0	2%
3-C9-OLE	4.6	4.8	4%	1.7	1.8	2%
13-BUTDE	10.9	11.3	3%	4.2	4.2	1%
ISOPRENE	9.1	9.4	4%	3.4	3.5	1%
CYC-PNTE	7.7	8.0	4%	2.8	2.8	2%
CYC-HEXE	5.7	5.9	4%	2.2	2.2	1%
A-PINENE	3.3	3.4	4%	1.28	1.29	1%
B-PINENE	4.4	4.6	4%	1.7	1.7	1%
ACETYLEN	0.50	0.52	3%	0.33	0.33	
ME-ACTYL	4.1	4.2	3%	2.2	2.2	1%
BENZENE	0.42	0.44	4%	0.138	0.137	-1%
TOLUENE	2.7	2.8	3%	0.63	0.59	-5%
C2-BENZ	2.7	2.8	3%	0.63	0.59	-6%

Table C-3 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	All 39	Avg Cond	(diff)	All 39	Avg Cond	(diff)
N-C3-BEN	2.1	2.2	3%	0.49	0.46	-5%
I-C3-BEN	2.2	2.3	3%	0.52	0.50	-4%
S-C4-BEN	1.9	1.9	3%	0.44	0.41	-6%
O-XYLENE	6.5	6.7	3%	2.0	1.9	-1%
P-XYLENE	6.6	6.8	3%	2.0	2.0	-1%
M-XYLENE	8.2	8.4	3%	2.5	2.4	
135-TMB	10.1	10.5	3%	3.1	3.1	
123-TMB	8.9	9.1	3%	2.7	2.7	
124-TMB	8.8	9.1	3%	2.7	2.7	-1%
TETRALIN	0.94	1.00	6%	0.129	0.115	-10%
NAPHTHAL	1.17	1.23	5%	0.093	0.073	-22%
ME-NAPH	3.3	3.4	4%	0.76	0.75	-2%
23-DMN	5.1	5.3	4%	1.36	1.35	-1%
STYRENE	2.2	2.3	5%	-0.30	-0.35	18%
MEOH	0.56	0.57	2%	0.28	0.28	
ETOH	1.34	1.38	3%	0.72	0.73	1%
N-C3-OH	2.3	2.3	3%	1.13	1.13	1%
I-C3-OH	0.54	0.56	5%	0.32	0.32	
N-C4-OH	2.7	2.8	3%	1.30	1.30	1%
I-C4-OH	1.9	2.0	3%	0.94	0.95	
T-C4-OH	0.42	0.43	2%	0.25	0.25	
ME-O-ME	0.77	0.80	4%	0.56	0.57	1%
MTBE	0.62	0.64	3%	0.41	0.41	1%
ETBE	2.0	2.0	3%	1.03	1.03	
FORMALD	7.2	7.4	4%	2.1	2.1	
ACETALD	5.5	5.7	4%	2.2	2.2	2%
PROPALD	6.5	6.8	4%	2.5	2.5	1%
GLYOXAL	2.2	2.3	4%	0.71	0.71	1%
MEGLYOX	14.8	15%	4%	4.5	4.6	2%
ACETONE	0.56	0.57	2%	0.20	0.20	-2%
MEK	1.18	1.22	3%	0.55	0.55	
BENZALD	-0.57	-0.54	-4%	-1.24	-1.29	4%
PHENOL	1.12	1.18	5%	-0.47	-0.48	3%
CRESOL	2.3	2.4	4%	-0.58	-0.65	12%
Base ROG	3.2	3.3	3%	1.21	1.22	

Table C-4. Differences in RAFs and reactivities in the MIR and MOIR scales compared to values calculated using a more detailed base ROG lumping. All calculations used the SAPRC-90 mechanism. (Only differences greater than 0.5% are shown for the RAFs and greater than 1.5% are shown for the model species.)

DMS or Mix	MIR Scale			MOIR Scale		
	Standard	Detailed	(diff)	Standard	Detailed	(diff)
LEV and TLEV Exhaust RAFs						
CNG-TLEV	0.18	0.17	-1%	0.22	0.22	
Relative Reactivities (gram basis).						
N-C8	0.19	0.19	-2%	0.34	0.34	1%
N-C12	0.119	0.123	4%	0.21	0.21	
N-C14	0.101	0.097	-4%	0.18	0.18	2%
224TM-C5	0.29	0.28	-4%	0.45	0.42	-6%
4-ME-C7	0.38	0.39	2%	0.57	0.58	1%
2M-2-BUT	2.0	2.0	-2%	1.9	1.9	-1%
NAPHTHAL	0.37	0.38	2%	0.077	0.074	-4%
ME-NAPH	1.03	1.03		0.63	0.63	
23-DMN	1.6	1.6		1.12	1.12	
STYRENE	0.70	0.69	-1%	-0.24	-0.26	7%
FORMALD	2.3	2.2	-2%	1.7	1.7	-2%
MEGLYOX	4.7	4.6	-2%	3.7	3.7	-2%
BENZALD	-0.18	-0.18	2%	-1.02	-1.03	
Incremental Reactivities (gm O3/gm VOC)						
N-C10	0.46	0.48	2%	0.31	0.31	
N-C12	0.38	0.39	4%	0.25	0.25	
N-C14	0.32	0.31	-3%	0.22	0.22	2%
2-ME-C5	1.5	1.6	2%	0.90	0.90	
224TM-C5	0.93	0.89	-4%	0.54	0.51	-6%
4-ME-C7	1.20	1.23	3%	0.70	0.70	
1E4MCYC6	2.3	2.3	2%	1.18	1.18	
13DECYC6	1.8	1.8	2%	0.93	0.93	
1-C9-OLE	2.2	2.3	2%	0.89	0.89	
I-C3-BEN	2.2	2.3	2%	0.52	0.51	
S-C4-BEN	1.9	1.9	2%	0.44	0.43	-2%
TETRALIN	0.94	0.96	2%	0.129	0.130	
NAPHTHAL	1.17	1.21	3%	0.093	0.089	-5%
I-C3-OH	0.54	0.54	2%	0.32	0.32	
T-C4-OH	0.42	0.42	2%	0.25	0.25	
BENZALD	-0.57	-0.58	3%	-1.24	-1.25	
PHENOL	1.12	1.14	2%	-0.47	-0.48	2%
CRESOL	2.3	2.4	2%	-0.58	-0.58	
Base ROG	3.2	3.2		1.21	1.21	

Table C-5. Differences in RAFs and reactivities from the SAPRC-90 mechanism, compared to the values from the updated (SAPRC-91) mechanism.

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	SAPRC91	(diff)	SAPRC90	SAPRC91	(diff)
LEV and TLEV Exhaust RAFs						
M85-TLEV	0.37	0.37	-1%	0.38	0.36	-5%
CNG-TLEV	0.18	0.18	2%	0.22	0.23	4%
LPG-TLEV	0.50	0.51	1%	0.59	0.61	2%
E85-TLEV	0.63	0.65	4%	0.77	0.82	6%
PH2-TLEV	0.98	0.98	0%	0.99	1.00	0%
PH2-LEV	0.94	0.95	1%	0.97	0.98	1%
Relative Reactivities (gram basis)						
CO	0.017	0.017	-3%	0.031	0.029	-9%
METHANE	0.0047	0.0046	-2%	0.0076	0.0071	-7%
ETHANE	0.078	0.082	6%	0.136	0.148	9%
PROPANE	0.15	0.16	6%	0.26	0.28	10%
N-C4	0.32	0.34	6%	0.55	0.60	11%
N-C5	0.33	0.35	6%	0.56	0.61	10%
N-C6	0.31	0.33	5%	0.53	0.59	10%
N-C7	0.26	0.27	6%	0.44	0.50	13%
N-C8	0.19	0.21	9%	0.34	0.39	17%
N-C9	0.17	0.19	9%	0.29	0.36	21%
N-C10	0.147	0.16	11%	0.25	0.32	24%
N-C11	0.132	0.148	12%	0.23	0.29	25%
N-C12	0.119	0.133	13%	0.21	0.26	27%
N-C13	0.110	0.125	13%	0.19	0.25	28%
N-C14	0.101	0.115	14%	0.18	0.23	29%
2-ME-C3	0.38	0.39	2%	0.60	0.61	1%
22-DM-C3	0.116	0.131	12%	0.18	0.23	28%
2-ME-C4	0.44	0.46	5%	0.71	0.77	7%
22-DM-C4	0.26	0.28	7%	0.42	0.47	12%
23-DM-C4	0.34	0.34	2%	0.55	0.56	1%
2-ME-C5	0.48	0.52	8%	0.74	0.85	15%
3-ME-C5	0.48	0.51	5%	0.78	0.84	8%
223TM-C4	0.42	0.43	3%	0.65	0.66	3%
23-DM-C6	0.42	0.44	6%	0.64	0.72	11%
24-DM-C6	0.47	0.51	7%	0.71	0.80	12%
33-DM-C5	0.22	0.24	8%	0.38	0.43	14%
2-ME-C6	0.34	0.36	6%	0.56	0.62	10%
3-ME-C6	0.44	0.48	8%	0.68	0.77	14%
224TM-C5	0.29	0.31	4%	0.45	0.51	14%
234TM-C5	0.51	0.53	6%	0.76	0.83	9%
23-DM-C6	0.42	0.44	6%	0.64	0.72	11%
24-DM-C6	0.47	0.51	7%	0.71	0.80	12%
25-DM-C6	0.51	0.53	3%	0.76	0.80	5%
2-ME-C7	0.30	0.32	7%	0.49	0.56	13%
3-ME-C7	0.31	0.33	6%	0.51	0.57	12%
4-ME-C7	0.38	0.41	9%	0.57	0.67	17%
24-DM-C7	0.42	0.46	8%	0.62	0.71	15%
225TM-C6	0.31	0.33	9%	0.48	0.55	17%
4-ET-C7	0.36	0.39	9%	0.53	0.62	17%
4-PR-C7	0.32	0.35	10%	0.46	0.55	19%
24-DM-C7	0.42	0.46	8%	0.62	0.71	15%
36-DE-C8	0.39	0.41	6%	0.57	0.63	10%
CYCC5	0.75	0.81	8%	1.16	1.32	14%
ME-CYCC5	0.89	0.95	6%	1.28	1.40	10%

