CALCULATION OF REACTIVITY SCALES USING AN UPDATED CARBON BOND IV MECHANISM

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by

William P. L. Carter

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ABSTRACT

This report describes a calculation of the Maximum Incremental Reactivity (MIR) and the Maximum Ozone Incremental Reactivity (MOIR) scales using an updated version of the Carbon Bond IV chemical mechanism which is being used in the air quality modeling in Phase II of the Auto/Oil Air Quality Improvement Research Program. Except for the mechanism, the methodology and model scenarios employed are essentially the same as used to calculate the MIR and MOIR scales used in the California Air Resources Board "Clean Fuels/Low Emissions Vehicle" regulations.

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TABLE OF CONTENTS

LIST OF TABLES

INTRODUCTION

In 1991 the California Air Resources Board adopted the Maximum Incremental Reactivity (MIR) scale for deriving reactivity adjustment factors (RAFs) in its "Clean Fuels/Low Emissions Vehicle" regulations (CARB, 1991). These RAFs are intended to place regulation of volatile organic compounds (VOCs) in exhausts from alternatively-fueled vehicles on an equal ozone impact basis. The ozone impact is quantified by the MIR scale, which gives the amount of additional ozone calculated to be formed when small amounts of various VOCs are added to the emissions, divided by the amount of VOC emitted, for environmental conditions where the VOCs have their greatest effect on ozone formation (Carter, 1993a,b). The MIR scale was calculated using simple one-cell model scenarios representing 39 different urban areas in the United States (Bauges, 1990), and the atmospheric chemical reactions of the VOCs were represented in these calculations using SAPRC-90 chemical mechanism (Carter, 1990; 1993a).

As part of the work being carried out for the Auto/Oil Air Quality Improvement Research Program, Systems Applications International (SAI) is conducting a series of airshed model calculations to estimate the ozone impacts of different fuel/vehicle systems. In addition, SAI and the Auto/Oil Program are calculating reactivity-weighted VOC emissions for comparison to mass emissions and airshed model results. Most of the model calculations which are to be conducted for Phase II of this program will utilize an updated version of the Carbon Bond IV mechanism (Gery et al., 1988) implemented in the Urban Airshed Model (UAM). This updated version of the mechanism is somewhat different from that used in Phase I of the Auto/Oil Program and is different from that used in the regulatory version of the UAM (UAM 6.2). All versions of the Carbon Bond IV mechanism have significant differences with the SAPRC-90 mechanism which was used to calculate the MIR scale adopted by the CARB. To be able to compare UAM predictions with reactivity-weighted VOC emissions for a consistent chemical mechanism, it is necessary to develop modified reactivity scales using the Carbon Bond mechanism. For a consistent comparison, the modified scale should be developed using the same methodology as used when developing MIR and the other SAPRC-90 scales, except for the different chemical mechanism.

To address this need, SAI contracted the author to develop the MIR and other reactivity scales using the same version of the Carbon Bond mechanism which will be used in Phase II of the Auto/Oil Program. This report gives the mechanism and methodology used and the resulting reactivity scales.

CHEMICAL MECHANISM

A description of the Carbon Bond mechanism and the model species it uses is given by Gery et al. (1988), and that discussion is not duplicated here. Table 1 gives a listing of the version of the Carbon Bond IV mechanism which was used in this study. The assignments of Carbon Bond species to SAPRC detailed model species are given in Table 2. Table 3 gives the photolysis rates, as a function of zenith angle, which were used in the simulations. These were supplied by SAI and are based on recent literature values (Yarwood, private communication). Computer files implementing this mechanism are being sent to SAI along with this report, and are available from the author upon request.

The implementation procedure used in this study is as follows. An earlier version of the mechanism, adopted from OZIPR input files, had already been implemented in SAPRC software. These were sent to Greg Yarwood of SAI for correction and updates. The corrected files were returned, both in hardcopy and computer-readable form, and were implemented in the software used for reactivity calculations.

A discussion of the changes made to the Carbon Bond mechanism for this study is beyond the scope of this report. The major changes were the updates in the PAN rate constants, the addition of XO2+HO2 and other peroxy + peroxy reactions, correction to the methanol rate constant, and re-assignments of the Carbon Bond species to detailed model species. The re-assignments of the Carbon Bond species to detailed model species were necessary to achieve consistency with the assignments used to develop emissions inventories for the UAM in the Auto/Oil modeling. Some of the re-assignments caused significant changes in predicted reactivities of individual model species, as will be seen later.

Table 1. Listing of the Carbon Bond Mechanism as used in the Base Case Simulations.

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
Standard Mechanism					
1	(Phot. Set = NO2CB)				NO2 + HV = NO + O
2	4.21E+06	8.38E+04	-2.33	0.00	O = O3
3	2.75E+01	2.64E+03	2.72	0.00	O3 + NO = NO2
4	1.37E+04	(No T Dependence)			O + NO2 = NO
5	2.27E+03	2.30E+02	-1.37	0.00	O + NO2 = NO3
6	2.40E+03	3.23E+02	-1.20	0.00	O + NO = NO2
7	5.00E-02	1.76E+02	4.87	0.00	O3 + NO2 = NO3
8	(Same k as Reaction 1)				O3 + HV + #5.3E-2 = O
9	(Phot. Set = O3O1DCB)				O3 + HV = O1D
10	4.21E+05	1.15E+05	-0.78	0.00	O1D = O
11	3.26E+00	(No T Dependence)			H2O + O1D = #2 OH
12	1.02E+02	2.34E+03	1.87	0.00	O3 + OH = HO2
13	3.04E+00	2.10E+01	1.15	0.00	O3 + HO2 = OH
14	(Same k as Reaction 1)				NO3 + HV + #33.9 = #.89 NO2 + #.89 O + #.11 NO
15	4.39E+04	1.91E+04	-0.50	0.00	NO3 + NO = #2 NO2
16	6.07E-01	3.66E+01	2.44	0.00	NO3 + NO2 = NO + NO2
17	1.84E+03	7.85E+02	-0.51	0.00	NO3 + NO2 = N2O5
18	1.90E-06	(No T Dependence)			N2O5 + H2O = #2 HNO3
19	3.54E+00	2.11E+16	21.65	0.00	N2O5 = NO3 + NO2
20	1.52E-04	2.60E-05	-1.05	0.00	NO + NO = #2 NO2
21	2.60E-08	1.68E-17	-12.61	0.00	NO + NO2 + H2O = #2 HONO
22	9.62E+03	6.55E+02	-1.60	0.00	OH + NO = HONO
23	(Same k as Reaction 1)				HONO + HV + #.1975 = OH + NO
24	9.77E+03	(No T Dependence)			OH + HONO = NO2
25	1.50E-05	(No T Dependence)			HONO + HONO = NO + NO2
26	1.65E+04	1.54E+03	-1.42	0.00	OH + NO2 = HNO3
27	2.13E+02	7.60E+00	-1.99	0.00	OH + HNO3 = NO3
28	1.22E+04	5.48E+03	-0.48	0.00	HO2 + NO = OH + NO2
29	1.99E+03	1.64E+02	-1.49	0.00	HO2 + NO2 = PNA
30	6.41E+00	2.88E+15	20.11	0.00	PNA = HO2 + NO2
31	6.77E+03	1.91E+03	-0.76	0.00	OH + PNA = NO2
32	4.04E+03	8.74E+01	-2.29	0.00	HO2 + HO2 = H2O2
33	1.92E-01	7.69E-10	-11.53	0.00	HO2 + HO2 + H2O = H2O2
34	(Phot. Set = HCHOMCB)				H2O2 + HV + #.189 = #2 OH
35	2.53E+03	4.72E+03	0.37	0.00	OH + H2O2 = HO2
36	3.22E+02	(No T Dependence)			OH + CO = HO2
37	1.50E+04	(No T Dependence)			HCHO + OH = HO2 + CO
38	(Phot. Set = HCHORCB)				HCHO + HV = #2 HO2 + CO
39	(Phot. Set = HCHOMCB)				HCHO + HV = CO
40	2.45E+02	4.30E+04	3.08	0.00	HCHO + O = OH + HO2 + CO
41	9.30E-01	(No T Dependence)			HCHO + NO3 = HNO3 + HO2 + CO
42	6.50E+02	1.74E+04	1.96	0.00	ALD2 + O = C2O3 + OH
43	2.39E+04	1.04E+04	-0.50	0.00	ALD2 + OH = C2O3
44	3.70E+00	(No T Dependence)			ALD2 + NO3 = C2O3 + HNO3
45	(Phot. Set = ALD2RCB)				ALD2 + HV = XO2 + #2 HO2 + CO + HCHO
46	2.83E+04	5.15E+04	0.36	0.00	C2O3 + NO = NO2 + XO2 + HCHO + HO2
47	1.36E+04	3.84E+03	-0.76	0.00	C2O3 + NO2 = PAN
48	3.44E-02	1.20E+18	26.83	0.00	PAN = C2O3 + NO2
49	3.70E+03	(No T Dependence)			C2O3 + C2O3 = #2 XO2 + #2 HCHO + #2 HO2
50	9.60E+03	(No T Dependence)			C2O3 + HO2 = #.79 HCHO + #.79 XO2 + #.79 HO2 + #.79 OH
51	2.18E+01	6.52E+03	3.40	0.00	OH = XO2 + HCHO + HO2
52	1.20E+03	(No T Dependence)			PAR + OH = #.87 XO2 + #.13 XO2N + #.11 HO2 + #.11 ALD2 + #.76 ROR + #-.11 PAR
53	1.64E+05	6.25E+16	15.90	0.00	ROR = #1.1 ALD2 + #.96 XO2 + #.94 HO2 + #-2.1 PAR + #.04 XO2N + #.02 ROR
54	9.54E+04	(No T Dependence)			ROR = HO2
55	2.20E+04	(No T Dependence)			ROR + NO2 =
56	5.96E+03	1.76E+04	0.64	0.00	O + OLE = #.63 ALD2 + #.38 HO2 + #.28 XO2 + #.3 CO + #.2 HCHO + #.02 XO2N + #.22 PAR + #.2 OH
57	4.15E+04	7.74E+03	-1.00	0.00	OH + OLE = HCHO + ALD2 + XO2 + HO2 + #-1 PAR
58	1.89E-02	2.10E+01	4.18	0.00	O3 + OLE = #.5 ALD2 + #.74 HCHO + #.33 CO + #.44 HO2 + #.22 XO2 + #.1 OH + #-1 PAR
59	1.14E+01	(No T Dependence)			NO3 + OLE = #.91 XO2 + #.09 XO2N + HCHO + ALD2 + #-1 PAR + NO2
60	1.10E+03	1.54E+04	1.57	0.00	O + ETH = HCHO + #.7 XO2 + CO + #1.7 HO2 + #.3 OH
61	1.18E+04	3.00E+03	-0.82	0.00	OH + ETH = XO2 + #1.56 HCHO + HO2 + #.22 ALD2
62	2.86E-03	1.86E+01	5.23	0.00	O3 + ETH = HCHO + #.42 CO + #.12 HO2
63	9.08E+03	3.11E+03	-0.64	0.00	OH + TOL = #.08 XO2 + #.36 CRES + #.44 HO2 + #.56 TO2
64	1.20E+04	(No T Dependence)			TO2 + NO = #.9 NO2 + #.9 HO2 + #.9 OPEN
65	2.50E+02	(No T Dependence)			TO2 = CRES + HO2
66	6.10E+04	(No T Dependence)			OH + CRES = #.4 CRO + #.6 XO2 + #.6 HO2 + #.3 OPEN
67	3.25E+04	(No T Dependence)			NO3 + CRES = CRO + HNO3
68	2.00E+04	(No T Dependence)			CRO + NO2 =
69	(Same k as Reaction 38)				OPEN + HV + #8.40 = C2O3 + HO2 + CO
70	4.40E+04	(No T Dependence)			OPEN + OH = XO2 + #2 CO + #2 HO2 + C2O3 + HCHO
71	1.52E-02	8.03E-02	0.99	0.00	OPEN + O3 = #.03 ALD2 + #.62 C2O3 + #.7 HCHO + #.03 XO2 + #.69 CO + #.08 OH + #.76 HO2 + #.2 MGLY
72	3.61E+04	2.45E+04	-0.23	0.00	OH +XYL = #.7 HO2 + #.5 XO2 + #.2 CRES + #.8 MGLY + #1.1 PAR + #.3 TO2

Table 1 (continued)