Table C-5 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	SAPRC91	(diff)	SAPRC90	SAPRC91	(diff)
CYCC6	0.40	0.44	9%	0.61	0.71	17%
13DMCYC5	0.80	0.84	5%	1.14	1.22	7%
ME-CYCC6	0.58	0.63	8%	0.82	0.94	15%
ET-CYCC5	0.73	0.78	7%	1.07	1.19	11%
ET-CYCC6	0.61	0.65	7%	0.84	0.94	12%
1E4MCYC6	0.73	0.77	6%	0.97	1.07	10%
13DECYC6	0.56	0.59	5%	0.77	0.84	9%
13E5MCC6	0.60	0.63	5%	0.82	0.89	8%
135ECYC6	0.53	0.56	5%	0.72	0.78	8%
ETHENE	2.3	2.3	0%	2.6	2.5	-5%
PROPENE	3.0	3.0	1%	3.1	3.1	-1%
1-BUTENE	2.8	2.9	4%	2.9	3.1	6%
1-PENTEN	2.0	2.1	5%	2.0	2.2	8%
3M-1-BUT	2.0	2.1	5%	2.0	2.2	8%
1-HEXENE	1.40	1.48	6%	1.44	1.6	10%
1-C7-OLE	1.10	1.17	6%	1.13	1.26	11%
1-C8-OLE	0.85	0.91	7%	0.88	0.99	13%
1-C9-OLE	0.70	0.76	8%	0.73	0.84	15%
ISOBUTEN	1.7	1.6	-2%	1.6	1.48	-7%
2M-1-BUT	1.5	1.5	0%	1.6	1.5	-2%
T-2-BUTE	3.1	3.2	1%	3.1	3.0	-2%
C-2-BUTE	3.1	3.2	1%	3.1	3.0	-2%
2-C5-OLE	2.8	2.9	3%	2.7	2.8	3%
2M-2-BUT	2.0	2.0	0%	1.9	1.8	-4%
2-C6-OLE	2.1	2.2	3%	2.1	2.1	3%
2-C7-OLE	1.7	1.8	3%	1.7	1.8	4%
3-C8-OLE	1.7	1.7	5%	1.6	1.8	7%
3-C9-OLE	1.45	1.5	5%	1.43	1.5	7%
13-BUTDE	3.4	3.6	3%	3.4	3.6	4%
ISOPRENE	2.9	3.0	3%	2.8	2.9	3%
CYC-PNTE	2.4	2.5	2%	2.3	2.3	2%
CYC-HEXE	1.8	1.9	4%	1.8	1.9	5%
A-PINENE	1.04	1.08	5%	1.06	1.11	5%
B-PINENE	1.39	1.00	-28%	1.37	1.03	-25%
ACETYLEN	0.16	0.16	-1%	0.27	0.26	-4%
ME-ACTYL	1.30	1.43	10%	1.8	2.1	19%
BENZENE	0.134	0.17	25%	0.113	0.149	32%
TOLUENE	0.86	0.84	-3%	0.52	0.46	-11%
C2-BENZ	0.85	0.83	-3%	0.52	0.46	-11%
N-C3-BEN	0.67	0.65	-3%	0.40	0.36	-11%
I-C3-BEN	0.71	0.69	-3%	0.43	0.38	-11%
S-C4-BEN	0.60	0.58	-3%	0.36	0.32	-11%
O-XYLENE	2.0	2.0	-3%	1.6	1.49	-7%
P-XYLENE	2.1	2.0	-3%	1.6	1.5	-8%
M-XYLENE	2.6	2.5	-4%	2.0	1.8	-9%
135-TMB	3.2	3.0	-8%	2.5	2.2	-14%
123-TMB	2.8	2.6	-7%	2.2	1.9	-13%
124-TMB	2.8	2.6	-7%	2.2	1.9	-13%
TETRALIN	0.30	0.23	-21%	0.106	0.057	-46%
NAPHTHAL	0.37	0.26	-29%	0.077	-2.8E-04	-100%
ME-NAPH	1.03	0.77	-25%	0.63	0.44	-31%
23-DMN	1.6	1.24	-24%	1.12	0.82	-27%
STYRENE	0.70	0.73	5%	-0.24	-0.39	61%

Table C-5 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	SAPRC91	(diff)	SAPRC90	SAPRC91	(diff)
MEOH	0.18	0.18	0%	0.23	0.21	-7%
ETOH	0.42	0.45	7%	0.60	0.66	10%
N-C3-OH	0.71	0.79	10%	0.93	1.11	20%
I-C3-OH	0.17	0.17	-1%	0.26	0.25	-5%
N-C4-OH	0.85	0.93	9%	1.07	1.25	17%
I-C4-OH	0.61	0.66	8%	0.78	0.89	14%
T-C4-OH	0.132	0.132	0%	0.20	0.19	-5%
ME-O-ME	0.24	0.24	-2%	0.46	0.44	-4%
MTBE	0.20	0.20	0%	0.33	0.32	-3%
ETBE	0.63	0.63	0%	0.85	0.82	-4%
FORMALD	2.3	2.2	-3%	1.7	1.5	-11%
ACETALD	1.7	1.8	3%	1.8	1.8	1%
PROPALD	2.1	2.2	6%	2.1	2.2	9%
GLYOXAL	0.70	0.68	-3%	0.58	0.53	-9%
MEGLYOX	4.7	4.5	-3%	3.7	3.3	-10%
ACETONE	0.18	0.18	0%	0.17	0.17	0%
MEK	0.37	0.40	7%	0.45	0.51	13%
BENZALD	-0.18	-0.123	-31%	-1.02	-1.08	6%
PHENOL	0.35	0.37	4%	-0.39	-0.38	-1%
CRESOL	0.73	0.74	2%	-0.47	-0.46	-2%
Incremental Reactivities (gm O3/gm VOC)						
CO	0.054	0.059	9%	0.038	0.039	1%
METHANE	0.0150	0.016	10%	0.0093	0.0096	3%
ETHANE	0.25	0.29	18%	0.17	0.20	21%
PROPANE	0.48	0.57	18%	0.31	0.38	22%
N-C4	1.02	1.22	19%	0.66	0.81	23%
N-C5	1.04	1.22	18%	0.68	0.83	22%
N-C6	0.98	1.16	18%	0.65	0.79	22%
N-C7	0.81	0.96	19%	0.53	0.67	26%
N-C8	0.60	0.74	22%	0.41	0.53	29%
N-C9	0.54	0.66	23%	0.36	0.48	34%
N-C10	0.46	0.58	24%	0.31	0.42	37%
N-C11	0.42	0.52	25%	0.28	0.39	39%
N-C12	0.38	0.47	26%	0.25	0.35	41%
N-C13	0.35	0.44	27%	0.23	0.33	42%
N-C14	0.32	0.41	27%	0.22	0.31	43%
2-ME-C3	1.21	1.38	14%	0.73	0.82	12%
22-DM-C3	0.37	0.46	26%	0.22	0.31	42%
2-ME-C4	1.38	1.6	18%	0.87	1.03	19%
22-DM-C4	0.82	0.98	19%	0.51	0.63	24%
23-DM-C4	1.07	1.22	14%	0.67	0.75	12%
2-ME-C5	1.5	1.9	21%	0.90	1.14	27%
3-ME-C5	1.5	1.8	18%	0.94	1.13	20%
223TM-C4	1.32	1.5	15%	0.79	0.89	14%
23-DM-C6	1.31	1.6	19%	0.78	0.96	23%
24-DM-C6	1.5	1.8	20%	0.86	1.07	25%
33-DM-C5	0.71	0.85	20%	0.46	0.58	26%
2-ME-C6	1.08	1.27	18%	0.68	0.83	22%
3-ME-C6	1.40	1.7	21%	0.83	1.04	26%
224TM-C5	0.93	1.08	17%	0.54	0.68	26%
234TM-C5	1.6	1.9	18%	0.92	1.11	21%
23-DM-C6	1.31	1.6	19%	0.78	0.96	23%
24-DM-C6	1.5	1.8	20%	0.86	1.07	25%