Rxn. Label	Kinetic Parameters [a] k(300)	A	Ea	B	Reactions [b]
73	2.60E+04	(No T Dependence)			OH + MGLY = XO2 + C2O3
74	(Same k as Reaction 38)				MGLY + HV + #8.96 = C2O3 + HO2 + CO
75	2.70E+04	(No T Dependence)			O + ISOP = #.6 HO2 + #.8 ALD2 + #.55 OLE + #.5 XO2 + #.5 CO + #.45 ETH + #.9 PAR
76	1.42E+05	(No T Dependence)			OH + ISOP = XO2 + HCHO + #.67 HO2 + #.13 XO2N + ETH + #.4 MGLY + #.2 C2O3 + #.2 ALD2
77	1.80E-02	(No T Dependence)			O3 + ISOP = HCHO + #.4 ALD2 + #.55 ETH + #.2 MGLY + #.1 PAR + #.06 CO + #.44 HO2 + #.1 OH
78	4.70E+02	(No T Dependence)			NO3 + ISOP = XO2N
79	1.20E+04	(No T Dependence)			XO2 + NO = NO2
80	1.94E+03	2.55E+01	-2.58	0.00	XO2 + XO2 =
81	1.20E+04	(No T Dependence)			XO2N + NO =
82	8.64E+03	1.13E+02	-2.58	0.00	XO2 + HO2 =
83	8.64E+03	1.13E+02	-2.58	0.00	XO2N + HO2 =
84	1.94E+03	2.55E+01	-2.58	0.00	XO2N + XO2N =
85	3.89E+03	5.10E+01	-2.58	0.00	XO2N + XO2 =
86	1.62E+05	7.03E+04	-0.50	0.00	HO2 + OH =
Added Species for Auto/Oil					
101	1.37E+03	4.88E+03	0.76	0.00	MEOH + OH = HCHO + HO2
102	4.80E+03	6.06E+03	0.14	0.00	ETOH + OH = #.078 HCHO + #.961 ALD2 + HO2 + #.05 XO2
103	4.18E+03	(No T Dependence)			MTBE + OH = #1.37 XO2 + #.98 HO2 + #.42 HCHO + #.97 PAR + #.02 XO2N
Added Biogenics for EKMA Scenarios (from detailed model species assignment file)					
83	1.00E+10	(No T Dependence)			APIN = #6 PAR + #1.5 ALD2 + #.5 OLE
84	1.00E+10	(No T Dependence)			UNKN = #7 PAR + #.75 ALD2 + #.75 OLE
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)			OH + T.3 = OH + T.3PROD
R01	1.00E+03	(No T Dependence)			OH + T01 = OH + T01PROD
R03	3.00E+03	(No T Dependence)			OH + T03 = OH + T03PROD
R10	1.00E+04	(No T Dependence)			OH + T10 = OH + T10PROD
R30	3.00E+04	(No T Dependence)			OH + T30 = OH + T30PROD
R1C	1.00E+05	(No T Dependence)			OH + T1C = OH + T1CPROD
R3C	3.00E+05	(No T Dependence)			OH + T3C = OH + T3CPROD
	Counter species used for computing mechansitic reactivities for species which are represented explicitly.				
T37	1.50E+04	(No T Dependence)			OH + T_HCHO = OH + R_HCHO
T38	(Phot. Set = HCHORCB)				T_HCHO = R_HCHO
T39	(Phot. Set = HCHOMCB)				T_HCHO = R_HCHO
T40	1.35E+00	2.37E+02	3.08	0.00	O + T_HCHO = O + R_HCHO
T41	9.30E-01	(No T Dependence)			NO3 + T_HCHO = NO3 + R_HCHO
T42	2.38E+01	6.36E+02	1.96	0.00	O + T_ALD2 = O + R_ALD2
T43	5.52E+04	2.40E+04	-0.50	0.00	OH + T_ALD2 = OH + R_ALD2
T44	3.70E+00	(No T Dependence)			NO3 + T_ALD2 = NO3 + R_ALD2
T45	(Phot. Set = ALD2RCB)				T_ALD2 = R_ALD2
T60	7.71E+01	1.08E+03	1.57	0.00	O + T_ETH = O + R_ETH
T61	4.69E+04	1.19E+04	-0.82	0.00	OH + T_ETH = OH + R_ETH
T62	4.17E-07	2.70E-03	5.23	0.00	O3 + T_ETH = O3 + R_ETH
Counter species used for computing integrated O3 or OH					
	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
IOH	1.00E+00	(No T Dependence)			OH = OH + INTOH

[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 values used as a function of zenith angle being as shown on Table 3.

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

Table 2. Assignment of Carbon Bond species to SAPRC detailed model species.

Description	DMS Name	Carbon Bond Assignment			
Alkanes					
Methane	METHANE	#.01	PAR	#.99	INERT
Carbon Monoxide	CO		CO		
Ethane	ETHANE	#0.4	PAR	#1.6	INERT
Propane	PROPANE	#1.5	PAR	#1.5	INERT
n-Butane	N-C4	#4	PAR		
n-Pentane	N-C5	#5	PAR		
n-Hexane	N-C6	#6	PAR		
n-Heptane	N-C7	#7	PAR		
n-Octane	N-C8	#7	PAR		INERT
n-Nonane	N-C9	#7	PAR	#2	INERT
n-Decane	N-C10	#7	PAR	#3	INERT
n-Undecane	N-C11	#8	PAR	#3	INERT
n-Dodecane	N-C12	#8	PAR	#4	INERT
n-Tridecane	N-C13	#9	PAR	#4	INERT
n-Tetradecane	N-C14	#10	PAR	#4	INERT
n-Pentadecane	N-C15	#10	PAR	#5	INERT
n-C16	N-C16	#11	PAR	#5	INERT
n-C17	N-C17	#11	PAR	#6	INERT
n-C18	N-C18	#12	PAR	#6	INERT
n-C19	N-C19	#13	PAR	#6	INERT
n-C20	N-C20	#13	PAR	#7	INERT
n-C21	N-C21	#14	PAR	#7	INERT
n-C22	N-C22	#14	PAR	#8	INERT
Isobutane	2-ME-C3	#4	PAR		
Iso-Pentane	2-ME-C4	#5	PAR		
Neopentane	22-DM-C3	#4	PAR		INERT
2-Methyl Pentane	2-ME-C5	#6	PAR		
3-Methylpentane	3-ME-C5	#6	PAR		
2,2-Dimethyl Butane	22-DM-C4	#5	PAR		INERT
2,3-Dimethyl Butane	23-DM-C4	#6	PAR		
2,4-Dimethyl Pentane	24-DM-C5	#7	PAR		
3-Methyl Hexane	3-ME-C6	#7	PAR		
2-Methyl Hexane	2-ME-C6	#7	PAR		
2,3-Dimethyl Pentane	23-DM-C5	#7	PAR		
3,3-Dimethyl Pentane	33-DM-C5	#6	PAR		INERT
2,2,3-Trimethyl Butane	223TM-C4	#6	PAR		INERT
2-Methyl Heptane	2-ME-C7	#8	PAR		
3-Methyl Heptane	3-ME-C7	#8	PAR		
4-Methyl Heptane	4-ME-C7	#8	PAR		
2,3-Dimethyl Hexane	23-DM-C6	#8	PAR		
2,4-Dimethyl Hexane	24-DM-C6	#8	PAR		
2,5-Dimethyl Hexane	25-DM-C6	#8	PAR		
2,2,4-Trimethyl Pentane	224TM-C5	#7	PAR		INERT
2,3,4-Trimethyl Pentane	234TM-C5	#8	PAR		
2,2,3,3-Tetrame. Butane	2233M-C4	#6	PAR	#2	INERT
2,4-Dimethyl Heptane	24-DM-C7	#9	PAR		
4-Ethyl Heptane	4-ET-C7	#9	PAR		
2,2,5-Trimethyl Hexane	225TM-C6	#8	PAR		INERT
3,4-Propyl Heptane	4-PR-C7	#10	PAR		
3,5-Diethyl Heptane	35-DE-C7	#11	PAR		
2,6-Diethyl Octane	36-DE-C8	#12	PAR		
3,7-Diethyl Nonane	37-DE-C9	#13	PAR		
3,8-Diethyl Decane	38DE-C10	#14	PAR		
3,9-Diethyl Undecane	39DE-C11	#15	PAR		
Cyclopropane	CYCC3	#3	INERT		
Cyclobutane	CYCC4	#4	INERT		

Table 2 (continued)

Description	DMS Name	Carbon Bond Assignment
Cyclopentane	CYCC5	#5 PAR
Methylcyclopentane	ME-CYCC5	#6 PAR
Cyclohexane	CYCC6	#6 PAR
Methylcyclohexane	ME-CYCC6	#7 PAR
1,3-Dimeth. Cyclopentane	13DMCYC5	#7 PAR
Ethyl Cyclopentane	ET-CYCC5	#7 PAR
Propyl Cyclopentane	PR-CYCC5	#8 PAR
Ethylcyclohexane	ET-CYCC6	#8 PAR
1,3-Dimethyl Cyclohexane	13DMCYC6	#8 PAR
1-Eth.-4-Meth. Cyclohex.	1E4MCYC6	#9 PAR
1,3-Diethyl-Cyclohexane	13DECYC6	#10 PAR
13-Dieth-5-Me. Cyclohex.	13E5MCC6	#11 PAR
1,3,5-Triethyl Cyclohex.	135ECYC6	#12 PAR
13-Dieth-5-Pent Cyclohx.	13E5PCC6	#13 PAR
13-Diprop-5-Eth Cyclohx.	13P5ECC6	#14 PAR
135-Tripropyl Cyclohex.	135PCYC6	#15 PAR
Lumped C4-C5 Alkanes	C4C5	#4.5 PAR
Lumped C6+ Alkanes	C6PLUS	#7 PAR
Branched C5 Alkanes	BR-C5	#5 PAR
Branched C6 Alkanes	BR-C6	#6 PAR
Branched C7 Alkanes	BR-C7	#7 PAR
Branched C8 Alkanes	BR-C8	#8 PAR
Branched C9 Alkanes	BR-C9	#9 PAR
Branched C10 Alkanes	BR-C10	#10 PAR
Branched C11 alkanes	BR-C11	#11 PAR
Branched C12 Alkanes	BR-C12	#12 PAR
Branched C13 Alkanes	BR-C13	#13 PAR
Branched C14 Alkanes	BR-C14	#14 PAR
Branched C15 Alkanes	BR-C15	#15 PAR
Branched C16 Alkanes	BR-C16	#16 PAR
Branched C17 Alkanes	BR-C17	#17 PAR
Branched C18 Alkanes	BR-C18	#18 PAR
C6 Cycloalkanes	CYC-C6	#6 PAR
C7 Cycloalkanes	CYC-C7	#7 PAR
C8 Cycloalkanes	CYC-C8	#8 PAR
C9 Cycloalkanes	CYC-C9	#9 PAR
C10 Cycloalkanes	CYC-C10	#10 PAR
C11 Cycloalkanes	CYC-C11	#11 PAR
C12 Cycloalkanes	CYC-C12	#12 PAR
C13 Cycloalkanes	CYC-C13	#13 PAR
C14 Cycloalkanes	CYC-C14	#14 PAR
C15 Cycloalkanes	CYC-C15	#15 PAR
C9 Bicycloalkanes	BCYC-C9	#9 PAR
C10 Bicycloalkanes	BCYC-C10	#10 PAR
C11 Bicycloalkanes	BCYC-C11	#11 PAR
C12 Bicycloalkanes	BCYC-C12	#12 PAR
C13 Bicycloalkanes	BCYC-C13	#13 PAR
C14 Bicycloalkanes	BCYC-C14	#14 PAR
C15 Bicycloalkanes	BCYC-C15	#15 PAR
Following "old" names should be removed from .CMP files, but are kept temporarily for so they can be processed.		
Isobutane	ISO-C4	#4 PAR
Iso-Pentane	ISO-C5	#5 PAR
Neopentane	NEO-C5	#4 PAR INERT

Table 2 (continued)

Description	DMS Name	Carbon Bond Assignment				
2,2-Dimethyl Butane	22-DMB	#5	PAR		INERT	
2,3-Dimethyl Butane	23-DMB	#6	PAR			
2,2,4-Trimethyl Pentane	ISO-C8	#7	PAR		INERT	
Alkenes						
Ethene	ETHENE		ETH			
Propene	PROPENE		OLE		PAR	
1-Butene	1-BUTENE		OLE	#2	PAR	
C4 Terminal Alkanes	C4-OLE1		OLE	#2	PAR	
1-Pentene	1-PENTEN		OLE	#3	PAR	
C5 Terminal Alkanes	C5-OLE1		OLE	#3	PAR	
1-Hexene	1-HEXENE		OLE	#4	PAR	
C6 Terminal Alkanes	C6-OLE1		OLE	#4	PAR	
C7 Terminal Alkanes	C7-OLE1		OLE	#5	PAR	
C8 Terminal Alkanes	C8-OLE1		OLE	#6	PAR	
C9 Terminal Alkanes	C9-OLE1		OLE	#7	PAR	
C10 Terminal Alkanes	C10-OLE1		OLE	#8	PAR	
C11 Terminal Alkanes	C11-OLE1		OLE	#9	PAR	
C12 Terminal Alkanes	C12-OLE1		OLE	#10	PAR	
C13 Terminal Alkanes	C13-OLE1		OLE	#11	PAR	
C14 Terminal Alkanes	C14-OLE1		OLE	#12	PAR	
C15 Terminal Alkanes	C15-OLE1		OLE	#13	PAR	
Isobutene	ISOBUTEN		HCHO	#3	PAR	
2-Methyl-1-Butene	2M-1-BUT		HCHO	#4	PAR	
3-Methyl-1-Butene	3M-1-BUT		OLE	#3	PAR	
trans-2-Butene	T-2-BUTE	#2	ALD2			
cis-2-Butene	C-2-BUTE	#2	ALD2			
C4 Internal Alkenes	C4-OLE2	#2	ALD2			
2-Methyl-2-Butene	2M-2-BUT	#3	PAR		ALD2	
C5 Internal Alkenes	C5-OLE2		PAR	#2	ALD2	
C6 Internal Alkenes	C6-OLE2	#2	PAR	#2	ALD2	
C7 Internal Alkenes	C7-OLE2	#3	PAR	#2	ALD2	
C8 Internal Alkenes	C8-OLE2	#4	PAR	#2	ALD2	
C9 Internal Alkenes	C9-OLE2	#5	PAR	#2	ALD2	
C10 Internal Alkenes	C10-OLE2	#6	PAR	#2	ALD2	
C11 Internal Alkenes	C11-OLE2	#7	PAR	#2	ALD2	
C12 Internal Alkenes	C12-OLE2	#8	PAR	#2	ALD2	
C13 Internal Alkenes	C13-OLE2	#9	PAR	#2	ALD2	
C14 Internal Alkenes	C14-OLE2	#10	PAR	#2	ALD2	
C15 Internal Alkenes	C15-OLE2	#11	PAR	#2	ALD2	
1,3-Butadiene	13-BUTDE	#2	OLE			
Isoprene	ISOPRENE		ISOP			
Cyclopentene	CYC-PNTE		PAR	#2	ALD2	
Cyclohexene	CYC-HEXE	#2	PAR	#2	ALD2	
a-Pinene	A-PINENE	#0.5	OLE	#6	PAR	#1.5 ALD2
b-Pinene	B-PINENE		OLE	#8	PAR	
3-Carene	3-CARENE		OLE	#8	PAR	
d-Limonene	D-LIMONE		OLE	#4	PAR	#2 ALD2
Myrcene	MYRCENE	#3	OLE	#4	PAR	
C4 Olefins (unspeciated)	C4-OLE		OLE	#2	PAR	
C5 Olefins (unspeciated)	C5-OLE		OLE	#3	PAR	
C6 Olefins (unspeciated)	C6-OLE		OLE	#4	PAR	
C7 Olefins (unspeciated)	C7-OLE		OLE	#5	PAR	
C8 Olefins (unspeciated)	C8-OLE		OLE	#6	PAR	
C9 Olefins (unspeciated)	C9-OLE		OLE	#7	PAR	

Table 2 (continued)

Description	DMS Name	Carbon Bond Assignment			
C10 Olefins (unspeciated)	C10-OLE		OLE	#8	PAR
C11 Olefins (unspeciated)	C11-OLE		OLE	#9	PAR
Assume these are cyclic olefins: split 2 ALD2 + n PAR					
C6 Cyclic or di-olefins	C6-OL2D	#2	PAR	#2	ALD2
C7 Cyclic or di-olefins	C7-OL2D	#3	PAR	#2	ALD2
C8 Cyclic or di-olefins	C8-OL2D	#4	PAR	#2	ALD2
C9 Cyclic or di-olefins	C9-OL2D	#5	PAR	#2	ALD2
C10 Cyclic or di-olefins	C10-OL2D	#6	PAR	#2	ALD2
C11 Cyclic or di-olefins	C11-OL2D	#7	PAR	#2	ALD2
C12 Cyclic or di-olefins	C12-OL2D	#8	PAR	#2	ALD2
C13 Cyclic or di-olefins	C13-OL2D	#9	PAR	#2	ALD2
C14 Cyclic or di-olefins	C14-OL2D	#10	PAR	#2	ALD2
C15 Cyclic or di-olefins	C15-OL2D	#11	PAR	#2	ALD2
Aromatics					
Benzene	BENZENE		PAR	#5	INERT
Toluene	TOLUENE		TOL		
Ethyl Benzene	C2-BENZ		PAR		TOL
n-Propyl Benzene	N-C3-BEN	#2	PAR		TOL
Isopropyl Benzene	I-C3-BEN	#2	PAR		TOL
Butyl Benzene	C4-BENZ	#3	PAR		TOL
C9 Monosub. Benzenes	C9-BEN1	#2	PAR		TOL
s-Butyl Benzene	S-C4-BEN	#3	PAR		TOL
C10 Monosub. Benzenes	C10-BEN1	#3	PAR		TOL
C11 Monosub. Benzenes	C11-BEN1	#4	PAR		TOL
C12 Monosub. Benzenes	C12-BEN1	#5	PAR		TOL
o-Xylene	O-XYLENE		XYL		
p-Xylene	P-XYLENE		XYL		
m-Xylene	M-XYLENE		XYL		
C8 Disub. Benzenes	C8-BEN2		XYL		
C9 Disub. Benzenes	C9-BEN2		PAR		XYL
C10 Disub. Benzenes	C10-BEN2	#2	PAR		XYL
C11 Disub. Benzenes	C11-BEN2	#3	PAR		XYL
C12 Disub. Benzenes	C12-BEN2	#4	PAR		XYL
1,3,5-Trimethyl Benzene	135-TMB		PAR		XYL
1,2,3-Trimethyl Benzene	123-TMB		PAR		XYL
1,2,4-Trimethyl Benzene	124-TMB		PAR		XYL
C9 Trisub. Benzenes	C9-BEN3		PAR		XYL
C10 Trisub. Benzenes	C10-BEN3	#2	PAR		XYL
C11 Trisub. Benzenes	C11-BEN3	#3	PAR		XYL
C12 Trisub. Benzenes	C12-BEN3	#4	PAR		XYL
C10 Tetrasub. Benzenes	C10-BEN4	#2	PAR		XYL
C11 Tetrasub. Benzenes	C11-BEN4	#3	PAR		XYL
C12 Tetrasub. Benzenes	C12-BEN4	#4	PAR		XYL
C11 Pentasub. Benzenes	C11-BEN5	#3	PAR		XYL
C11 Pentasub. Benzenes	C12-BEN5	#4	PAR		XYL
C12 Hexaasub. Benzenes	C12-BEN6	#4	PAR		XYL
Indan	INDAN		PAR		XYL
Indane	INDANE		PAR		XYL
Tetralin	TETRALIN	#2	PAR		XYL
Naphthalene	NAPHTHAL	#2	PAR		XYL
Methyl Naphthalenes	ME-NAPH	#3	PAR		XYL
2,3-Dimethyl Naphth.	23-DMN	#4	PAR		XYL
C11 Tetralin or Indane	C11-TET	#3	PAR		XYL

Table 2 (continued)

Description	DMS Name	Carbon Bond Assignment					
Styrene	STYRENE		TOL	#0.5	OLE		
C9 Styrenes	C9-STY1		TOL		OLE		
C10 Styrenes	C10-STY2		PAR		TOL		OLE
C9 Styrenes	C9-STYR		TOL		OLE		
C10 Styrenes	C10-STYR		PAR		TOL		OLE
C9 Aromatics (unspeciated)	C9-ARO	#1.5	PAR	#0.5	TOL	#0.5	XYL
C10 Aromatics (unspeciated)	C10-ARO	#2.5	PAR	#0.5	TOL	#0.5	XYL
C11 Aromatics (unspeciated)	C11-ARO	#3	PAR		XYL		
C12 Aromatics (unspeciated)	C12-ARO	#4	PAR		XYL		
Acetylenes							
Acetylene	ACETYLEN		PAR		INERT		
Butyne	BUTYNE	#2	PAR		ALD2		
Pentyne	PENTYNE	#3	PAR		ALD2		
Methyl Acetylene	ME-ACTYL		PAR		ALD2		
Aldehydes, Ketones							
Formaldehyde	FORMALD		HCHO				
Acetaldehyde	ACETALD		ALD2				
C3 Aldehydes	PROPALD		PAR		ALD2		
C4 Aldehydes	C4-RCHO	#2	PAR		ALD2		
C5 Aldehydes	C5-RCHO	#3	PAR		ALD2		
C6 Aldehydes	C6-RCHO	#4	PAR		ALD2		
C7 Aldehydes	C7-RCHO	#5	PAR		ALD2		
C8 Aldehydes	C8-RCHO	#6	PAR		ALD2		
Methyl Glyoxal	MEGLYOX		FORM		ALD2		
Acrolein	ACROLEIN	#0.5	OLE		ALD2		
Methacrolein	METHACRO		OLE		ALD2		
Crotonaldehyde	CROTALD		OLE		ALD2		
Alkyl Phenols	CRESOL		TOL				
Phenol	PHENOL		PAR	#5	INERT		
Benzaldehyde	BENZALD	#7	INERT				
Acetone	ACETONE	#3	PAR				
C4 Ketones	MEK	#4	PAR				
Methyl Vinyl Ketone	MVK		OLE	#2	PAR		
C5 Ketones	KET5	#5	PAR				
C6 Ketones	KET6	#6	PAR				
C7 Ketones	KET7	#7	PAR				
C8 Ketones	KET8	#8	PAR				
C9 Ketones	KET9	#9	PAR				
C10 Ketones	KET10	#10	PAR				
C5 Cyclic Ketones	KET5C	#5	PAR				
C6 Cyclic Ketones	KET6C	#6	PAR				
C7 Cyclic Ketones	KET7C	#7	PAR				
C8 Cyclic Ketones	KET8C	#8	PAR				
C9 Cyclic Ketones	KET9C	#9	PAR				
C10 Cyclic Ketones	KET10C	#10	PAR				
Others							
Methanol	MEOH		MEOH				
Ethanol	ETOH		ETOH				

Table 2 (continued)

Description	DMS Name	Carbon Bond Assignment					
n-Propyl Alcohol	N-C3-OH	#3	PAR				
Isopropyl Alcohol	I-C3-OH	#3	PAR				
Isobutyl Alcohol	I-C4-OH	#4	PAR				
n-Butyl Alcohol	N-C4-OH	#4	PAR				
t-Butyl Alcohol	T-C4-OH	#3	PAR		INERT		
s-Butyl Alcohol	S-C4-OH	#4	PAR				
Pentyl Alcohol	C5OH	#5	PAR				
1-Heptanol	1-C7OH	#7	PAR				
2-Ethyl-1-Hexanol	2-ETC6OH	#8	PAR				
Ethylene Glycol	ET-GLYCL	#0.4	PAR	#1.6	INERT		
Propylene Glycol	PR-GLYCL	#1.5	PAR	#1.5	INERT		
1,2-Butandiol	12-C4OH2	#4	PAR				
1,2-Dihydroxy Hexane	C6-GLYCL	#6	PAR				
Dimethyl Ether	ME-O-ME	#2	PAR				
Diethyl Ether	ET-O-ET	#2	PAR		ALD2		
Methyl t-Butyl Ether	MTBE		MTBE				
Ethyl Isopropyl Ether	S-098106	#3	PAR		ALD2		
Ethyl t-Butyl Ether	ETBE		ETH	#4	INERT		
2-Butyltetrahydrofuran	S-098108	#6	PAR		ALD2		
Dibutyl Ether	S-098107	#6	PAR		ALD2		
2-Methoxy-Ethanol	MEO-ETOH		PAR		ALD2		
2-Ethoxy-Ethanol	ETO-ETOH	#2	PAR		ALD2		
1-Ethoxy-2-Propanol	ETOC3OH	#3	PAR		ALD2		
2-Butoxy-Ethanol	BUO-ETOH	#4	PAR		ALD2		
Butyl Cellosolve	BU-CELSV	#4	PAR		ALD2		
2-(2-Ethoxyethoxy) EtOH	CARBITOL	#2	PAR	#2	ALD2		
2-(2-Butoxyethoxy)-EtOH	C8-CELSV	#8	PAR		ALD2		
Methyl Acetate	ME-ACET	#2	PAR		INERT		
Methyl Acrylate	ME-ACRYL		PAR		OLE		INERT
Vinyl Acetate	VIN-ACET		PAR		OLE		INERT
Ethyl Acetate	ET-ACET	#3	PAR		INERT		
Ethyl Acrylate	ET-ACRYL	#2	PAR		OLE		INERT
Propyl Acetate	PR-ACET	#4	PAR		INERT		
Methyl Isobutyrate	ME-IBUAT	#4	PAR		INERT		
Isopropyl Acetate	IPR-ACET	#4	PAR		INERT		
n-Butyl Acetate	BU-ACET	#5	PAR		INERT		
Isobutyl Acetate	IBU-ACET	#5	PAR		INERT		
2-Ethoxyethyl Acetate	CSV-ACET	#3	PAR		ALD2		INERT
Isobutyl Isobutyrate	IBU-IBTR	#7	PAR		INERT		
Isoamyl Isobutyrate	IC5IBUAT	#8	PAR		INERT		
Subst. C7 Ester (C12)	S-098116	#11	PAR		INERT		
Subst. C9 Ester (C12)	S-098117	#11	PAR		INERT		
Ethylene Oxide	ETOX		PAR		INERT		
Propylene Oxide	PROX	#2	PAR		INERT		
Furan	FURAN	#2	OLE				
Ethyl Amine	ET-AMINE	#0.4	PAR		ALD2	#1.6	INERT
Acrylonitrile	ACRYLNIT		PAR		OLE		
Trimethyl Amine	TM-AMINE		PAR		OLE		
Methyl Chloride	S-043801	#1	INERT				
Dichloromethane	S-043802	#1	INERT				

Table 2 (continued)

Description	DMS Name	Carbon Bond Assignment		
Methyl Bromide	S-243819	#1	INERT	
Chloroform	S-043803	#1	INERT	
Methylene Bromide	S-043805	#1	INERT	
Ethyl Chloride	S-043812	#2	INERT	
Trans-1,2-Dichloroethene	S-099018	#2	INERT	
1,1-Dichloroethane	S-043813	#2	INERT	
1,1,2-Trichloroethane	S-043820	#2	INERT	
1,1,1-Trichloroethane	S-043814	#2	INERT	
1,2-Dichloropropane	S-099016	#3	INERT	
1-Chlorobutane	S-098104	#4	PAR	
3-(Chloromethyl)-Heptane	S-098105	#8	PAR	
Vinyl Chloride	CL-ETHE		ETH	
1,1-Dichloroethene	S-099013	#2	INERT	
Ethylene Dichloride	S-043815	#2	INERT	
Trichloroethylene	CL3-ETHE	#2	INERT	
Perchloroethylene	CL4-ETHE	#2	INERT	
Ethylene Dibromide	S-099014	#2	INERT	
Haloaromatics and Nitrobenzene represented like Benzene				
Monochlorobenzene	CL-BEN	PAR	#5	INERT
p-Dichlorobenzene	CL2-BEN	PAR	#5	INERT
Nitrobenzene	S-099009	PAR	#5	INERT

Table 3. Photolysis rates as a function of zenith angle.

Zenith	Photolysis File				
Angle	NO2CB	O3O1DCB	HCHORCB	HCHOMCB	ALD2RCB
0.	5.962e-1	2.646e-3	2.222e-3	2.972e-3	4.082e-4
10.	5.910e-1	2.555e-3	2.186e-3	2.937e-3	3.986e-4
20.	5.754e-1	2.292e-3	2.079e-3	2.831e-3	3.705e-4
30.	5.483e-1	1.889e-3	1.901e-3	2.650e-3	3.252e-4
40.	5.080e-1	1.397e-3	1.651e-3	2.387e-3	2.657e-4
50.	4.514e-1	8.880e-4	1.331e-3	2.031e-3	1.960e-4
60.	3.727e-1	4.445e-4	9.496e-4	1.568e-3	1.232e-4
70.	2.628e-1	1.481e-4	5.329e-4	9.899e-4	5.765e-5
78.	1.484e-1	3.846e-5	2.258e-4	4.829e-4	2.018e-5
86.	4.402e-2	4.664e-6	3.923e-5	1.064e-4	2.810e-6

METHODS

Scenarios Used for Reactivity Assessment

The development of a comprehensive set of pollution scenarios representing a realistic distribution of ozone pollution conditions requires an analysis of the range of conditions in airsheds where ozone is a problem. This is beyond the scope of this study. However, an extensive set of idealized pollution scenarios has been developed for a number of urban areas for conducting EKMA model analyses of effects of ROG and NO_x controls on ozone formation (e.g., see Gipson et al., 1981; Gipson and Freas, 1983; EPA, 1984; Gery et al., 1987; Bauges, 1990). The EKMA modeling approach involves use of single-cell box models to simulate ozone formation in one day episodes. Such models cannot represent realistic pollution episodes in great detail, and do not incorporate processes such as carry-over of pollutants from one day to the next. However, they can represent dynamic injection of pollutants, time-varying changes of inversion heights with entrainment of pollutants from aloft as the inversion height increases throughout the day, and time-varying photolysis rates, temperatures, and humidities (Gipson et al, 1981; Gipson, 1984; EPA, 1984). Thus they can represent a wide range of chemical conditions which may affect predictions of effects of ROG and NO_x control on ozone formation. These chemical conditions are the same as those affecting VOC reactivity. Therefore, at least to the extent they are suitable for their intended purpose, an appropriate set of EKMA scenarios should also be suitable for assessing methods to develop reactivity scales encompassing a wide range of conditions.