Table C-5 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	SAPRC91	(diff)	SAPRC90	SAPRC91	(diff)
25-DM-C6	1.6	1.9	16%	0.93	1.08	16%
2-ME-C7	0.96	1.15	20%	0.59	0.75	26%
3-ME-C7	0.99	1.18	19%	0.62	0.77	24%
4-ME-C7	1.20	1.46	22%	0.70	0.90	29%
24-DM-C7	1.33	1.6	21%	0.75	0.95	27%
225TM-C6	0.97	1.18	22%	0.58	0.75	29%
4-ET-C7	1.13	1.38	22%	0.64	0.83	29%
4-PR-C7	1.01	1.24	23%	0.56	0.74	31%
24-DM-C7	1.33	1.6	21%	0.75	0.95	27%
36-DE-C8	1.23	1.45	18%	0.69	0.84	22%
CYCC5	2.4	2.9	21%	1.41	1.8	26%
ME-CYCC5	2.8	3.4	19%	1.6	1.9	22%
CYCC6	1.28	1.6	22%	0.74	0.95	29%
13DMCYC5	2.5	3.0	17%	1.38	1.6	19%
ME-CYCC6	1.8	2.2	21%	1.00	1.27	27%
ET-CYCC5	2.3	2.8	20%	1.30	1.6	23%
ET-CYCC6	1.9	2.3	19%	1.02	1.26	24%
1E4MCYC6	2.3	2.7	19%	1.18	1.44	22%
13DECYC6	1.8	2.1	18%	0.93	1.13	21%
13E5MCC6	1.9	2.2	17%	1.00	1.19	20%
135ECYC6	1.7	2.0	17%	0.87	1.05	20%
ETHENE	7.4	8.3	12%	3.2	3.4	5%
PROPENE	9.4	10.7	13%	3.8	4.1	9%
1-BUTENE	8.9	10.4	17%	3.5	4.1	18%
1-PENTEN	6.2	7.3	18%	2.5	2.9	19%
3M-1-BUT	6.2	7.3	18%	2.5	2.9	19%
1-HEXENE	4.4	5.2	18%	1.7	2.1	22%
1-C7-OLE	3.5	4.1	19%	1.38	1.7	23%
1-C8-OLE	2.7	3.2	20%	1.07	1.34	25%
1-C9-OLE	2.2	2.7	20%	0.89	1.13	27%
ISOBUTEN	5.3	5.8	10%	1.9	2.0	3%
2M-1-BUT	4.9	5.5	12%	1.9	2.1	8%
T-2-BUTE	10.0	11.3	13%	3.8	4.1	9%
C-2-BUTE	10.0	11.3	13%	3.8	4.1	9%
2-C5-OLE	8.8	10.2	15%	3.3	3.8	14%
2M-2-BUT	6.4	7.2	12%	2.3	2.5	7%
2-C6-OLE	6.7	7.7	15%	2.5	2.9	15%
2-C7-OLE	5.5	6.4	15%	2.1	2.4	15%
3-C8-OLE	5.3	6.2	17%	2.0	2.4	19%
3-C9-OLE	4.6	5.4	17%	1.7	2.1	19%
13-BUTDE	10.9	12.6	16%	4.2	4.8	15%
ISOPRENE	9.1	10.5	15%	3.4	3.9	14%
CYC-PNTE	7.7	8.8	14%	2.8	3.1	13%
CYC-HEXE	5.7	6.6	16%	2.2	2.6	16%
A-PINENE	3.3	3.8	17%	1.28	1.50	17%
B-PINENE	4.4	3.5	-20%	1.7	1.39	-17%
ACETYLEN	0.50	0.56	11%	0.33	0.35	6%
ME-ACTYL	4.1	5.1	24%	2.2	2.9	32%
BENZENE	0.42	0.59	40%	0.138	0.20	46%
TOLUENE	2.7	3.0	9%	0.63	0.62	-1%
C2-BENZ	2.7	2.9	9%	0.63	0.62	-2%
N-C3-BEN	2.1	2.3	9%	0.49	0.48	-1%
I-C3-BEN	2.2	2.4	9%	0.52	0.51	-1%

Table C-5 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	SAPRC91	(diff)	SAPRC90	SAPRC91	(diff)
S-C4-BEN	1.9	2.1	9%	0.44	0.44	-1%
O-XYLENE	6.5	7.0	8%	2.0	2.0	3%
P-XYLENE	6.6	7.1	8%	2.0	2.0	2%
M-XYLENE	8.2	8.8	7%	2.5	2.5	0%
135-TMB	10.1	10.5	3%	3.1	2.9	-4%
123-TMB	8.9	9.2	4%	2.7	2.6	-3%
124-TMB	8.8	9.2	4%	2.7	2.6	-3%
TETRALIN	0.94	0.83	-12%	0.129	0.077	-40%
NAPHTHAL	1.17	0.93	-21%	0.093	-3.7E-04	-100%
ME-NAPH	3.3	2.7	-16%	0.76	0.59	-23%
23-DMN	5.1	4.4	-15%	1.36	1.11	-19%
STYRENE	2.2	2.6	17%	-0.30	-0.53	79%
MEOH	0.56	0.63	12%	0.28	0.28	3%
ETOH	1.34	1.6	19%	0.72	0.88	22%
N-C3-OH	2.3	2.8	24%	1.13	1.50	33%
I-C3-OH	0.54	0.60	11%	0.32	0.33	6%
N-C4-OH	2.7	3.3	23%	1.30	1.7	29%
I-C4-OH	1.9	2.3	21%	0.94	1.19	26%
T-C4-OH	0.42	0.47	12%	0.25	0.26	5%
ME-O-ME	0.77	0.85	10%	0.56	0.59	6%
MTBE	0.62	0.69	12%	0.41	0.44	8%
ETBE	2.0	2.2	12%	1.03	1.10	7%
FORMALD	7.2	7.8	8%	2.1	2.1	-1%
ACETALD	5.5	6.4	15%	2.2	2.4	12%
PROPALD	6.5	7.8	19%	2.5	3.0	20%
GLYOXAL	2.2	2.4	8%	0.71	0.71	1%
MEGLYOX	14.8	16%	9%	4.5	4.5	-1%
ACETONE	0.56	0.63	12%	0.20	0.22	10%
MEK	1.18	1.41	19%	0.55	0.69	25%
BENZALD	-0.57	-0.43	-23%	-1.24	-1.45	17%
PHENOL	1.12	1.31	17%	-0.47	-0.52	10%
CRESOL	2.3	2.6	14%	-0.58	-0.62	9%
Base ROG	3.2	3.5	12%	1.21	1.34	11%

Table C-6. Differences in RAFs and reactivities from the standard SAPRC-90 mechanism compared to values from the mechanism with aromatics parameters re-optimized after correcting the experimental NOx data. (Only maximum reactivity calculation done. Only differences greater than 0.5% are shown for the RAFs and greater than 1.5% are shown for the model species.)

DMS or Mix	MIR Scale		
	Standard	NOx-Corr	(diff)
LEV and TLEV Exhaust RAFs			
LPG-TLEV	0.50	0.50	1%
E85-TLEV	0.63	0.64	1%
Relative Reactivities (gram basis)			
CO	0.017	0.018	2%
N-C8	0.19	0.20	4%
N-C9	0.17	0.17	2%
N-C10	0.147	0.150	2%
N-C11	0.132	0.136	3%
N-C12	0.119	0.126	6%
N-C13	0.110	0.113	3%
N-C14	0.101	0.098	-3%
23-DM-C4	0.34	0.35	2%
224TM-C5	0.29	0.28	-3%
2-ME-C7	0.30	0.31	2%
36-DE-C8	0.39	0.40	2%
13DMCYC5	0.80	0.82	2%
ET-CYCC6	0.61	0.62	2%
1-C9-OLE	0.70	0.72	2%
BENZENE	0.134	0.137	2%
N-C3-BEN	0.67	0.68	2%
I-C3-BEN	0.71	0.72	2%
O-XYLENE	2.0	2.0	-3%
P-XYLENE	2.1	2.0	-3%
M-XYLENE	2.6	2.5	-3%
TETRALIN	0.30	0.31	6%
NAPHTHAL	0.37	0.39	5%
ME-NAPH	1.03	1.05	2%
STYRENE	0.70	0.71	2%
I-C3-OH	0.17	0.18	4%
BENZALD	-0.18	-0.17	-3%
PHENOL	0.35	0.36	3%
CRESOL	0.73	0.74	
Incremental Reactivities (gm O3/gm VOC)			
CO	0.054	0.056	3%
N-C8	0.60	0.63	5%
N-C9	0.54	0.55	2%
N-C10	0.46	0.47	2%
N-C11	0.42	0.43	3%
N-C12	0.38	0.40	6%
N-C13	0.35	0.36	3%
N-C14	0.32	0.31	-3%

Table C-6 (continued)

DMS or Mix	MIR Scale		
	Standard	NOx-Corr	(diff)
23-DM-C4	1.07	1.10	3%
224TM-C5	0.93	0.90	-3%
2-ME-C7	0.96	0.98	2%
4-ME-C7	1.20	1.22	2%
36-DE-C8	1.23	1.25	2%
13DMCYC5	2.5	2.6	2%
ET-CYCC6	1.9	2.0	2%
13DECYC6	1.8	1.8	2%
1-C8-OLE	2.7	2.7	2%
1-C9-OLE	2.2	2.3	3%
ISOBUTEN	5.3	5.4	2%
BENZENE	0.42	0.43	2%
N-C3-BEN	2.1	2.2	2%
I-C3-BEN	2.2	2.3	2%
S-C4-BEN	1.9	1.9	2%
O-XYLENE	6.5	6.3	-3%
P-XYLENE	6.6	6.4	-3%
M-XYLENE	8.2	8.0	-3%
TETRALIN	0.94	1.00	6%
NAPHTHAL	1.17	1.23	5%
ME-NAPH	3.3	3.3	2%
STYRENE	2.2	2.3	2%
I-C3-OH	0.54	0.56	4%
GLYOXAL	2.2	2.3	2%
BENZALD	-0.57	-0.55	-3%
PHENOL	1.12	1.15	3%
CRESOL	2.3	2.3	2%

Table C-7. Differences in RAFs and reactivities for selected species from the SAPRC-91 mechanism and the "averaged conditions" scenarios, compared to values calculated using the preliminary alternative aromatics mechanism.

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC91	New Aro.	(diff)	SAPRC91	New Aro.	(diff)
LEV and TLEV Exhaust RAFs						
M85	0.37	0.33	-9.	0.36	0.33	-10.
CNG	0.18	0.16	-13.	0.24	0.21	-13.
LPG	0.52	0.46	-12.	0.62	0.54	-13.
E85	0.65	0.59	-10.	0.83	0.73	-12.
PH2	0.97	0.95	-2.	0.99	0.97	-2.
PH2-L	0.96	0.91	-5.	0.98	0.94	-4.
Relative Reactivities (gram basis)						
CO	0.017	0.016	-7.	0.029	0.027	-6.
ETHANE	0.083	0.078	-5.	0.15	0.143	-7.
N-C4	0.35	0.33	-6.	0.62	0.58	-6.
N-C8	0.21	0.21	-2.	0.40	0.40	1.
BR-C8	0.39	0.37	-6.	0.66	0.62	-5.
N-C15	0.109	0.113	5.	0.23	0.23	3.
ETHENE	2.4	2.1	-11.	2.6	2.2	-15.
PROPENE	3.0	2.6	-13.	3.2	2.7	-15.
T-2-BUTE	3.2	2.7	-15.	3.2	2.6	-17.
1-HEXENE	1.49	1.30	-13.	1.6	1.43	-13.
BENZENE	0.17	0.17	2.	0.15	0.19	23.
TOLUENE	0.84	0.89	6.	0.44	0.75	70.
M-XYLENE	2.5	3.1	24.	1.8	2.4	32.
135-TMB	3.0	2.7	-9.	2.2	2.0	-8.
MEOH	0.18	0.16	-9.	0.21	0.19	-12.
ETOH	0.45	0.42	-7.	0.68	0.63	-8.
FORMALD	2.2	1.8	-21.	1.6	1.16	-26.
ACETALD	1.8	1.6	-15.	1.9	1.6	-15.
ACETONE	0.18	0.15	-14.	0.17	0.142	-16.
BENZALD	-0.123	-0.067	-46.	-1.18	-1.05	-11.
CRESOL	0.75	0.65	-13.	-0.54	-0.49	-9.
Incremental Reactivities (gm O3/gm VOC)						
CO	0.061	0.064	6.	0.039	0.042	9.
ETHANE	0.30	0.32	8.	0.20	0.22	9.
N-C4	1.25	1.34	7.	0.82	0.89	9.
N-C8	0.77	0.85	11.	0.52	0.61	17.
BR-C8	1.43	1.5	7.	0.86	0.95	11.
N-C15	0.39	0.47	19.	0.30	0.36	19.
ETHENE	8.5	8.6	1.	3.4	3.4	-1.
PROPENE	11.0	10.9	-1.	4.2	4.1	-2.
T-2-BUTE	11.7	11.3	-4.	4.2	4.0	-3.
1-HEXENE	5.4	5.4	-1.	2.2	2.2	1.

Table C-7 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC91	New Aro.	(diff)	SAPRC91	New Aro.	(diff)
BENZENE	0.61	0.70	16.	0.20	0.29	43.
TOLUENE	3.0	3.7	21.	0.58	1.15	98.
M-XYLENE	9.0	12.7	41.	2.4	3.7	53.
135-TMB	10.8	11.2	4.	2.9	3.1	7.
MEOH	0.64	0.66	3.	0.28	0.29	3.
ETOH	1.6	1.7	6.	0.90	0.96	7.
FORMALD	8.1	7.3	-10.	2.1	1.8	-14.
ACETALD	6.6	6.5	-3.	2.5	2.4	-2.
ACETONE	0.64	0.63	-2.	0.22	0.22	-2.
BENZALD	-0.45	-0.27	-39.	-1.5	-1.6	4.
CRESOL	2.7	2.7	-1.	-0.71	-0.76	6.
Base ROG	3.6	4.1	14.	1.32	1.5	16.