Base Case Scenarios.

The set of EKMA scenarios used in this study were based on those developed by the United States EPA for determining, for planning purposes, how various ROG and NO_x control strategies would affect ozone nonattainment in various areas of the country (Bauges, 1990). For this purpose, Bauges (1990, 1991) selected 39 urban areas in the United States based on geographical distribution and coverage of ozone nonattainment areas and based on the availability of the ambient non-methane organic carbon (NMOC) and the local climatological data needed to provide input into the model. For each area, an episode was selected based on how well it represents the ozone design value for the city, which is usually the fourth highest ozone day if three complete years of ozone data are available (Bauges, 1990). The initial NMOC and NO_x concentrations in the scenarios were based on the median of all levels measured during all days exceeding 0.124 ppm O_3 or the top ten episodes if more than ten exceedences were measured during the NMOC sampling period. Ozone concentrations aloft were based on downwind measurements made just after the morning increase in the mixing height. The mixing height inputs were prepared based on upper air soundings recommended by the EPA EKMA

guidance documents (EPA, 1984). A constant 30 ppb of NMOC aloft was assumed in all scenarios. Hourly emissions by county were obtained from 1985 NAPAP emissions inventory. Biogenic emissions estimates were also included; with separate estimates being made for isoprene, α-pinene and "unknowns". The scenarios also had estimates of initial and emitted CO, and hourly temperature and humidity values. The major characteristics of each of these scenarios are listed in Table 4. Complete tabulations of the scenario conditions and listings of the data files as received from Bauges are given in Appendix B to this report.

Several changes were made to these EPA scenarios based on discussions with the California ARB staff and members of the ARB's reactivity advisory panel (Croes, 1991; CARB, 1991). Based on a suggestion by Pitts (private communication), and analyses of ambient nitrous acid (HONO) measurements, 2% of the initial NO_x and 0.1% of the emitted NO_x in all the scenarios was assumed to be converted to HONO. Methane was assumed to be constant at the global background value of 1.79 ppm. NO_x aloft was assumed to be zero rather than the EPA's default of 2 ppb. The solar light intensities and spectral distributions used to calculate rates of photolysis reactions were those calculated by Jeffries (private communication, 1991) for 640 meters, the approximate mid-point of the mixed layer during daylight hours. The composition of the NMOCs entrained from aloft was derived based on the analysis of aircraft data conducted by Jeffries et al. (1989), and is the same as used by Carter (1991).

Consistent with the treatment in original EPA scenarios (Bauges 1991), the same NMOC composition profile was used to represent the initial and emitted anthropogenic NMOCs for all scenarios. The profile used in this study was developed by Croes (personal communication, 1991) based on an analysis of ambient hydrocarbon and aldehyde measurements from the EPA data base (Jeffries et al. 1991, and references therein) and obtained from the 1987 Southern California Air Quality Study (SCAQS) (Croes et al., 1993; Lurmann et al. 1992). The hydrocarbons was based on the 1987-88 all-city profile derived from the measurement data of Lonneman (Jeffries et al., 1991), while the oxygenates were based on the SCAQS data (Croes et al. 1993; Lurmann et al. 1992). (The EPA data were preferred for the hydrocarbons because the data set is more robust and very similar to the SCAQS hydrocarbon data, while the SCAQS oxygenate data were preferred because they include measurements for the higher oxygenates which are not in the EPA data base, but are consistent with the EPA data in terms of formaldehyde and acetaldehyde levels.) The oxygenates constituted 4.5% of initial and emitted NMOC's, of which slightly under half were formaldehyde and acetaldehyde. The NMOC inputs in the EKMA scenarios were increased by 4.7% to correct for the fact that the oxygenates are not included in the ambient measurements used to the NMOC inputs for these EKMA scenarios. The composition of the ROG surrogate used is given in Table 5. This can be compared with the composition of the ROG's aloft, which is given in Table 6.

Table 4. Summary of conditions of the EPA base case scenarios.

Scenario		Calc. O_3^{max} (ppb)	ROG/NO_x	NO_x/ NO_x^{MOR}	Final H [M]	Input flux (m.mol-m^{-2}) (% emitted)				Aloft O_3 (ppb)
City, State	Date					HC		NOx		
Atlanta, GA	6/6/88	158	7.25	0.74	2146	11.76	(44%)	1.62	(56%)	63
Austin, TX	9/9/88	155	9.30	0.55	2108	11.22	(17%)	1.21	(39%)	85
Baltimore, MD	7/7/88	279	5.15	1.10	1169	16.79	(42%)	3.26	(58%)	84
Baton Rouge, LA	4/26/88	210	6.83	0.98	968	11.13	(44%)	1.63	(73%)	62
Birmingham, AL	7/31/87	214	6.94	0.56	1770	12.83	(9%)	1.85	(33%)	81
Boston, MA	6/16/88	176	6.50	0.62	2598	14.26	(52%)	2.19	(57%)	105
Charlotte, NC	6/8/88	130	7.79	0.33	3046	7.46	(47%)	0.96	(52%)	92
Chicago, IL	8/11/88	235	11.63	0.55	1392	24.97	(33%)	2.15	(59%)	40
Cincinnati, OH	8/18/88	177	6.37	0.77	2816	17.29	(34%)	2.71	(35%)	70
Cleveland, OH	7/5/88	214	6.62	1.00	1650	15.68	(51%)	2.37	(50%)	89
Dallas, TX	9/9/87	163	4.74	1.34	2250	17.51	(49%)	3.70	(72%)	75
Denver, CO	7/26/88	165	6.33	1.20	3358	29.33	(57%)	4.64	(64%)	57
Detroit, MI	8/2/88	210	6.82	0.79	1844	17.29	(49%)	2.54	(55%)	68
El Paso, TX	9/7/88	156	6.59	1.11	2000	12.27	(15%)	1.86	(23%)	65
Hartford, CT	7/8/88	150	8.39	0.49	2318	10.71	(25%)	1.28	(30%)	78
Houston, TX	8/26/88	267	6.08	0.98	1748	25.47	(32%)	4.19	(55%)	65
Indianapolis, IN	7/28/88	179	6.64	0.93	1675	12.06	(41%)	1.82	(68%)	52
Jacksonville, FL	5/7/87	136	7.62	0.69	1485	7.73	(37%)	1.01	(59%)	40
Kansas City, MO	8/7/87	138	7.09	0.63	2200	9.07	(26%)	1.28	(39%)	65
Lake Charles, LA	7/26/88	251	7.42	0.69	457	6.96	(27%)	0.94	(75%)	40
Los Angeles, CA	9/3/88	488	7.59	1.01	503	23.05	(29%)	3.04	(30%)	100
Louisville, KY	6/13/88	185	5.53	0.88	2518	13.74	(40%)	2.48	(78%)	75
Memphis, TN	6/24/87	197	6.78	0.70	1750	14.90	(24%)	2.20	(45%)	58
Miami, FL	4/22/87	117	9.63	0.43	2720	9.47	(25%)	0.98	(38%)	57
Nashville, TN	6/22/86	146	8.05	0.45	1608	7.36	(23%)	0.91	(63%)	50
New York, NY	6/22/88	306	8.09	0.77	1512	39.19	(48%)	4.85	(50%)	103
Philadelphia, PA	7/29/88	208	6.19	0.97	1800	19.01	(75%)	3.07	(76%)	53
Phoenix, AZ	9/9/88	236	7.58	1.00	3250	39.87	(2%)	5.26	(3%)	60
Portland, OR	6/29/87	146	6.46	0.72	1575	6.23	(53%)	0.96	(66%)	66
Richmond, VA	7/10/88	205	6.18	0.81	1932	16.36	(78%)	2.65	(84%)	64
Sacramento, CA	7/23/88	178	6.59	0.89	1103	7.40	(36%)	1.12	(45%)	60
St Louis, MO	7/8/88	264	6.08	1.13	1625	25.63	(81%)	4.21	(86%)	82
Salt Lake City, UT	7/22/88	164	8.47	0.62	2150	10.69	(22%)	1.26	(32%)	85
San Antonio, TX	9/26/88	118	3.92	1.13	2308	6.00	(46%)	1.53	(60%)	60
San Diego, CA	10/3/88	169	7.09	1.00	850	7.67	(33%)	1.08	(37%)	90
San Francisco, CA	5/20/88	156	4.78	1.93	650	25.01	(77%)	5.24	(85%)	70
Tampa, FL	4/23/87	195	4.36	1.15	991	7.90	(29%)	1.81	(67%)	68
Tulsa, OK	7/22/86	197	5.31	0.94	1830	14.86	(29%)	2.80	(42%)	70
Washington, DC	7/30/88	248	5.32	0.84	1421	13.48	(66%)	2.54	(81%)	99
Averaged Conditions		201	6.57	0.85	1823	15.38	(60%)	2.34	(46%)	70

No claim is made as to the accuracy of these scenarios in representing any real episode, though clearly they were developed with an attempt to make their input data and predictions as consistent as possible with the available (though generally limited) data. However, even if they are not accurate in representing their particular episodes, they represent the EPA's best efforts to represent, as accurately as possible given the available data and the limitations of the formulation of the EKMA model, the range of conditions occurring in urban areas throughout the United States. For the purpose of investigating reactivity scales, it is more important that the scenarios represent a realistic distribu-

Table 5. 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 5 (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 6. 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

tion of chemical conditions than any one accurately represent the details of any particular episode.

These scenarios are referred to as "base case" to distinguish them from the scenarios derived by adjusting NO_x inputs to yield standard conditions of NO_x availability as discussed below.

Adjusted NO_x Scenarios.

It has been shown previously that incremental reactivities — and even ratios of incremental reactivities — can depend significantly on the NO_x levels in the scenarios (E.g., Dodge, 1984; Carter and Atkinson, 1989; Carter, 1991).

This is because NO_x is required for ozone formation, and if NO_x is consumed before the end of the episode or simulation, then VOCs cannot achieve their full ozone formation potential. Table 4 shows that the NO_x inputs and the ROG/NO_x ratios vary widely among the 39 EPA scenarios, suggesting that NO_x availability, and thus incremental reactivities, are also highly variable. However, if the NO_x inputs to these scenarios were adjusted to yield consistent conditions of NO_x availability, one might expect the incremental reactivities, or at least the ratios of incremental reactivities, to be much less variable. If so, the set of incremental reactivities (or reactivity ratios) so obtained may provide a general reactivity scale which is at least applicable to that particular condition of NO_x availability. Comparing different reactivity scales for different NO_x conditions would provide a systematic means to assess how reactivity scales, and control strategies based on them, would vary with NO_x.

To develop a set of scenarios for this purpose, one needs an appropriate means to quantify NO_x availability, or at least appropriate criteria to establish equivalency in NO_x conditions. NO_x availability is determined both by the amount of NO_x input into the scenario and by the rate of which it is consumed. The ROG/NO_x ratio is obviously an important factor affecting this, but it is not the only one. For example, light intensity, temperature, and the reactivity of the ROGs present will also affect the rate at which NO_x is removed, and thus different scenarios with the same ROG/NO_x ratio may have significantly different conditions of NO_x availability. Because of this, the amount of NO_x input or the ROG/NO_x ratio are not by themselves useful for measuring NO_x availability or establishing equivalency or comparability in NO_x conditions.

A more reliable way to establish comparability in NO_x conditions is to assess similarities or differences in sensitivities, both in sign and magnitude, of ozone formation to changes in NO_x and ROG inputs. If one examines how these sensitivities change as NO_x inputs are varied while holding other scenario conditions constant, we find that a consistent pattern is observed for essentially all scenarios. In all cases there is a NO_x level where the ROG input has the highest and most positive effect on ozone which is near or the same as the point where the effect of NO_x is the most negative, there is a lower NO_x level which yield the maximum ozone concentration and where the effect of NO_x on ozone changes sign, and there is a yet lower NO_x level where the effects of fractional changes of VOC and NO_x on ozone formation are equal. Although these three points in general occur at different NO_x inputs or ROG/NO_x ratios for conditions of different scenarios, they clearly represent consistent NO_x conditions at least in terms of how ozone formation is affected by ROG and NO_x changes. Thus, these served as the basis for deriving the adjusted NO_x scenarios for this study.

In the "Maximum Incremental Reactivity" (MIR) scenarios, the NO_x inputs are adjusted so that the base ROG mixture had the highest incremental reactivity. This represents NO_x conditions where emissions of VOCs have the greatest effect on ozone formation, and also where NO_x has the strongest ozone inhibiting effect. Note also that MIR conditions can be thought of as representing approximately the highest NO_x levels which are relevant in considering control strategies for ozone, because ozone becomes suppressed if NO_x inputs are increased significantly above this level.

In the "Maximum Ozone Reactivity" (MOR) scenarios, the NO_x inputs are adjusted to yield the highest peak ozone concentration. This represents the dividing line between conditions where NO_x is in excess and where ozone is NO_x limited, or the "ridgeline" on ozone isopleth plots (Dodge, 1977). It is also, by definition, the optimum NO_x condition for ozone formation.

In the "Equal Benefit Incremental Reactivity" (EBIR) scenarios, the NO_x inputs are adjusted so that the effect on ozone of a given percentage incremental change in ROG input is the same as the effect of an equal percentage change in NO_x. In other words, this is the point where the incremental reactivity of the base ROG mixture, multiplied by the total amount of ROG input (excluding aloft or biogenic ROGs), equals the incremental reactivity of NO_x, multiplied by the amount of NO_x input. These are refereed to as equal benefit scenarios because a NO_x reductions and VOC reductions are of equal benefit in reducing ozone. It represents the lowest NO_x conditions where VOC control is of equal or greater effectiveness for reducing ozone than NO_x control. (Carbon Bond calculations were not conducted for EBIR conditions.)

In each of these three cases, the NO_x adjustment was done by varying both the initial NO_x and the emitted NO_x by the same factor. The exact NO_x input levels where ozone or base ROG reactivity were maximized, or where the equal benefit point occurred, were determined to within 1% by an iterative procedure where the ozone and the derivatives of ozone with respect to ROG or NO_x were calculated and then fit to polynomial curves near the points of interest.

Averaged Conditions Scenarios.

It is useful for sensitivity studies and example calculations to have a single scenario or set of scenario conditions which can be taken as being representative of the larger set. For this purpose, we derived an "averaged conditions" scenario from the averages of all the relevant inputs of the 39 base case scenarios. The inputs which were averaged to derive this scenario included the latitude, longitude, initial and aloft ozone, CO, biogenic levels, fractions of total non-biogenic and non-aloft ROGs present initially, fractions of total NO_x present initially, hourly emission fluxes of ROG, NO_x, biogenics, and CO, and hourly temperatures, humidities, and inversion heights. The major inputs for

this scenario are also given in Table 4. The MIR, MOR, or EBIR versions of this scenario are determined using the exact same procedure as discussed above for the base case scenarios.

Detailed 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 this program and its 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 Appendix A.

The OZIPM4 computer program was not used in this work 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 Appendix A 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 also given in Appendix A.

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. In these scenarios, there was no ground-layer background ozone, NMOCs or NO_x. (Ground-layer background O_3 was not used because it would react rapidly with the initial NO, and the ground-layer background NMOCs are assumed to be small compared to controllable NMOC or NO_x.) The aloft layer contained 30 ppb of a mixture of ROGs 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 in Appendix A 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 in Appendix A 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 Appendix A 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 NO_x levels yielding maximum incremental reactivity (for the MIR scenarios), maximum ozone concentration (for MOIR), and equal effects of fractional changes of NO_x and ROG inputs on ozone (for EBIR) were determined by a computer program (called MROPT2). This program calculated the maximum ozone concentrations and base ROG incremental reactivities at varying NO_x levels to determine these three NO_x levels for each scenario. The program initially used large stepwise changes in NO_x to determine the approximate points, then used increasingly smaller changes, then quadratic fitting functions, to determine the points fairly precisely. Note that the MIR, MOR, and EBIR NO_x levels depend on the chemical mechanism as well as the scenario, so in general they are different for the Carbon Bond mechanism than those used when calculating the reactivity scale with SAPRC-90. The NO_x inputs for the base case and adjusted NO_x scenarios for the SAPRC-90 and the Carbon Bond mechanism are given in Table 7.

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 emitted. Table 5 gives the detailed composition of the base ROG mixture which was used to represent the initially present and emitted NMOCs, and Table 8 gives them in terms of Carbon Bond model species used in the EKMA calculations. Detailed and model species compositions used for the NMOCs aloft are given in Tables 6 and 8, respectively.

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 given in Appendix A. The values for intermediate times are determined by linear interpolation.

The photolysis rates used were given as a function of solar zenith angle by SAI, and are tabulated in Table 3. In the model simulations, 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 photolysis rates given for the 10 zenith angles were then used as inputs to a non-linear optimization program to

Table 7. NO_x Inputs (in mmol m^{-2} day^{-1}) in the base case and adjusted NO_x scenarios for the reactivity calculations using the SAPRC-90 and the Carbon Bond mechanisms.

Scenario	Base Case	Adjusted NOx					
		SAPRC-90			Carbon Bond		
		MIR	MOIR	EBIR	MIR	MOIR	EBIR
ATL GA	1.62	3.09	2.06	1.51	3.11	2.18	1.75
AUS TX	1.21	3.15	2.09	1.44	3.14	2.19	1.69
BAL MD	3.26	3.97	2.71	1.79	4.06	2.97	2.34
BAT LA	1.63	2.32	1.60	1.25	2.32	1.66	1.40
BIR AL	1.85	4.42	3.00	2.14	4.63	3.28	2.59
BOS MA	2.19	5.05	3.34	2.32	5.09	3.55	2.76
CHA NC	0.96	4.07	2.66	2.07	4.21	2.88	2.38
CHI IL	2.15	5.26	3.66	2.60	5.30	3.92	3.17
CIN OH	2.71	4.91	3.26	2.03	5.02	3.53	2.63
CLE OH	2.37	3.41	2.21	1.56	3.38	2.37	1.87
DAL TX	3.70	4.03	2.67	1.96	3.96	2.75	2.20
DEN CO	4.64	5.56	3.71	2.58	5.39	3.85	3.13
DET MI	2.54	4.41	2.95	1.83	4.48	3.20	2.39
ELP TX	1.86	2.51	1.65	1.24	2.44	1.68	1.35
HAR CT	1.28	3.72	2.40	1.55	3.81	2.62	1.97
HOU TX	4.19	5.88	4.00	2.76	5.92	4.29	3.34
IND IN	1.82	2.89	1.81	1.22	2.89	1.96	1.44
JAC FL	1.01	2.09	1.40	1.04	2.08	1.47	1.18
KAN MO	1.28	2.92	1.91	1.14	2.91	2.02	1.48
LAK LA	0.94	1.84	1.27	0.95	1.84	1.36	1.10
LOS CA	3.04	4.03	2.83	2.25	4.09	3.02	2.60
LOU KY	2.48	4.15	2.69	1.93	4.14	2.81	2.19
MEM TN	2.20	4.32	2.95	1.98	4.37	3.16	2.42
MIA FL	0.98	3.35	2.18	1.59	3.37	2.31	1.82
NAS TN	0.92	2.82	1.88	1.28	2.91	2.04	1.55
NEW NY	4.85	7.73	5.91	4.39	7.83	6.27	5.51
PHI PA	3.07	4.42	2.97	1.99	4.41	3.18	2.43
PHO AZ	5.26	7.53	5.00	3.31	7.45	5.27	4.03
POR OR	0.96	2.04	1.27	0.93	2.04	1.34	1.05
RIC VA	2.65	4.43	2.96	1.83	4.53	3.26	2.51
SAC CA	1.12	1.84	1.21	0.81	1.83	1.27	0.96
SAI MO	4.22	5.17	3.52	2.39	5.09	3.72	3.05
SAL UT	1.26	3.03	1.93	1.24	2.99	2.05	1.53
SAN TX	1.53	2.02	1.31	1.00	2.02	1.35	1.10
SDO CA	1.08	1.53	1.02	0.77	1.53	1.08	0.89
SFO CA	5.24	3.73	2.66	2.17	3.64	2.71	2.44
TAM FL	1.81	2.18	1.45	1.13	2.22	1.57	1.29
TUL OK	2.80	4.21	2.78	1.77	4.21	2.98	2.24
WAS DC	2.54	4.05	2.76	1.93	4.20	3.02	2.40

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.

Table 8. Composition of the Base ROG and Aloft mixtures in terms of Carbon Bond Species.

CB4 Species	mol Species/mol C Mix Base ROG	Aloft ROG
PAR	0.59861	0.48392
ETH	0.01410	0.01555
OLE	0.13992	0.00270
TOL	0.13773	0.00614
XYL	0.17204	0.00372
HCHO	0.10460	0.74862
ALD2	0.25866	0.10754
ISOP	0.00136	0.00363

Reactivity Calculation Methods

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.

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 various 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. In the case of the Carbon Bond mechanism these included "T_HCHO", "T_ALD2" and "T_ETH". (The kinetic reactivities of the explicit Carbon Bond species which react only with OH radicals VOCs were calculated from their OH rate constants as discussed below.) The ratio of the final concentration of the reactive species to the TRACE species is used as the kinetic reactivity of the reactive test species, i.e.,

$$KR(Txx) = 1 - \frac{\text{final [Txx]}}{\text{final [TRACE]}},$$

where "Txx" is Tnn or T_name. (Note that the initial and emitted Txx and TRACE are the same and thus cancel out.) 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 represented in the model using a species with adjustable parameters. In this case, the program knows the compound's OH radical 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 corresponding model species. (In these calculations, this was done for all the Carbon Bond VOC species except for HCHO, ALD2, and ETH, whose kinetic reactivities were calculated explicitly as discussed above.)

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 $5x10^{-4}$ 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 incremental reactivities (IR) are then computed as:

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

where (VOC added) is in units of mmol m^{-2} day^{-1}, nC is the number of carbons in the VOC, $MaxO_3$ is in units of ppm, and the superscripts "base" and "test" refer to the results of the base case and the added test VOC calculation, respectively. The use of (final TRACE) in the denominator serves to convert the units of (VOC added) to final ppmC units, so both the numerator and denominator have molar units, giving a result whose units are moles of ozone formed per mole of carbon input.

Note that all incremental reactivities calculated in this work are based on ozone yields. Incremental reactivities can also be based on integrated ozone or integrated ozone above the standard (Carter, 1993a,b), but these are not reported here because they are not needed for the Auto/Oil Program.

Table 9 gives examples of the selected raw calculation results of 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).

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 mechanistic reactivities of "NULL-3" (a species which reacts with OH with a rate constant of 3 x 10^{-3} ppm^{-1} min^{-1} and only regenerates OH) in these scenarios (calculated using the SAPRC-90 mechanism) have magnitudes of less than 0.003. Based on this, we conclude that the numerical uncertainty corresponds to uncertainty in mechanistic reactivities of less than 0.005.

Table 9. Kinetic reactivities, amounts added, percent ozone changes, and molar mechanistic reactivities for the MIR and MOR "averaged conditions" scenario calculations.

CB4 Species	MIR Scenario				MOR Scenario			
	K.Rct.	Added	ΔO3 (%)	M.Rct	K.Rct.	Added	ΔO3 (%)	M.Rct
CO	0.030	1.20	0.29	0.98	0.047	0.78	0.10	0.414
PAR	0.108	0.34	0.98	3.22	0.164	0.23	0.30	1.22
ETH	0.954	0.019	0.74	4.95	0.968	0.019	0.24	1.97
OLE	1.00	0.019	1.57	9.95	1.00	0.019	0.46	3.63
TOL	0.569	0.093	0.28	6.30	0.723	0.0073	-0.03	-0.718
XYL	0.936	0.0049	0.79	20.8	0.968	0.0049	0.17	5.53
HCHO	0.925	0.040	2.01	6.54	0.944	0.040	0.43	1.77
ALD2	0.964	0.019	0.98	6.44	0.972	0.019	0.29	2.38
ISOP	1.00	0.0074	1.39	22.7	1.00	0.0074	0.36	7.40
MEOH	0.122	0.300	1.03	3.38	0.185	0.20	0.24	0.98
ETOH	0.362	0.051	0.56	3.66	0.503	0.037	0.17	1.37
MTBE	0.325	0.023	0.22	3.57	0.457	0.016	0.07	1.54

Incremental reactivities were calculated as described above for each of the Carbon Bond VOC species for each of the 39 sets of base case, MIR, and MOR scenarios. The incremental reactivities for these Carbon Bond VOC species in the MIR scale were then computed by averaging the incremental reactivities of these species in the MIR scenarios. Likewise, the incremental reactivities for these species in the maximum ozone incremental reactivity (MOIR) scale were calculated by averaging the incremental reactivities in the MOR scenarios.

The Carbon Bond mechanism represents detailed model species by mixtures of Carbon Bond species. In this work, only reactivities of the carbon bond model species were calculated explicitly. The reactivities of the detailed model species were calculated from those of the Carbon Bond species and using the principle that incremental reactivities of mixtures are equal to the sum of the incremental reactivities of the components, times the fraction of the components present. Thus, if $f_{j,i}$ is the amount of Carbon Bond species i used to represent detailed model species j, and IR_i is the incremental reactivity of Carbon Bond species i in a particular reactivity scale, then IR_j, the incremental reactivity of detailed model species j in that scale, is given by $IR_j = \sum_i IR_i \, f_{j,i}$.

Note that the method used for deriving Carbon Bond MIR or MOIR incremental reactivities from those in the individual scenarios is somewhat different from the method used for the SAPRC-90 mechanism. In the latter case, the kinetic, mechanistic, and incremental reactivities were calculated for each detailed model species in each scenario, and then the incremental reactivities for the scales were derived by averaging the products of the average kinetic and the average mechanistic reactivities for each model species. This approach is not

appropriate for the Carbon Bond mechanism because the concept of separating kinetic and mechanistic reactivities is not compatible with the concept of different parts of the molecules reacting independently, which is the basis for the Carbon Bond representation of many detailed model species. However, use of the SAPRC-90 reactivity aggregation approach gives incremental reactivities which are within ~2% of those calculated using the approach in this work, except for cases, such as the C_{8+} alkylbenzenes under maximum ozone conditions, which the detailed model species are represented as combinations of carbon bond species with both negative and positive reactivities (e.g, TOL and PAR, respectively).

RESULTS

Tables 10-12 give the listings of incremental reactivities (in units of mol O_3/mol C) of the Carbon Bond species and the base ROG mixture (B.ROG) in all the individual maximum reactivity, maximum ozone, and base case scenarios, respectively. Table 13 gives the incremental reactivities of the carbon bond species and the individual SAPRC detailed model species in the MIR and MOIR scales calculated using the Carbon Bond mechanism. The data in the columns labeled "1991" are the reactivities calculated using a previous version of the Carbon Bond mechanism, which was presented to the CARB's Reactivity Advisory Panel in 1991, and which is given in the report to the CARB on the reactivity scale calculation (Carter 1993a). The data in the column labeled "1993" are the reactivities calculated in this work.

The MIR and MOIR incremental reactivities for the Carbon Bond model species are essentially unchanged relative to the previous (1991) calculation except for MTBE and, to a lesser extent, methanol. The MTBE reactivity is changed because in the 1991 calculation it was represented by PAR, while in this calculation it was represented explicitly. The MEOH reactivity changed because of the change in its OH radical rate constant. The relatively large percentage change in TOL reactivity in the MOIR scale is not significant, because the magnitude of the reactivity is small.

Much larger changes can be seen in the reactivities for individual detailed model species relative to the 1991 calculation. This is because of the differences in assignments of Carbon Bond species to the detailed model species which were provided by SAI, compared to those we used previously. As expected, the differences are largest for those species whose Carbon Bond assignments are the most uncertain.