Table C-8. Differences in RAFs and reactivities from the SAPRC-90 mechanism, compared to values from the LCC Mechanism. (The SAPRC-90 values were those calculated in September, 1991.)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	LCC	(diff)	SAPRC90	LCC	(diff)
LEV and TLEV Exhaust RAFs						
M85-TLEV	0.37	0.36	-2%	0.38	0.38	0%
CNG-TLEV	0.18	0.17	-2%	0.22	0.21	-4%
LPG-TLEV	0.50	0.50	1%	0.59	0.60	1%
E85-TLEV	0.63	0.60	-5%	0.77	0.69	-11%
PH2-TLEV	0.98	0.98	0%	1.00	0.99	-1%
PH2-LEV	0.94	0.95	0%	0.97	0.97	0%
Relative Reactivities (gram basis)						
METHANE	0.0047	0.0	-100%	0.0077	0.0	-100%
ETHANE	0.078	0.081	4%	0.136	0.128	-6%
PROPANE	0.15	0.16	8%	0.26	0.28	10%
N-C4	0.32	0.53	63%	0.55	0.83	51%
N-C5	0.33	0.43	30%	0.56	0.67	19%
N-C6	0.31	0.36	14%	0.53	0.56	4%
N-C7	0.26	0.31	19%	0.44	0.48	9%
N-C8	0.19	0.27	38%	0.34	0.42	25%
N-C9	0.17	0.24	40%	0.30	0.37	27%
N-C10	0.148	0.22	46%	0.26	0.34	32%
N-C11	0.134	0.20	47%	0.23	0.31	33%
N-C12	0.120	0.18	50%	0.21	0.28	35%
N-C13	0.111	0.17	50%	0.19	0.26	34%
N-C14	0.102	0.15	52%	0.18	0.24	36%
2-ME-C3	0.38	0.53	38%	0.60	0.83	37%
22-DM-C3	0.117	0.43	265%	0.18	0.67	271%
2-ME-C4	0.44	0.43	-3%	0.72	0.67	-7%
22-DM-C4	0.26	0.36	37%	0.42	0.56	33%
23-DM-C4	0.34	0.36	5%	0.55	0.56	1%
2-ME-C5	0.48	0.36	-27%	0.74	0.56	-25%
3-ME-C5	0.48	0.36	-26%	0.78	0.56	-28%
223TM-C4	0.42	0.31	-27%	0.65	0.48	-26%
23-DM-C6	0.42	0.27	-35%	0.65	0.42	-35%
24-DM-C6	0.48	0.27	-44%	0.71	0.42	-41%
33-DM-C5	0.22	0.31	36%	0.38	0.48	27%
2-ME-C6	0.34	0.31	-10%	0.56	0.48	-15%
3-ME-C6	0.44	0.31	-31%	0.68	0.48	-30%
224TM-C5	0.29	0.27	-9%	0.45	0.42	-6%
234TM-C5	0.51	0.27	-47%	0.76	0.42	-45%
23-DM-C6	0.42	0.27	-35%	0.65	0.42	-35%
24-DM-C6	0.48	0.27	-44%	0.71	0.42	-41%
25-DM-C6	0.52	0.27	-48%	0.77	0.42	-45%
2-ME-C7	0.30	0.27	-12%	0.49	0.42	-14%
3-ME-C7	0.31	0.27	-15%	0.51	0.42	-18%
4-ME-C7	0.38	0.27	-29%	0.58	0.42	-27%
24-DM-C7	0.42	0.24	-43%	0.62	0.37	-39%
225TM-C6	0.31	0.24	-22%	0.48	0.37	-21%
4-ET-C7	0.36	0.24	-33%	0.53	0.37	-29%
4-PR-C7	0.32	0.22	-33%	0.46	0.34	-27%
24-DM-C7	0.42	0.24	-43%	0.62	0.37	-39%
36-DE-C8	0.39	0.18	-54%	0.57	0.28	-51%
CYCC5	0.75	0.44	-42%	1.16	0.68	-41%
ME-CYCC5	0.89	0.36	-59%	1.28	0.57	-55%

Table C-8 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	LCC	(diff)	SAPRC90	LCC	(diff)
CYCC6	0.41	0.36	-10%	0.61	0.57	-7%
13DMCYC5	0.81	0.31	-61%	1.14	0.49	-57%
ME-CYCC6	0.58	0.31	-46%	0.83	0.49	-41%
ET-CYCC5	0.73	0.31	-57%	1.07	0.49	-54%
ET-CYCC6	0.61	0.27	-56%	0.84	0.43	-49%
1E4MCYC6	0.73	0.24	-67%	0.97	0.38	-61%
13DECYC6	0.56	0.22	-61%	0.77	0.34	-56%
13E5MCC6	0.60	0.20	-67%	0.82	0.31	-62%
135ECYC6	0.53	0.18	-66%	0.72	0.29	-60%
ETHENE	2.3	2.4	2%	2.6	2.7	4%
PROPENE	3.0	3.4	13%	3.1	3.3	5%
1-BUTENE	2.8	2.5	-11%	2.9	2.5	-15%
1-PENTEN	2.0	2.0	2%	2.0	2.0	-3%
3M-1-BUT	2.0	2.0	2%	2.0	2.0	-3%
1-HEXENE	1.40	1.7	20%	1.44	1.6	14%
1-C7-OLE	1.10	1.44	31%	1.14	1.41	24%
1-C8-OLE	0.85	1.26	48%	0.88	1.23	40%
1-C9-OLE	0.71	1.12	58%	0.73	1.09	49%
ISOBUTEN	1.7	2.5	50%	1.6	2.5	54%
2M-1-BUT	1.6	2.0	30%	1.6	2.0	25%
T-2-BUTE	3.1	2.5	-20%	3.1	2.5	-21%
C-2-BUTE	3.1	2.5	-20%	3.1	2.5	-21%
2-C5-OLE	2.8	2.0	-28%	2.7	2.0	-28%
2M-2-BUT	2.0	2.0	-1%	1.9	2.0	4%
2-C6-OLE	2.1	1.7	-21%	2.1	1.6	-21%
2-C7-OLE	1.8	1.44	-18%	1.7	1.41	-18%
3-C8-OLE	1.7	1.26	-25%	1.6	1.23	-25%
3-C9-OLE	1.45	1.12	-23%	1.43	1.09	-23%
13-BUTDE	3.4	2.6	-24%	3.4	2.6	-26%
ISOPRENE	2.9	2.1	-28%	2.8	2.0	-28%
CYC-PNTE	2.4	2.1	-14%	2.3	2.0	-12%
CYC-HEXE	1.8	1.7	-4%	1.8	1.7	-7%
A-PINENE	1.04	1.04	0%	1.06	1.01	-4%
B-PINENE	1.39	1.04	-26%	1.37	1.01	-26%
ACETYLEN	0.16	0.0	-100%	0.27	0.0	-100%
ME-ACTYL	1.30	0.0	-100%	1.8	0.0	-100%
BENZENE	0.134	0.131	-3%	0.113	0.20	81%
TOLUENE	0.86	0.84	-2%	0.52	0.60	15%
C2-BENZ	0.85	0.73	-14%	0.52	0.52	0%
N-C3-BEN	0.67	0.65	-3%	0.40	0.46	13%
I-C3-BEN	0.71	0.65	-9%	0.43	0.46	7%
S-C4-BEN	0.60	0.58	-3%	0.36	0.41	13%
O-XYLENE	2.0	2.9	43%	1.6	2.3	41%
P-XYLENE	2.1	2.9	40%	1.6	2.3	38%
M-XYLENE	2.6	2.9	13%	2.0	2.3	12%
135-TMB	3.2	2.6	-19%	2.5	2.0	-21%
123-TMB	2.8	2.6	-8%	2.2	2.0	-9%
124-TMB	2.8	2.6	-8%	2.2	2.0	-9%
TETRALIN	0.30	2.3	680%	0.106	1.8	1616%
NAPHTHAL	0.37	2.4	550%	0.075	1.9	2411%
ME-NAPH	1.04	2.2	111%	0.63	1.7	169%
23-DMN	1.6	2.0	22%	1.12	1.5	38%
STYRENE	0.70	1.36	94%	-0.24	1.33	-644%

Table C-8 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	LCC	(diff)	SAPRC90	LCC	(diff)
MEOH	0.18	0.18	3%	0.23	0.23	2%
ETOH	0.42	0.41	-2%	0.60	0.51	-14%
N-C3-OH	0.71	0.51	-28%	0.93	0.80	-14%
I-C3-OH	0.17	0.51	200%	0.26	0.80	207%
N-C4-OH	0.85	0.41	-51%	1.07	0.65	-39%
I-C4-OH	0.61	0.41	-32%	0.78	0.65	-17%
T-C4-OH	0.132	0.41	214%	0.20	0.65	218%
ME-O-ME	0.24	0.67	173%	0.46	1.04	126%
MTBE	0.20	0.22	11%	0.33	0.37	10%
ETBE	0.63	0.30	-52%	0.85	0.47	-45%
FORMALD	2.3	2.2	-3%	1.7	1.8	3%
ACETALD	1.7	1.8	1%	1.8	1.7	-3%
PROPALD	2.1	1.34	-35%	2.1	1.32	-36%
ACETONE	0.18	0.77	333%	0.17	0.80	381%
MEK	0.37	0.62	65%	0.45	0.65	43%
BENZALD	-0.18	0.0	-100%	-1.02	0.0	-100%
PHENOL	0.36	0.83	131%	-0.39	0.58	-250%
CRESOL	0.73	0.83	13%	-0.47	-0.88	86%
Incremental Reactivities (gm O3/gm VOC)						
CO	0.054			0.038		
METHANE	0.0150	0.0	-100%	0.0093	0.0	-100%
ETHANE	0.25	0.22	-11%	0.17	0.135	-18%
PROPANE	0.48	0.44	-8%	0.31	0.30	-4%
N-C4	1.02	1.43	39%	0.66	0.87	32%
N-C5	1.04	1.15	11%	0.68	0.70	3%
N-C6	0.98	0.96	-2%	0.65	0.59	-9%
N-C7	0.81	0.83	2%	0.53	0.51	-5%
N-C8	0.61	0.73	18%	0.41	0.44	9%
N-C9	0.54	0.65	20%	0.36	0.40	10%
N-C10	0.47	0.58	25%	0.31	0.36	15%
N-C11	0.42	0.53	25%	0.28	0.32	16%
N-C12	0.38	0.49	28%	0.25	0.30	18%
N-C13	0.35	0.45	28%	0.24	0.27	17%
N-C14	0.32	0.42	29%	0.22	0.26	18%
2-ME-C3	1.21	1.43	18%	0.73	0.87	20%
22-DM-C3	0.37	1.15	211%	0.22	0.70	223%
2-ME-C4	1.38	1.15	-17%	0.87	0.70	-19%
22-DM-C4	0.82	0.96	17%	0.51	0.59	16%
23-DM-C4	1.07	0.96	-10%	0.67	0.59	-12%
2-ME-C5	1.5	0.96	-37%	0.90	0.59	-34%
3-ME-C5	1.5	0.96	-37%	0.94	0.59	-38%
223TM-C4	1.32	0.83	-37%	0.79	0.51	-36%
23-DM-C6	1.32	0.73	-45%	0.78	0.44	-43%
24-DM-C6	1.5	0.73	-52%	0.86	0.44	-48%
33-DM-C5	0.71	0.83	16%	0.46	0.51	11%
2-ME-C6	1.08	0.83	-23%	0.68	0.51	-26%
3-ME-C6	1.40	0.83	-41%	0.83	0.51	-39%
224TM-C5	0.93	0.73	-22%	0.54	0.44	-18%
234TM-C5	1.6	0.73	-55%	0.92	0.44	-52%
23-DM-C6	1.32	0.73	-45%	0.78	0.44	-43%
24-DM-C6	1.5	0.73	-52%	0.86	0.44	-48%
25-DM-C6	1.6	0.73	-56%	0.93	0.44	-52%
2-ME-C7	0.96	0.73	-25%	0.60	0.44	-25%