Table 10. Incremental Reactivities for Carbon Bond model species and the base ROG mixture in the individual Maximum Reactivity scenarios. Units are mol O_3/mol

Scen.	CO	PAR	ETH	OLE	TOL	XYL	HCHO	ALD2	ISOP	MEOH	ETOH	MTBE	B.ROG
ATL GA	0.0270	0.308	4.39	8.89	3.10	16.87	5.06	5.38	19.77	0.390	1.239	1.064	0.882
AUS TX	0.0300	0.363	4.54	9.53	3.25	17.87	5.26	5.83	20.93	0.399	1.371	1.153	0.958
BAL MD	0.0330	0.358	4.99	10.37	4.54	21.59	6.38	6.88	23.58	0.420	1.415	1.406	1.046
BAT LA	0.0230	0.236	4.05	7.93	2.96	16.09	5.25	4.41	18.33	0.357	1.001	0.944	0.786
BIR AL	0.0350	0.468	5.51	11.67	4.47	22.97	6.71	7.59	26.08	0.496	1.729	1.370	1.224
BOS MA	0.0320	0.388	4.21	8.52	3.13	15.65	4.49	5.37	18.79	0.388	1.332	1.197	0.894
CHA NC	0.0330	0.432	4.32	8.59	3.14	15.40	4.01	5.53	18.24	0.407	1.502	1.246	0.916
CHI IL	0.0270	0.312	4.65	9.56	4.01	20.46	5.95	5.81	21.83	0.408	1.240	1.090	0.989
CIN OH	0.0350	0.418	4.93	10.50	3.93	20.40	5.83	6.86	23.58	0.431	1.531	1.373	1.075
CLE OH	0.0240	0.272	4.05	8.71	2.74	16.61	5.32	5.38	19.90	0.347	1.023	0.965	0.848
DAL TX	0.0250	0.292	4.12	8.74	2.90	16.80	5.38	5.08	19.76	0.361	1.152	1.001	0.860
DEN CO	0.0210	0.211	4.01	8.48	2.73	16.96	5.86	5.16	20.10	0.333	0.881	0.877	0.816
DET MI	0.0310	0.389	4.66	10.20	3.63	19.82	5.89	6.57	23.12	0.410	1.399	1.192	1.047
ELP TX	0.0210	0.213	4.14	8.96	2.75	17.72	5.87	5.32	20.71	0.338	0.952	0.875	0.842
HAR CT	0.0350	0.447	5.19	10.90	3.98	20.60	5.89	7.10	23.99	0.461	1.650	1.342	1.130
HOU TX	0.0360	0.391	5.07	10.33	4.58	21.47	6.17	6.42	23.50	0.451	1.519	1.446	1.065
IND IN	0.0300	0.344	4.98	10.56	3.65	20.80	6.52	6.54	24.01	0.435	1.365	1.172	1.055
JAC FL	0.0310	0.333	5.02	9.81	3.80	19.59	5.83	5.88	22.40	0.453	1.383	1.211	0.995
KAN MO	0.0350	0.460	5.27	11.12	4.03	20.98	5.95	7.20	24.39	0.468	1.714	1.349	1.152
LAK LA	0.0360	0.392	5.57	10.40	4.65	22.39	6.61	6.02	23.92	0.525	1.562	1.403	1.116
LOS CA	0.0160	0.180	3.13	6.76	2.68	14.47	4.31	3.99	15.56	0.263	0.705	0.658	0.669
LOU KY	0.0350	0.424	5.26	10.64	3.77	19.81	6.11	6.35	23.24	0.478	1.617	1.360	1.081
MEM TN	0.0380	0.451	5.71	11.58	4.80	23.34	6.84	7.34	26.34	0.518	1.710	1.470	1.219
MIA FL	0.0320	0.376	5.00	10.24	3.67	19.54	5.68	6.44	22.97	0.444	1.443	1.249	1.037
NAS TN	0.0440	0.594	6.61	13.09	5.51	26.04	7.46	8.32	29.16	0.631	2.269	1.695	1.427
NEW NY	0.0230	0.215	3.63	7.19	2.89	15.08	4.92	4.29	17.17	0.309	0.768	0.882	0.730
PHI PA	0.0310	0.351	4.73	10.05	3.78	20.10	6.29	6.38	23.36	0.413	1.325	1.178	1.031
PHO AZ	0.0230	0.321	4.65	10.36	3.65	21.16	6.14	6.47	22.95	0.399	1.306	0.994	1.032
POR OR	0.0320	0.374	4.95	10.28	3.51	19.24	5.68	6.38	22.70	0.429	1.464	1.232	1.025
RIC VA	0.0300	0.362	4.74	10.38	3.76	20.40	6.75	6.99	24.00	0.408	1.343	1.171	1.067
SAC CA	0.0370	0.415	5.94	11.86	5.20	24.54	6.84	7.58	26.60	0.519	1.831	1.650	1.186
SAI MO	0.0230	0.265	4.02	8.95	2.96	17.66	6.17	5.71	21.08	0.341	1.003	0.925	0.886
SAL UT	0.0270	0.356	4.56	9.98	3.12	18.58	5.66	6.40	21.80	0.398	1.355	1.087	0.989
SAN TX	0.0260	0.319	4.08	8.57	2.80	16.06	4.60	5.21	18.93	0.359	1.247	1.021	0.854
SDO CA	0.0210	0.193	3.25	6.91	2.37	14.37	4.81	4.03	17.07	0.270	0.737	0.796	0.683
SFO CA	0.0180	0.145	3.29	6.44	2.92	14.13	4.26	3.86	15.02	0.252	0.700	0.868	0.595
TAM FL	0.0310	0.317	4.77	9.50	3.59	18.82	6.13	5.51	21.98	0.423	1.253	1.185	0.956
TUL OK	0.0360	0.419	5.05	10.47	3.94	20.26	5.98	6.62	23.74	0.456	1.485	1.341	1.088
WAS DC	0.0310	0.383	4.54	9.78	3.46	18.81	6.19	6.31	22.53	0.406	1.350	1.192	1.013
Average	**0.0296**	**0.346**	**4.66**	**9.66**	**3.60**	**19.06**	**5.77**	**6.01**	**21.88**	**0.410**	**1.330**	**1.170**	**0.981**
Std. Dev	**0.0062**	**0.093**	**0.73**	**1.44**	**0.74**	**2.86**	**0.79**	**1.05**	**3.05**	**0.076**	**0.331**	**0.230**	**0.167**

Table 11. Incremental Reactivities for Carbon Bond model species and the base ROG mixture in the individual Maximum Ozone scenarios. Units are mol O_3/mol C.

Scen.	CO	PAR	ETH	OLE	TOL	XYL	HCHO	ALD2	ISOP	MEOH	ETOH	MTBE	B.ROG
ATL GA	0.0190	0.189	2.00	3.68	-0.05	5.50	1.65	2.25	7.55	0.192	0.691	0.701	0.353
AUS TX	0.0200	0.233	2.04	3.91	-0.38	5.49	1.61	2.53	7.78	0.191	0.815	0.753	0.385
BAL MD	0.0190	0.203	1.76	3.47	-0.95	4.88	1.45	2.32	6.70	0.167	0.676	0.672	0.333
BAT LA	0.0160	0.130	1.72	2.95	-0.17	4.80	1.73	1.58	6.52	0.168	0.455	0.597	0.276
BIR AL	0.0220	0.291	2.14	4.13	-0.64	6.13	1.70	2.77	8.09	0.211	0.983	0.800	0.438
BOS MA	0.0210	0.235	1.73	3.14	-0.37	4.20	1.18	2.03	6.21	0.177	0.728	0.748	0.333
CHA NC	0.0230	0.292	1.99	3.58	-0.13	4.82	1.12	2.42	6.80	0.203	0.950	0.839	0.397
CHI IL	0.0170	0.166	1.70	3.16	-0.64	5.12	1.58	1.96	6.59	0.165	0.546	0.617	0.307
CIN OH	0.0210	0.260	1.99	3.94	-0.65	5.40	1.44	2.66	7.55	0.188	0.876	0.776	0.396
CLE OH	0.0180	0.164	1.79	3.48	-0.93	4.72	1.68	2.18	7.30	0.167	0.549	0.647	0.308
DAL TX	0.0150	0.178	1.78	3.40	-0.29	4.93	1.68	2.00	7.02	0.167	0.636	0.624	0.322
DEN CO	0.0170	0.121	1.81	3.40	-0.56	5.14	1.93	2.05	7.60	0.163	0.419	0.604	0.294
DET MI	0.0190	0.233	1.78	3.49	-0.75	4.77	1.34	2.32	6.75	0.170	0.769	0.693	0.350
ELP TX	0.0150	0.131	2.01	3.95	-0.33	6.13	2.20	2.35	8.60	0.174	0.534	0.603	0.339
HAR CT	0.0240	0.283	2.17	4.17	-0.39	5.87	1.50	2.78	7.87	0.209	0.990	0.827	0.431
HOU TX	0.0180	0.205	1.74	3.27	-0.57	4.98	1.55	2.05	6.71	0.172	0.675	0.675	0.333
IND IN	0.0210	0.192	2.05	3.98	-0.61	5.92	1.93	2.48	8.14	0.194	0.707	0.723	0.369
JAC FL	0.0210	0.178	2.08	3.68	0.26	5.98	1.77	2.18	7.76	0.207	0.652	0.733	0.361
KAN MO	0.0240	0.290	2.19	4.21	-0.19	5.87	1.41	2.82	7.78	0.206	1.041	0.847	0.437
LAK LA	0.0200	0.177	1.79	2.93	-0.14	5.23	1.65	1.68	6.45	0.199	0.555	0.717	0.313
LOS CA	0.0110	0.106	1.18	2.32	-0.52	3.82	1.29	1.40	5.03	0.114	0.307	0.435	0.212
LOU KY	0.0230	0.252	2.20	4.05	-0.26	6.00	1.93	2.45	8.22	0.220	0.887	0.840	0.412
MEM TN	0.0220	0.228	1.96	3.58	-0.27	5.58	1.58	2.30	7.24	0.202	0.761	0.777	0.374
MIA FL	0.0220	0.218	2.14	4.02	0.01	6.00	1.64	2.58	8.09	0.207	0.775	0.787	0.394
NAS TN	0.0270	0.343	2.44	4.38	0.21	7.04	1.86	2.85	8.71	0.262	1.203	0.969	0.504
NEW NY	0.0170	0.120	1.42	2.36	-0.60	3.75	1.38	1.43	5.51	0.140	0.287	0.570	0.228
PHI PA	0.0190	0.189	1.75	3.33	-0.52	4.85	1.47	2.13	6.75	0.168	0.631	0.672	0.323
PHO AZ	0.0160	0.215	1.99	4.24	-0.92	6.24	1.88	2.76	8.23	0.176	0.799	0.645	0.393
POR OR	0.0220	0.223	2.16	4.10	-0.27	5.92	1.74	2.56	8.14	0.204	0.837	0.789	0.394
RIC VA	0.0210	0.222	1.90	3.74	-0.70	5.22	1.47	2.53	7.18	0.180	0.751	0.725	0.364
SAC CA	0.0180	0.228	2.16	4.14	-0.16	6.45	1.83	2.61	8.19	0.204	0.904	0.718	0.409
SAI MO	0.0160	0.156	1.58	3.14	-1.03	4.24	1.56	2.03	6.54	0.146	0.510	0.577	0.282
SAL UT	0.0190	0.246	2.12	4.28	-0.66	5.93	1.77	2.87	8.40	0.193	0.882	0.741	0.412
SAN TX	0.0170	0.210	1.98	3.81	0.14	5.54	1.54	2.39	7.62	0.182	0.782	0.683	0.372
SDO CA	0.0140	0.110	1.47	2.78	-0.33	4.34	1.63	1.59	6.37	0.130	0.349	0.517	0.248
SFO CA	0.0110	0.081	1.26	2.30	-0.51	3.60	1.42	1.28	5.23	0.114	0.267	0.413	0.198
TAM FL	0.0200	0.168	1.92	3.37	-0.13	5.40	1.86	1.93	7.37	0.192	0.561	0.711	0.328
TUL OK	0.0220	0.221	1.89	3.50	-0.39	5.14	1.47	2.26	7.06	0.191	0.701	0.762	0.356
WAS DC	0.0200	0.229	1.75	3.35	-0.78	4.61	1.48	2.21	6.73	0.174	0.725	0.715	0.342
Average	**0.0192**	**0.203**	**1.89**	**3.56**	**-0.41**	**5.27**	**1.61**	**2.25**	**7.24**	**0.182**	**0.697**	**0.699**	**0.349**
Std. Dev	**0.0034**	**0.058**	**0.26**	**0.55**	**0.32**	**0.78**	**0.22**	**0.42**	**0.89**	**0.029**	**0.214**	**0.111**	**0.065**

Table 12. Incremental Reactivities for Carbon Bond model species and the base ROG mixture in the individual base case scenarios. Units are mol O_3/mol C.

Scen.	CO	PAR	ETH	OLE	TOL	XYL	HCHO	ALD2	ISOP	MEOH	ETOH	MTBE	B.ROG
ATL GA	0.0160	0.116	1.29	2.36	-1.23	2.28	0.81	1.50	4.38	0.126	0.461	0.528	0.185
AUS TX	0.0140	0.097	1.04	2.05	-2.32	0.76	0.50	1.50	3.49	0.095	0.426	0.472	0.124
BAL MD	0.0210	0.238	2.32	4.66	0.16	7.91	2.37	3.06	9.76	0.215	0.798	0.770	0.471
BAT LA	0.0150	0.124	1.63	2.78	-0.30	4.37	1.62	1.48	6.11	0.160	0.431	0.572	0.258
BIR AL	0.0150	0.143	1.07	2.19	-3.35	0.72	0.34	1.63	3.15	0.105	0.606	0.504	0.139
BOS MA	0.0150	0.132	1.04	1.92	-1.74	1.21	0.49	1.29	3.28	0.107	0.461	0.511	0.153
CHA NC	0.0120	0.075	0.84	1.74	-2.47	-0.07	0.21	1.35	2.56	0.078	0.390	0.400	0.081
CHI IL	0.0110	0.044	0.66	1.24	-2.82	-0.17	0.40	0.87	2.07	0.072	0.215	0.322	0.039
CIN OH	0.0180	0.196	1.43	2.86	-1.93	2.58	0.68	2.05	4.79	0.135	0.720	0.613	0.249
CLE OH	0.0180	0.163	1.79	3.48	-0.93	4.72	1.68	2.18	7.30	0.167	0.546	0.641	0.308
DAL TX	0.0250	0.294	3.98	8.14	2.75	15.75	4.98	4.70	18.42	0.358	1.147	1.016	0.812
DEN CO	0.0200	0.184	3.21	6.34	1.57	12.28	4.20	3.79	14.92	0.278	0.714	0.809	0.605
DET MI	0.0160	0.177	1.28	2.52	-1.88	2.26	0.69	1.72	4.28	0.124	0.630	0.550	0.219
ELP TX	0.0170	0.158	2.57	5.12	0.56	9.04	3.07	3.01	11.49	0.220	0.653	0.691	0.464
HAR CT	0.0160	0.121	1.12	2.36	-2.59	1.10	0.39	1.71	3.42	0.105	0.591	0.495	0.149
HOU TX	0.0180	0.197	1.64	3.08	-0.76	4.50	1.42	1.94	6.23	0.163	0.649	0.652	0.309
IND IN	0.0200	0.172	1.84	3.57	-1.00	4.92	1.67	2.24	7.14	0.176	0.649	0.669	0.318
JAC FL	0.0160	0.085	1.23	2.14	-1.08	2.21	0.80	1.28	4.01	0.127	0.363	0.507	0.159
KAN MO	0.0180	0.179	1.36	2.80	-1.87	2.12	0.45	2.00	4.18	0.127	0.763	0.589	0.227
LAK LA	0.0150	0.074	0.92	1.42	-1.61	1.41	0.69	0.81	2.82	0.114	0.244	0.463	0.105
LOS CA	0.0110	0.106	1.20	2.37	-0.51	3.90	1.35	1.37	5.21	0.113	0.318	0.424	0.220
LOU KY	0.0210	0.213	1.81	3.30	-0.89	4.26	1.45	2.03	6.45	0.183	0.770	0.740	0.320
MEM TN	0.0170	0.131	1.19	2.20	-1.77	2.05	0.66	1.46	3.79	0.128	0.500	0.541	0.178
MIA FL	0.0130	0.048	0.95	1.90	-2.18	0.47	0.37	1.37	2.97	0.090	0.321	0.405	0.085
NAS TN	0.0160	0.110	1.09	2.14	-2.61	0.97	0.47	1.51	3.14	0.113	0.585	0.489	0.132
NEW NY	0.0150	0.062	0.75	1.08	-1.99	0.34	0.45	0.68	2.32	0.088	0.116	0.411	0.063
PHI PA	0.0180	0.178	1.63	3.09	-0.76	4.26	1.30	1.98	6.16	0.158	0.598	0.641	0.294
PHO AZ	0.0160	0.214	1.97	4.20	-0.96	6.17	1.86	2.73	8.15	0.175	0.792	0.642	0.389
POR OR	0.0180	0.142	1.45	2.77	-1.41	2.72	0.93	1.78	4.94	0.138	0.605	0.591	0.223
RIC VA	0.0190	0.172	1.40	2.78	-1.82	2.70	0.66	1.95	4.58	0.136	0.633	0.606	0.233
SAC CA	0.0170	0.192	1.74	3.35	-0.85	4.48	1.29	2.14	6.23	0.165	0.786	0.628	0.312
SAI MO	0.0190	0.201	2.37	4.88	0.45	8.50	2.95	3.09	10.98	0.213	0.681	0.717	0.475
SAL UT	0.0140	0.141	1.24	2.62	-2.65	1.39	0.67	1.90	4.33	0.109	0.598	0.511	0.178
SAN TX	0.0190	0.249	2.51	4.87	0.91	8.02	2.21	3.00	10.18	0.229	0.923	0.788	0.490
SDO CA	0.0140	0.110	1.45	2.76	-0.35	4.29	1.61	1.58	6.28	0.129	0.350	0.511	0.246
SFO CA	0.0080	0.083	1.81	4.37	1.52	8.77	2.87	2.80	9.96	0.134	0.396	0.335	0.406
TAM FL	0.0240	0.235	2.97	5.40	1.38	10.12	3.31	3.06	12.35	0.285	0.829	0.920	0.553
TUL OK	0.0210	0.201	1.69	3.13	-0.75	4.23	1.23	2.03	6.14	0.174	0.649	0.709	0.309
WAS DC	0.0170	0.183	1.32	2.51	-1.73	2.50	0.87	1.70	4.61	0.134	0.598	0.594	0.230
Average	**0.0167**	**0.152**	**1.61**	**3.14**	**-1.02**	**4.10**	**1.38**	**2.01**	**6.22**	**0.152**	**0.577**	**0.589**	**0.275**
Std. Dev	**0.0034**	**0.059**	**0.71**	**1.45**	**1.38**	**3.61**	**1.12**	**0.82**	**3.65**	**0.060**	**0.207**	**0.150**	**0.164**

Table 13. Incremental Reactivities calculated using two versions of the Carbon Bond IV Mechanism. The "1991" version is from Carter (1993a), and the "1993" version was calculated in this work.

Name	-- Maximum Reactivity -- 1991	1993	chg.	---- Maximum Ozone ---- 1991	1993	chg.
Carbon Bond Species (mol O_3/mol C VOC)						
CO	0.03030	0.02955	-2%	0.01920	0.01923	0%
PAR	0.3445	0.3458	0%	0.2005	0.2030	1%
ETH	2.386	2.328	-2%	0.9404	0.9427	0%
OLE	4.953	4.831	-2%	1.747	1.778	2%
TOL	0.5360	0.5139	-4%	-0.07590	-0.05907	-22%
XYL	2.515	2.383	-5%	0.6599	0.6587	0%
HCHO	6.121	5.771	-6%	1.629	1.612	-1%
ALD2	2.961	3.007	2%	1.072	1.123	5%
ISOP	4.603	4.375	-5%	1.453	1.448	0%
MEOH	0.3947	0.4101	4%	0.1677	0.1818	8%
ETOH	0.6729	0.6650	-1%	0.3351	0.3483	4%
MTBE	0.3445	0.2340	-32%	0.2005	0.1397	-30%
Detailed Model Species (gm O_3/gm VOC)						
CO	0.053	0.051	-4%	0.033	0.033	0%
METHANE	0.0	0.0104		0.0	0.0061	
ETHANE	0.22	0.22	-2%	0.131	0.130	-1%
PROPANE	0.57	0.56	-2%	0.33	0.33	-1%
N-C4	1.16	1.14	-2%	0.68	0.67	-1%
N-C5	1.17	1.15	-2%	0.68	0.68	-1%
N-C6	1.18	1.16	-2%	0.68	0.68	-1%
N-C7	1.18	1.16	-2%	0.69	0.68	-1%
N-C8	1.18	1.02	-14%	0.69	0.60	-13%
N-C9	1.19	0.91	-24%	0.69	0.53	-23%
N-C10	1.19	0.82	-31%	0.69	0.48	-31%
N-C11	1.19	0.85	-29%	0.69	0.50	-28%
N-C12	1.19	0.78	-35%	0.69	0.46	-34%
N-C13	1.19	0.81	-32%	0.69	0.48	-31%
N-C14	1.19	0.84	-30%	0.69	0.49	-29%
N-C15	1.19	0.78	-35%	0.69	0.46	-34%
N-C16	1.19	0.81	-32%	0.69	0.47	-32%
N-C17	1.19	0.76	-36%	0.69	0.45	-36%
N-C18	1.20	0.78	-35%	0.70	0.46	-34%
N-C19	1.20	0.80	-33%	0.70	0.47	-32%
N-C20	1.20	0.76	-36%	0.70	0.45	-36%
N-C21	1.20	0.78	-35%	0.70	0.46	-34%
N-C22	1.20	0.75	-37%	0.70	0.44	-37%
2-ME-C3	1.16	1.14	-2%	0.68	0.67	-1%
2-ME-C4	1.17	1.15	-2%	0.68	0.68	-1%
22-DM-C3	0.94	0.92	-2%	0.54	0.54	-1%
2-ME-C5	1.18	1.16	-2%	0.68	0.68	-1%
3-ME-C5	1.18	1.16	-2%	0.68	0.68	-1%
22-DM-C4	1.18	0.96	-18%	0.68	0.57	-17%
23-DM-C4	1.18	1.16	-2%	0.68	0.68	-1%
24-DM-C5	1.18	1.16	-2%	0.69	0.68	-1%
3-ME-C6	1.18	1.16	-2%	0.69	0.68	-1%
2-ME-C6	1.18	1.16	-2%	0.69	0.68	-1%
23-DM-C5	1.18	1.16	-2%	0.69	0.68	-1%
33-DM-C5	1.18	0.99	-16%	0.69	0.58	-15%
223TM-C4	1.18	0.99	-16%	0.69	0.58	-15%
2-ME-C7	1.18	1.16	-2%	0.69	0.68	-1%

Table 13 (continued)

Name	-- Maximum Reactivity -- 1991	1993	chg.	---- Maximum Ozone ---- 1991	1993	chg.
3-ME-C7	1.18	1.16	-2%	0.69	0.68	-1%
4-ME-C7	1.18	1.16	-2%	0.69	0.68	-1%
23-DM-C6	1.18	1.16	-2%	0.69	0.68	-1%
24-DM-C6	1.18	1.16	-2%	0.69	0.68	-1%
25-DM-C6	1.18	1.16	-2%	0.69	0.68	-1%
224TM-C5	1.18	1.02	-14%	0.69	0.60	-13%
234TM-C5	1.18	1.16	-2%	0.69	0.68	-1%
2233M-C4	1.18	0.87	-26%	0.69	0.51	-26%
24-DM-C7	1.19	1.16	-2%	0.69	0.68	-1%
4-ET-C7	1.19	1.16	-2%	0.69	0.68	-1%
225TM-C6	1.19	1.04	-13%	0.69	0.61	-12%
4-PR-C7	1.19	1.17	-2%	0.69	0.68	-1%
35-DE-C7	1.19	1.17	-2%	0.69	0.69	-1%
36-DE-C8	1.19	1.17	-2%	0.69	0.69	-1%
37-DE-C9	1.19	1.17	-2%	0.69	0.69	-1%
38DE-C10	1.19	1.17	-2%	0.69	0.69	-1%
39DE-C11	1.19	1.17	-2%	0.69	0.69	-1%
CYCC3	0.0	0.0		0.0	0.0	
CYCC4	0.0	0.0		0.0	0.0	
CYCC5	1.20	1.18	-2%	0.70	0.69	-1%
ME-CYCC5	1.20	1.18	-2%	0.70	0.69	-1%
CYCC6	1.20	1.18	-2%	0.70	0.69	-1%
ME-CYCC6	1.20	1.18	-2%	0.70	0.69	-1%
13DMCYC5	1.20	1.18	-2%	0.70	0.69	-1%
ET-CYCC5	1.20	1.18	-2%	0.70	0.69	-1%
PR-CYCC5	1.20	1.18	-2%	0.70	0.69	-1%
ET-CYCC6	1.20	1.18	-2%	0.70	0.69	-1%
13DMCYC6	1.20	1.18	-2%	0.70	0.69	-1%
1E4MCYC6	1.20	1.18	-2%	0.70	0.69	-1%
13DECYC6	1.20	1.18	-2%	0.70	0.69	-1%
13E5MCC6	1.20	1.18	-2%	0.70	0.69	-1%
135ECYC6	1.20	1.18	-2%	0.70	0.69	-1%
13E5PCC6	1.20	1.18	-2%	0.70	0.69	-1%
13P5ECC6	1.20	1.18	-2%	0.70	0.69	-1%
135PCYC6	1.20	1.18	-2%	0.70	0.69	-1%
C4C5	1.17	1.15	-2%	0.68	0.67	-1%
C6PLUS	1.20	1.18	-2%	0.70	0.69	-1%
BR-C5	1.17	1.15	-2%	0.68	0.68	-1%
BR-C6	1.18	1.16	-2%	0.68	0.68	-1%
BR-C7	1.18	1.16	-2%	0.69	0.68	-1%
BR-C8	1.18	1.16	-2%	0.69	0.68	-1%
BR-C9	1.19	1.16	-2%	0.69	0.68	-1%
BR-C10	1.19	1.17	-2%	0.69	0.68	-1%
BR-C11	1.19	1.17	-2%	0.69	0.69	-1%
BR-C12	1.19	1.17	-2%	0.69	0.69	-1%
BR-C13	1.19	1.17	-2%	0.69	0.69	-1%
BR-C14	1.19	1.17	-2%	0.69	0.69	-1%
BR-C15	1.19	1.17	-2%	0.69	0.69	-1%
BR-C16	1.19	1.17	-2%	0.69	0.69	-1%
BR-C17	1.19	1.17	-2%	0.69	0.69	-1%
BR-C18	1.20	1.17	-2%	0.70	0.69	-1%
CYC-C6	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C7	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C8	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C9	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C10	1.20	1.18	-2%	0.70	0.69	-1%

Table 13 (continued)

Name	-- Maximum Reactivity -- 1991	1993	chg.	---- Maximum Ozone ---- 1991	1993	chg.
CYC-C11	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C12	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C13	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C14	1.20	1.18	-2%	0.70	0.69	-1%
CYC-C15	1.20	1.18	-2%	0.70	0.69	-1%
BCYC-C9	1.22	1.20	-2%	0.71	0.71	-1%
BCYC-C10	1.22	1.20	-2%	0.71	0.70	-1%
BCYC-C11	1.22	1.20	-2%	0.71	0.70	-1%
BCYC-C12	1.22	1.20	-2%	0.71	0.70	-1%
BCYC-C13	1.22	1.20	-2%	0.71	0.70	-1%
BCYC-C14	1.22	1.20	-2%	0.71	0.70	-1%
BCYC-C15	1.22	1.19	-2%	0.71	0.70	-1%
ISO-C4	1.16	1.14	-2%	0.68	0.67	-1%
ISO-C5	1.17	1.15	-2%	0.68	0.68	-1%
NEO-C5	0.94	0.92	-2%	0.54	0.54	-1%
22-DMB	1.18	0.96	-18%	0.68	0.57	-17%
23-DMB	1.18	1.16	-2%	0.68	0.68	-1%
ISO-C8	1.18	1.02	-14%	0.69	0.60	-13%
ETHENE	8.2	8.0	-3%	3.2	3.2	0%
PROPENE	11.7	11.4	-2%	4.2	4.3	2%
1-BUTENE	9.1	8.9	-2%	3.3	3.4	1%
C4-OLE1	9.1	8.9	-2%	3.3	3.4	1%
3M-1-BUT	7.5	7.3	-2%	2.8	2.9	1%
1-PENTEN	7.5	7.3	-2%	2.8	2.9	1%
1-HEXENE	6.5	6.3	-2%	2.5	2.5	1%
ISOBUTEN	9.1	5.8	-36%	3.3	1.9	-43%
2M-1-BUT	7.5	4.9	-35%	2.8	1.7	-41%
T-2-BUTE	10.2	10.3	1%	3.7	3.8	5%
C-2-BUTE	10.2	10.3	1%	3.7	3.8	5%
2M-2-BUT	4.8	4.8	1%	1.9	2.0	3%
13-BUTDE	14.5	17.	18%	4.7	6.3	34%
ISOPRENE	16.	15.	-5%	5.1	5.1	0%
CYC-PNTE	7.7	8.7	13%	2.9	3.3	14%
CYC-HEXE	6.6	7.4	12%	2.5	2.9	13%
A-PINENE	4.5	5.6	25%	1.8	2.2	24%
B-PINENE	4.5	4.4	-2%	1.8	1.8	1%
D-LIMONE	4.5	8.1	81%	1.8	3.1	73%
3-CARENE	4.5	4.4	-2%	1.8	1.8	1%
MYRCENE	4.5	10.7	139%	1.8	4.0	124%
C5-OLE1	7.5	7.3	-2%	2.8	2.9	1%
C6-OLE1	6.5	6.3	-2%	2.5	2.5	1%
C7-OLE1	5.7	5.6	-2%	2.2	2.2	1%
C8-OLE1	5.1	5.0	-2%	2.0	2.0	1%
C9-OLE1	4.7	4.6	-2%	1.9	1.9	1%
C10-OLE1	4.4	4.3	-2%	1.8	1.8	1%
C11-OLE1	4.1	4.0	-2%	1.7	1.7	1%
C12-OLE1	3.8	3.7	-2%	1.6	1.6	1%
C13-OLE1	3.6	3.5	-2%	1.5	1.5	1%
C14-OLE1	3.5	3.4	-2%	1.45	1.46	1%
C15-OLE1	3.3	3.2	-2%	1.40	1.41	1%
C4-OLE2	10.2	10.3	1%	3.7	3.8	5%
C5-OLE2	8.4	8.5	1%	3.1	3.2	4%
C6-OLE2	7.2	7.3	1%	2.7	2.8	4%
C7-OLE2	6.3	6.4	1%	2.4	2.5	4%
C8-OLE2	5.7	5.7	1%	2.2	2.3	4%
C9-OLE2	5.2	5.2	1%	2.0	2.1	3%