Table C-8 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	LCC	(diff)	SAPRC90	LCC	(diff)
3-ME-C7	0.99	0.73	-27%	0.62	0.44	-28%
4-ME-C7	1.20	0.73	-40%	0.70	0.44	-36%
24-DM-C7	1.34	0.65	-52%	0.75	0.40	-47%
225TM-C6	0.97	0.65	-33%	0.58	0.40	-32%
4-ET-C7	1.14	0.65	-43%	0.64	0.40	-38%
4-PR-C7	1.01	0.58	-42%	0.56	0.36	-37%
24-DM-C7	1.34	0.65	-52%	0.75	0.40	-47%
36-DE-C8	1.23	0.49	-61%	0.69	0.30	-57%
CYCC5	2.4	1.18	-50%	1.41	0.72	-49%
ME-CYCC5	2.8	0.98	-65%	1.6	0.60	-61%
CYCC6	1.28	0.98	-23%	0.74	0.60	-19%
13DMCYC5	2.5	0.84	-67%	1.39	0.52	-63%
ME-CYCC6	1.8	0.84	-54%	1.00	0.52	-48%
ET-CYCC5	2.3	0.84	-63%	1.30	0.52	-60%
ET-CYCC6	1.9	0.74	-62%	1.02	0.45	-56%
1E4MCYC6	2.3	0.66	-71%	1.18	0.40	-66%
13DECYC6	1.8	0.59	-67%	0.93	0.36	-61%
13E5MCC6	1.9	0.54	-72%	1.00	0.33	-67%
135ECYC6	1.7	0.49	-71%	0.87	0.30	-65%
ETHENE	7.3	6.4	-13%	3.2	2.9	-9%
PROPENE	9.4	9.1	-4%	3.8	3.5	-8%
1-BUTENE	8.9	6.8	-24%	3.5	2.6	-26%
1-PENTEN	6.2	5.4	-13%	2.5	2.1	-16%
3M-1-BUT	6.2	5.4	-13%	2.5	2.1	-16%
1-HEXENE	4.4	4.5	2%	1.7	1.7	-1%
1-C7-OLE	3.5	3.9	11%	1.38	1.48	8%
1-C8-OLE	2.7	3.4	26%	1.07	1.30	22%
1-C9-OLE	2.2	3.0	35%	0.89	1.15	30%
ISOBUTEN	5.3	6.8	28%	1.9	2.6	34%
2M-1-BUT	4.9	5.4	11%	1.9	2.1	9%
T-2-BUTE	9.9	6.8	-32%	3.8	2.6	-31%
C-2-BUTE	9.9	6.8	-32%	3.8	2.6	-31%
2-C5-OLE	8.8	5.4	-38%	3.3	2.1	-37%
2M-2-BUT	6.4	5.4	-15%	2.3	2.1	-10%
2-C6-OLE	6.7	4.5	-32%	2.5	1.7	-31%
2-C7-OLE	5.5	3.9	-30%	2.1	1.48	-28%
3-C8-OLE	5.3	3.4	-36%	2.0	1.30	-35%
3-C9-OLE	4.6	3.0	-34%	1.7	1.15	-33%
13-BUTDE	10.9	7.0	-35%	4.2	2.7	-35%
ISOPRENE	9.1	5.6	-38%	3.4	2.1	-37%
CYC-PNTE	7.7	5.6	-27%	2.8	2.1	-23%
CYC-HEXE	5.7	4.6	-18%	2.2	1.8	-19%
A-PINENE	3.3	2.8	-15%	1.28	1.07	-16%
B-PINENE	4.4	2.8	-36%	1.7	1.07	-36%
ACETYLEN	0.50	0.0	-100%	0.33	0.0	-100%
ME-ACTYL	4.1	0.0	-100%	2.2	0.0	-100%
BENZENE	0.42	0.35	-17%	0.137	0.22	58%
TOLUENE	2.7	2.3	-17%	0.63	0.63	0%
C2-BENZ	2.7	2.0	-27%	0.63	0.55	-13%
N-C3-BEN	2.1	1.7	-18%	0.49	0.48	-1%
I-C3-BEN	2.2	1.7	-22%	0.52	0.48	-7%
S-C4-BEN	1.9	1.6	-17%	0.44	0.43	-1%
O-XYLENE	6.5	7.9	22%	1.9	2.4	23%

Table C-8 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	LCC	(diff)	SAPRC90	LCC	(diff)
P-XYLENE	6.6	7.9	19%	2.0	2.4	20%
M-XYLENE	8.2	7.9	-3%	2.5	2.4	-2%
135-TMB	10.1	7.0	-31%	3.1	2.1	-31%
123-TMB	8.8	7.0	-21%	2.7	2.1	-21%
124-TMB	8.8	7.0	-21%	2.7	2.1	-21%
TETRALIN	0.95	6.3	566%	0.129	1.9	1395%
NAPHTHAL	1.18	6.5	455%	0.091	2.0	2088%
ME-NAPH	3.3	5.9	80%	0.76	1.8	134%
23-DMN	5.1	5.4	4%	1.36	1.6	20%
STYRENE	2.2	3.7	65%	-0.30	1.40	-574%
MEOH	0.56	0.49	-12%	0.28	0.25	-11%
ETOH	1.34	1.12	-16%	0.73	0.54	-25%
N-C3-OH	2.3	1.38	-39%	1.13	0.84	-25%
I-C3-OH	0.54	1.38	156%	0.32	0.84	168%
N-C4-OH	2.7	1.12	-58%	1.30	0.68	-47%
I-C4-OH	1.9	1.12	-42%	0.94	0.68	-28%
T-C4-OH	0.42	1.12	168%	0.25	0.68	177%
ME-O-ME	0.77	1.8	133%	0.56	1.10	97%
MTBE	0.62	0.59	-5%	0.41	0.39	-5%
ETBE	2.0	0.81	-59%	1.03	0.50	-52%
FORMALD	7.2	5.9	-17%	2.1	1.9	-10%
ACETALD	5.5	4.8	-13%	2.2	1.8	-15%
PROPALD	6.5	3.6	-45%	2.5	1.40	-44%
GLYOXAL	2.2			0.70		
MEGLYOX	14.8			4.5		
ACETONE	0.56	2.1	270%	0.20	0.85	319%
MEK	1.18	1.7	41%	0.55	0.68	25%
BENZALD	-0.55	0.0	-100%	-1.23	0.0	-100%
PHENOL	1.13	2.2	97%	-0.47	0.62	-231%
CRESOL	2.3	2.2	-3%	-0.57	-0.93	62%
Base ROG	3.2	2.7	-15%	1.21	1.06	-13%

Table C-9. Differences in RAFs and reactivities from the SAPRC-90 mechanism, compared to values from the Carbon Bond IV (CB4) Mechanism. (The SAPRC-90 values were those calculated in September, 1991.)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	CB4	(diff)	SAPRC90	CB4	(diff)
LEV and TLEV Exhaust RAFs						
M85-TLEV	0.37	0.39	5%	0.38	0.40	4%
CNG-TLEV	0.18	0.18	2%	0.22	0.22	0%
LPG-TLEV	0.50	0.54	7%	0.59	0.66	11%
E85-TLEV	0.63	0.64	1%	0.77	0.82	6%
PH2-TLEV	0.98	1.01	3%	1.00	1.04	4%
Relative Reactivities (gram basis)						
CO	0.017	0.015	-12%	0.031	0.028	-11%
METHANE	0.0047	0.0	-100%	0.0077	0.0	-100%
ETHANE	0.078	0.064	-18%	0.136	0.109	-20%
PROPANE	0.15	0.16	7%	0.26	0.28	8%
N-C4	0.32	0.33	2%	0.55	0.56	3%
N-C5	0.33	0.33	2%	0.56	0.57	1%
N-C6	0.31	0.33	8%	0.53	0.57	7%
N-C7	0.26	0.34	31%	0.44	0.57	30%
N-C8	0.19	0.34	73%	0.34	0.57	70%
N-C9	0.17	0.34	97%	0.30	0.57	94%
N-C10	0.148	0.34	128%	0.26	0.57	124%
N-C11	0.134	0.34	153%	0.23	0.58	148%
N-C12	0.120	0.34	183%	0.21	0.58	176%
N-C13	0.111	0.34	205%	0.19	0.58	197%
N-C14	0.102	0.34	232%	0.18	0.58	223%
2-ME-C3	0.38	0.33	-13%	0.60	0.56	-7%
22-DM-C3	0.117	0.27	129%	0.18	0.45	152%
2-ME-C4	0.44	0.33	-24%	0.72	0.57	-21%
22-DM-C4	0.26	0.33	29%	0.42	0.57	36%
23-DM-C4	0.34	0.33	-1%	0.55	0.57	3%
2-ME-C5	0.48	0.33	-31%	0.74	0.57	-23%
3-ME-C5	0.48	0.33	-30%	0.78	0.57	-27%
223TM-C4	0.42	0.34	-20%	0.65	0.57	-12%
23-DM-C6	0.42	0.34	-19%	0.65	0.57	-11%
24-DM-C6	0.48	0.34	-29%	0.71	0.57	-19%
33-DM-C5	0.22	0.34	50%	0.38	0.57	51%
2-ME-C6	0.34	0.34	-2%	0.56	0.57	2%
3-ME-C6	0.44	0.34	-24%	0.68	0.57	-17%
224TM-C5	0.29	0.34	15%	0.45	0.57	28%
234TM-C5	0.51	0.34	-34%	0.76	0.57	-25%
23-DM-C6	0.42	0.34	-19%	0.65	0.57	-11%
24-DM-C6	0.48	0.34	-29%	0.71	0.57	-19%
25-DM-C6	0.52	0.34	-35%	0.77	0.57	-25%
2-ME-C7	0.30	0.34	10%	0.49	0.57	16%
3-ME-C7	0.31	0.34	7%	0.51	0.57	12%
4-ME-C7	0.38	0.34	-12%	0.58	0.57	-1%
24-DM-C7	0.42	0.34	-20%	0.62	0.57	-7%
225TM-C6	0.31	0.34	10%	0.48	0.57	20%
4-ET-C7	0.36	0.34	-6%	0.53	0.57	8%
4-PR-C7	0.32	0.34	6%	0.46	0.57	24%
24-DM-C7	0.42	0.34	-20%	0.62	0.57	-7%
36-DE-C8	0.39	0.34	-13%	0.57	0.58	1%
CYCC5	0.75	0.34	-54%	1.16	0.58	-50%
ME-CYCC5	0.89	0.34	-62%	1.28	0.58	-55%

Table C-9 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	CB4	(diff)	SAPRC90	CB4	(diff)
CYCC6	0.41	0.34	-15%	0.61	0.58	-5%
13DMCYC5	0.81	0.34	-57%	1.14	0.58	-49%
ME-CYCC6	0.58	0.34	-41%	0.83	0.58	-30%
ET-CYCC5	0.73	0.34	-53%	1.07	0.58	-46%
ET-CYCC6	0.61	0.34	-44%	0.84	0.58	-31%
1E4MCYC6	0.73	0.34	-53%	0.97	0.58	-40%
13DECYC6	0.56	0.34	-39%	0.77	0.58	-24%
13E5MCC6	0.60	0.34	-43%	0.82	0.58	-29%
135ECYC6	0.53	0.34	-36%	0.72	0.58	-19%
ETHENE	2.3	2.4	3%	2.6	2.7	5%
PROPENE	3.0	3.4	14%	3.1	3.6	15%
1-BUTENE	2.8	2.6	-7%	2.9	2.8	-3%
1-PENTEN	2.0	2.2	10%	2.0	2.4	17%
3M-1-BUT	2.0	2.2	10%	2.0	2.4	17%
1-HEXENE	1.40	1.9	33%	1.44	2.1	44%
ISOBUTEN	1.7	2.6	57%	1.6	2.8	77%
2M-1-BUT	1.6	2.2	40%	1.6	2.4	51%
T-2-BUTE	3.1	2.9	-6%	3.1	3.1	0%
C-2-BUTE	3.1	2.9	-6%	3.1	3.1	0%
2M-2-BUT	2.0	1.38	-32%	1.9	1.6	-16%
13-BUTDE	3.4	4.2	22%	3.4	4.0	16%
ISOPRENE	2.9	4.7	64%	2.8	4.3	54%
CYC-PNTE	2.4	2.2	-8%	2.3	2.4	6%
CYC-HEXE	1.8	1.9	7%	1.8	2.1	17%
A-PINENE	1.04	1.29	25%	1.06	1.5	44%
B-PINENE	1.39	1.29	-7%	1.37	1.5	11%
ACETYLEN	0.16	0.18	16%	0.27	0.31	16%
ME-ACTYL	1.30	1.8	37%	1.8	2.1	18%
BENZENE	0.134	0.062	-54%	0.113	0.105	-8%
TOLUENE	0.86	0.57	-34%	0.52	-0.23	-145%
C2-BENZ	0.85	0.54	-37%	0.52	-0.128	-125%
N-C3-BEN	0.67	0.52	-23%	0.40	-0.046	-111%
I-C3-BEN	0.71	0.52	-27%	0.43	-0.046	-111%
S-C4-BEN	0.60	0.50	-17%	0.36	0.019	-95%
O-XYLENE	2.0	2.6	29%	1.6	2.0	26%
P-XYLENE	2.1	2.6	27%	1.6	2.0	23%
M-XYLENE	2.6	2.6	2%	2.0	2.0	0%
135-TMB	3.2	2.4	-26%	2.5	1.9	-26%
123-TMB	2.8	2.4	-15%	2.2	1.9	-16%
124-TMB	2.8	2.4	-15%	2.2	1.9	-16%
TETRALIN	0.30	2.2	629%	0.106	1.8	1550%
NAPHTHAL	0.37	2.3	508%	0.075	1.8	2314%
ME-NAPH	1.04	2.1	100%	0.63	1.7	168%
23-DMN	1.6	1.9	18%	1.12	1.6	42%
STYRENE	0.70	1.32	89%	-0.24	0.43	-277%
MEOH	0.18	0.17	-3%	0.23	0.21	-7%
ETOH	0.42	0.41	-4%	0.60	0.59	-1%
N-C3-OH	0.71	0.24	-66%	0.93	0.41	-56%
I-C3-OH	0.17	0.24	41%	0.26	0.41	57%
N-C4-OH	0.85	0.26	-69%	1.07	0.44	-59%
I-C4-OH	0.61	0.26	-57%	0.78	0.44	-43%
T-C4-OH	0.132	0.26	97%	0.20	0.44	116%