Table 13 (continued)

Name	-- Maximum Reactivity -- 1991	1993	chg.	---- Maximum Ozone ---- 1991	1993	chg.
C10-OLE2	4.8	4.8	1%	1.9	2.0	3%
C11-OLE2	4.5	4.5	1%	1.8	1.8	3%
C12-OLE2	4.2	4.2	1%	1.7	1.7	3%
C13-OLE2	4.0	4.0	1%	1.6	1.7	3%
C14-OLE2	3.8	3.8	1%	1.6	1.6	3%
C15-OLE2	3.6	3.6	1%	1.49	1.5	3%
C6-OL2D	7.4	7.4	1%	2.7	2.9	4%
C7-OL2D	5.8	6.5	12%	2.3	2.5	13%
C8-OL2D	5.8	5.8	1%	2.2	2.3	4%
C9-OL2D	5.3	5.3	1%	2.1	2.1	3%
C10-OL2D	4.9	4.9	1%	1.9	2.0	3%
C11-OL2D	4.5	4.6	1%	1.8	1.9	3%
C12-OL2D	4.2	4.3	1%	1.7	1.8	3%
C13-OL2D	4.0	4.0	1%	1.6	1.7	3%
C14-OL2D	3.8	3.8	1%	1.6	1.6	3%
C15-OL2D	3.6	3.6	1%	1.5	1.5	3%
BENZENE	0.22	0.21	-2%	0.126	0.125	-1%
TOLUENE	2.0	1.9	-5%	-0.27	-0.22	-21%
C2-BENZ	1.9	1.8	-5%	-0.145	-0.095	-34%
N-C3-BEN	1.8	1.7	-4%	-0.046	-0.0030	-93%
I-C3-BEN	1.8	1.7	-4%	-0.046	-0.0030	-93%
C9-BEN1	1.8	1.7	-4%	-0.046	-0.0030	-93%
S-C4-BEN	1.7	1.7	-4%	0.032	0.070	119%
C10-BEN1	1.7	1.7	-4%	0.032	0.070	119%
C11-BEN1	1.7	1.6	-4%	0.095	0.129	36%
C12-BEN1	1.6	1.6	-4%	0.148	0.18	21%
O-XYLENE	9.1	8.6	-6%	2.4	2.4	0%
P-XYLENE	9.1	8.6	-6%	2.4	2.4	0%
M-XYLENE	9.1	8.6	-6%	2.4	2.4	0%
C8-BEN2	9.1	8.6	-6%	2.4	2.4	0%
C9-BEN2	8.2	7.8	-6%	2.2	2.2	0%
C10-BEN2	7.5	7.1	-5%	2.0	2.0	0%
C11-BEN2	6.9	6.5	-5%	1.9	1.9	0%
C12-BEN2	6.4	6.0	-5%	1.8	1.8	0%
135-TMB	8.2	7.8	-6%	2.2	2.2	0%
123-TMB	8.2	7.8	-6%	2.2	2.2	0%
124-TMB	8.2	7.8	-6%	2.2	2.2	0%
C9-BEN3	8.2	7.8	-6%	2.2	2.2	0%
C10-BEN3	7.7	7.1	-9%	2.2	2.0	-7%
C11-BEN3	6.9	6.5	-5%	1.9	1.9	0%
C12-BEN3	6.4	6.0	-5%	1.8	1.8	0%
C10-BEN4	7.5	7.1	-5%	2.0	2.0	0%
C11-BEN4	6.9	6.5	-5%	1.9	1.9	0%
C12-BEN4	6.4	6.0	-5%	1.8	1.8	0%
C11-BEN5	6.9	6.5	-5%	1.9	1.9	0%
C12-BEN5	6.4	6.0	-5%	1.8	1.8	0%
C12-BEN6	6.4	6.0	-5%	1.8	1.8	0%
INDAN	8.3	7.9	-6%	2.2	2.2	0%
TETRALIN	7.6	7.2	-5%	2.1	2.1	0%
C11-TET	7.0	6.6	-5%	1.9	1.9	0%
NAPHTHAL	7.8	7.4	-5%	2.1	2.1	0%
ME-NAPH	7.2	6.8	-5%	2.0	2.0	0%
23-DMN	6.6	6.3	-5%	1.9	1.9	0%
STYRENE	4.6	3.9	-15%	0.51	0.63	24%
C9-STYR	10.7	5.4	-50%	2.8	1.28	-55%
C10-STYR	9.6	4.9	-48%	2.5	1.21	-52%

Table 13 (continued)

Name	-- Maximum Reactivity -- 1991	1993	chg.	---- Maximum Ozone ---- 1991	1993	chg.
ACETYLEN	0.65	0.64	-2%	0.38	0.37	-1%
ME-ACTYL	6.2	7.6	24%	2.5	2.9	17%
MEOH	0.60	0.61	3%	0.25	0.27	9%
ETOH	1.43	1.39	-3%	0.71	0.73	2%
N-C3-OH	0.84	0.83	-2%	0.49	0.49	-1%
I-C3-OH	0.84	0.83	-2%	0.49	0.49	-1%
I-C4-OH	0.91	0.90	-2%	0.53	0.53	-1%
N-C4-OH	0.91	0.90	-2%	0.53	0.53	-1%
T-C4-OH	0.91	0.67	-26%	0.53	0.39	-26%
S-C4-OH	0.91	0.90	-2%	0.53	0.53	-1%
C5OH	0.96	0.94	-2%	0.56	0.55	-1%
1-C7OH	1.02	1.00	-2%	0.59	0.59	-1%
2-ETC6OH	1.04	1.02	-2%	0.60	0.60	-1%
ET-GLYCL	0.54	0.107	-80%	0.32	0.063	-80%
PR-GLYCL	0.67	0.33	-51%	0.39	0.19	-50%
12-C4OH2	0.75	0.74	-2%	0.44	0.43	-1%
C6-GLYCL	0.86	0.84	-2%	0.50	0.49	-1%
ME-O-ME	0.73	0.72	-2%	0.43	0.42	-1%
ET-O-ET	0.91	4.3	376%	0.53	1.7	224%
MTBE	0.96	0.64	-34%	0.56	0.38	-32%
S-098106	0.96	3.8	301%	0.56	1.6	179%
ETBE	0.99	2.2	120%	0.58	0.89	53%
S-098108	1.05	3.0	187%	0.61	1.30	111%
S-098107	1.04	3.0	187%	0.60	1.28	111%
MEO-ETOH	0.67	4.0	502%	0.39	1.5	298%
ETO-ETOH	0.75	3.6	376%	0.44	1.41	224%
ETOC3OH	0.81	3.2	301%	0.47	1.32	179%
BUO-ETOH	0.86	3.0	250%	0.50	1.24	149%
BU-CELSV	0.86	3.0	250%	0.50	1.24	149%
CARBITOL	0.76	4.5	502%	0.44	1.8	298%
C8-CELSV	0.83	2.6	212%	0.48	1.14	136%
ME-ACET	0.68	0.45	-35%	0.40	0.26	-34%
ME-ACRYL	0.79	5.6	611%	0.46	2.1	359%
VIN-ACET	0.79	5.6	611%	0.46	2.1	359%
ET-ACET	0.77	0.57	-26%	0.45	0.33	-26%
ET-ACRYL	0.84	5.0	488%	0.49	1.9	287%
PR-ACET	0.83	0.65	-21%	0.48	0.38	-21%
ME-IBUAT	0.83	0.65	-21%	0.48	0.38	-21%
IPR-ACET	0.81	0.64	-21%	0.47	0.37	-21%
BU-ACET	0.87	0.71	-18%	0.51	0.42	-17%
IBU-ACET	0.87	0.71	-18%	0.51	0.42	-17%
CSV-ACET	0.77	2.6	234%	0.45	1.04	132%
IBU-IBTR	0.94	0.81	-14%	0.55	0.47	-13%
IC5IBUAT	0.96	0.84	-13%	0.56	0.49	-12%
S-098116	0.96	0.86	-10%	0.56	0.51	-9%
S-098117	0.93	0.84	-10%	0.54	0.49	-9%
ETOX	0.77	0.38	-51%	0.45	0.22	-50%
PROX	0.87	0.57	-35%	0.51	0.34	-34%
FURAN	0.99	13.6	1272%	0.58	5.0	768%
FORMALD	9.8	9.2	-6%	2.6	2.6	-1%
ACETALD	6.5	6.6	1%	2.3	2.4	5%
PROPALD	5.2	5.3	1%	1.9	2.0	4%
C4-RCHO	4.4	4.5	1%	1.7	1.8	4%
C5-RCHO	3.9	3.9	1%	1.5	1.6	3%
C6-RCHO	3.5	3.5	1%	1.42	1.46	3%
C7-RCHO	3.2	3.3	1%	1.33	1.37	3%

Table 13 (continued)

Name	-- Maximum Reactivity -- 1991	1993	chg.	---- Maximum Ozone ---- 1991	1993	chg.
C8-RCHO	3.0	3.0	0%	1.26	1.30	3%
ACROLEIN	13.6	9.3	-32%	4.8	3.4	-29%
MEGLYOX	20.			5.6		
CROTALD	10.9	10.7	-1%	3.9	4.0	3%
ACETONE	0.58	0.86	47%	0.34	0.50	49%
MEK	0.70	0.92	31%	0.41	0.54	32%
KET5	0.78	0.96	23%	0.46	0.57	24%
KET6	0.84	0.99	18%	0.49	0.58	19%
KET7	0.89	1.02	15%	0.52	0.60	16%
KET8	0.92	1.04	12%	0.54	0.61	13%
KET9	0.95	1.05	10%	0.55	0.62	11%
KET10	0.97	1.06	9%	0.57	0.62	10%
KET5C	0.80	0.99	23%	0.47	0.58	24%
KET6C	0.86	1.01	18%	0.50	0.60	19%
KET7C	0.90	1.04	15%	0.53	0.61	16%
KET8C	0.94	1.05	12%	0.55	0.62	13%
KET9C	0.96	1.07	10%	0.56	0.63	11%
KET10C	0.99	1.08	9%	0.57	0.63	10%
BENZALD	0.0	0.0		0.0	0.0	
PHENOL	3.5	0.18	-95%	0.18	0.103	-43%
CRESOL	3.1	1.6	-48%	0.16	-0.18	-216%
ET-AMINE	0.75	6.5	774%	0.44	2.5	468%
ACRYLNIT	0.96	9.1	848%	0.56	3.4	512%
TM-AMINE	0.86	8.1	848%	0.50	3.1	512%
S-099009	0.137	0.135	-2%	0.080	0.079	-1%
S-043801	0.0	0.0		0.0	0.0	
S-043802	0.0	0.0		0.0	0.0	
S-243819	0.0	0.0		0.0	0.0	
S-043803	0.0	0.0		0.0	0.0	
S-043805	0.0	0.0		0.0	0.0	
S-043812	0.0	0.0		0.0	0.0	
S-099018	0.0	0.0		0.0	0.0	
S-043813	0.0	0.0		0.0	0.0	
S-043820	0.0	0.0		0.0	0.0	
S-043814	0.0	0.0		0.0	0.0	
S-099016	0.0	0.0		0.0	0.0	
S-098104	0.0	0.72		0.0	0.42	
S-098105	0.0	0.89		0.0	0.52	
S-043860	0.0	3.6		0.0	1.45	
S-099013	0.0	0.0		0.0	0.0	
S-043815	0.0	0.0		0.0	0.0	
S-043824	0.0	0.0		0.0	0.0	
S-043817	0.0	0.0		0.0	0.0	
S-099014	0.0	0.0		0.0	0.0	
CL-BEN	0.15	0.147	-2%	0.087	0.087	-1%
CL2-BEN	0.115	0.113	-2%	0.067	0.066	-1%
INERT	0.0	0.0		0.0	0.0	

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APPENDIX A.
DETAILED INPUT DATA AND OZIPM4 INPUT FILES FOR THE INDIVIDUAL SCENARIOS

Table A-1 gives the detailed input data for the "Averaged Conditions" scenario. Table A-2 gives the detailed input data and OZIPM4 input files for the individual base case scenarios.

Table A-1. 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) Base:	2.34	Initial NOx (% of input)	45.67
MIR:	3.86		
MOR:	2.79		
EBIR:	2.23		

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

Table B-1 (continued)

Table A-2. 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 A-2 (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 A-2 (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.      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 A-2 (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 A-2 (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.      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 A-2 (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 A-2 (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 A-2 (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 A-2 (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.      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 A-2 (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.      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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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.      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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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.      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 A-2 (continued)

Scenario ID	**POROR1**	**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 A-2 (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.       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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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 A-2 (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

```
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 A-2 (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 A-2 (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
```