Table C-9 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	CB4	(diff)	SAPRC90	CB4	(diff)
ME-O-ME	0.24	0.21	-15%	0.46	0.35	-23%
MTBE	0.20	0.27	39%	0.33	0.46	38%
ETBE	0.63	0.28	-55%	0.85	0.48	-43%
FORMALD	2.3	2.8	26%	1.7	2.2	29%
ACETALD	1.7	1.9	7%	1.8	2.0	11%
PROPALD	2.1	1.5	-27%	2.1	1.6	-20%
MEGLYOX	4.7	5.9	26%	3.7	4.7	27%
ACETONE	0.18	0.17	-6%	0.17	0.28	68%
MEK	0.37	0.20	-46%	0.45	0.34	-25%
BENZALD	-0.18	0.0	-100%	-1.02	0.0	-100%
PHENOL	0.36	0.0	-100%	-0.39	0.0	-100%
CRESOL	0.73	0.89	21%	-0.47	0.134	-128%
Incremental Reactivities (gm O3/gm VOC)						
CO	0.054	0.052	-5%	0.038	0.033	-14%
METHANE	0.0150	0.0	-100%	0.0093	0.0	-100%
ETHANE	0.25	0.22	-11%	0.17	0.128	-22%
PROPANE	0.48	0.56	17%	0.31	0.33	5%
N-C4	1.02	1.14	11%	0.66	0.66	0%
N-C5	1.04	1.15	11%	0.68	0.67	-2%
N-C6	0.98	1.15	17%	0.65	0.67	4%
N-C7	0.81	1.16	42%	0.53	0.67	26%
N-C8	0.61	1.16	89%	0.41	0.67	65%
N-C9	0.54	1.16	115%	0.36	0.68	89%
N-C10	0.47	1.16	149%	0.31	0.68	118%
N-C11	0.42	1.16	176%	0.28	0.68	142%
N-C12	0.38	1.16	208%	0.25	0.68	168%
N-C13	0.35	1.17	232%	0.24	0.68	188%
N-C14	0.32	1.17	261%	0.22	0.68	214%
2-ME-C3	1.21	1.14	-6%	0.73	0.66	-9%
22-DM-C3	0.37	0.92	149%	0.22	0.53	145%
2-ME-C4	1.38	1.15	-17%	0.87	0.67	-23%
22-DM-C4	0.82	1.15	40%	0.51	0.67	32%
23-DM-C4	1.07	1.15	8%	0.67	0.67	0%
2-ME-C5	1.5	1.15	-25%	0.90	0.67	-25%
3-ME-C5	1.5	1.15	-24%	0.94	0.67	-29%
223TM-C4	1.32	1.16	-12%	0.79	0.67	-14%
23-DM-C6	1.32	1.16	-12%	0.78	0.67	-14%
24-DM-C6	1.5	1.16	-23%	0.86	0.67	-22%
33-DM-C5	0.71	1.16	63%	0.46	0.67	47%
2-ME-C6	1.08	1.16	7%	0.68	0.67	-1%
3-ME-C6	1.40	1.16	-17%	0.83	0.67	-19%
224TM-C5	0.93	1.16	25%	0.54	0.67	24%
234TM-C5	1.6	1.16	-28%	0.92	0.67	-27%
23-DM-C6	1.32	1.16	-12%	0.78	0.67	-14%
24-DM-C6	1.5	1.16	-23%	0.86	0.67	-22%
25-DM-C6	1.6	1.16	-29%	0.93	0.67	-27%
2-ME-C7	0.96	1.16	20%	0.60	0.67	13%
3-ME-C7	0.99	1.16	17%	0.62	0.67	9%
4-ME-C7	1.20	1.16	-4%	0.70	0.67	-3%
24-DM-C7	1.34	1.16	-13%	0.75	0.68	-10%
225TM-C6	0.97	1.16	20%	0.58	0.68	17%
4-ET-C7	1.14	1.16	2%	0.64	0.68	5%
4-PR-C7	1.01	1.16	15%	0.56	0.68	20%

Table C-9 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	CB4	(diff)	SAPRC90	CB4	(diff)
24-DM-C7	1.34	1.16	-13%	0.75	0.68	-10%
36-DE-C8	1.23	1.16	-5%	0.69	0.68	-2%
CYCC5	2.4	1.18	-50%	1.41	0.69	-51%
ME-CYCC5	2.8	1.18	-58%	1.6	0.69	-56%
CYCC6	1.28	1.18	-8%	0.74	0.69	-7%
13DMCYC5	2.5	1.18	-54%	1.39	0.69	-50%
ME-CYCC6	1.8	1.18	-36%	1.00	0.69	-31%
ET-CYCC5	2.3	1.18	-49%	1.30	0.69	-47%
ET-CYCC6	1.9	1.18	-39%	1.02	0.69	-33%
1E4MCYC6	2.3	1.18	-49%	1.18	0.69	-42%
13DECYC6	1.8	1.18	-34%	0.93	0.69	-26%
13E5MCC6	1.9	1.18	-38%	1.00	0.69	-31%
135ECYC6	1.7	1.18	-30%	0.87	0.69	-21%
ETHENE	7.3	8.2	12%	3.2	3.2	2%
PROPENE	9.4	11.7	24%	3.8	4.2	12%
1-BUTENE	8.9	9.0	2%	3.5	3.3	-5%
1-PENTEN	6.2	7.5	20%	2.5	2.8	14%
3M-1-BUT	6.2	7.5	20%	2.5	2.8	14%
1-HEXENE	4.4	6.4	45%	1.7	2.4	40%
ISOBUTEN	5.3	9.0	71%	1.9	3.3	72%
2M-1-BUT	4.9	7.5	52%	1.9	2.8	47%
T-2-BUTE	9.9	10.1	2%	3.8	3.7	-2%
C-2-BUTE	9.9	10.1	2%	3.8	3.7	-2%
2M-2-BUT	6.4	4.8	-26%	2.3	1.9	-18%
13-BUTDE	10.9	14.5	33%	4.2	4.7	13%
ISOPRENE	9.1	16%	79%	3.4	5.1	50%
CYC-PNTE	7.7	7.7	0%	2.8	2.9	4%
CYC-HEXE	5.7	6.6	16%	2.2	2.5	14%
A-PINENE	3.3	4.5	36%	1.28	1.8	40%
B-PINENE	4.4	4.5	1%	1.7	1.8	8%
ACETYLEN	0.50	0.64	26%	0.33	0.37	12%
ME-ACTYL	4.1	6.1	49%	2.2	2.5	15%
BENZENE	0.42	0.21	-50%	0.137	0.123	-10%
TOLUENE	2.7	2.0	-28%	0,63	-0.28	-144%
C2-BENZ	2.7	1.9	-31%	0.63	-0.15	-124%
N-C3-BEN	2.1	1.8	-16%	0.49	-0.055	-111%
I-C3-BEN	2.2	1.8	-21%	0.52	-0.055	-111%
S-C4-BEN	1.9	1.7	-10%	0.44	0.022	-95%
O-XYLENE	6.5	9.1	41%	1.9	2.4	22%
P-XYLENE	6.6	9.1	38%	2.0	2.4	20%
M-XYLENE	8.2	9.1	12%	2.5	2.4	-3%
135-TMB	10.1	8.2	-19%	3.1	2.2	-28%
123-TMB	8.8	8.2	-8%	2.7	2.2	-18%
124-TMB	8.8	8.2	-7%	2.7	2.2	-18%
TETRALIN	0.95	7.5	693%	0.129	2.1	1505%
NAPHTHAL	1.18	7.8	561%	0.091	2.1	2247%
ME-NAPH	3.3	7.1	118%	0.76	2.0	160%
23-DMN	5.1	6.6	29%	1.36	1.9	38%
STYRENE	2.2	4.6	106%	-0.30	0.51	-272%
MEOH	0.56	0.59	5%	0.28	0.25	-9%
ETOH	1.34	1.40	5%	0.73	0.70	-4%
N-C3-OH	2.3	0.83	-63%	1.13	0.48	-57%

Table C-9 (continued)

DMS or Mix	MIR Scale			MOIR Scale		
	SAPRC90	CB4	(diff)	SAPRC90	CB4	(diff)
I-C3-OH	0.54	0.83	54%	0.32	0.48	52%
N-C4-OH	2.7	0.89	-67%	1.30	0.52	-60%
I-C4-OH	1.9	0.89	-54%	0.94	0.52	-45%
T-C4-OH	0.42	0.89	114%	0.25	0.52	110%
ME-O-ME	0.77	0.72	-7%	0.56	0.42	-25%
MTBE	0.62	0.94	51%	0.41	0.55	35%
ETBE	2.0	0.97	-51%	1.03	0.57	-45%
FORMALD	7.2	9.8	37%	2.1	2.6	25%
ACETALD	5.5	6.5	17%	2.2	2.3	8%
PROPALD	6.5	5.2	-21%	2.5	1.9	-22%
MEGLYOX	14.8	20.	38%	4.5	5.6	24%
ACETONE	0.56	0.57	2%	0.20	0.33	64%
MEK	1.18	0.69	-42%	0.55	0.40	-27%
BENZALD	-0.55	0.0	-100%	-1.23	0.0	-100%
PHENOL	1.13	0.0	-100%	-0.47	0.0	-100%
CRESOL	2.3	3.1	32%	-0.57	0.16	-128%
Base ROG	3.2	3.4	9%	1.21	1.18	-3%