PB87-180600

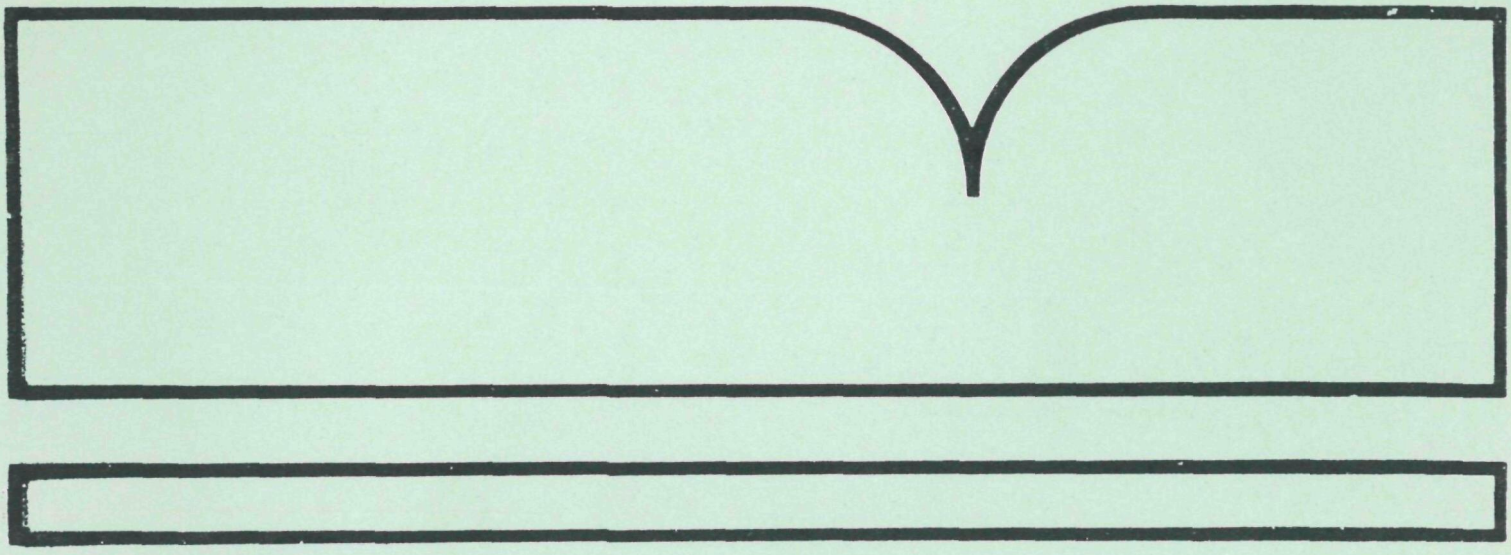
Surrogate Species Chemical Reaction Mechanism for Urban-Scale Air Quality Simulation Models. Volume 2 Guidelines for Using the Mechanism

Environmental Research and Technology, Inc.
Newbury Park, CA

Prepared for

Environmental Protection Agency
Research Triangle Park, NC

Apr 87



PB87-180600

EPA/600/3-87/014b
April 1987

A SURROGATE SPECIES CHEMICAL REACTION MECHANISM FOR URBAN-SCALE AIR QUALITY SIMULATION MODELS

VOLUME II - GUIDELINES FOR USING THE MECHANISM

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EPA Contract No. 68-02-4104

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The information in this document has been funded by the United States Environmental Protection Agency under Contract Number 68-02-4104 to ERT, Inc. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

ABSTRACT

A surrogate species chemical reaction mechanism for the photooxidation of nonmethane organic compounds (NMOC) and nitrogen oxides (NO_x) has been developed for use in urban-scale photochemical air quality simulation (AQS) models. The chemical mechanism has been evaluated against data from 491 environmental chamber experiments conducted in indoor and outdoor facilities. The results of the mechanism evaluation indicate good model performance for a large number of single organic-NO_x and multi-organic NO_x experiments.

Two versions of the chemical mechanism have been adapted for use in photochemical AQS models. One version of the mechanism incorporates detailed representation of the reactions of NMOC and is suitable for use in single-cell AQS models such as the OZIPM/EKMA model. Another version of the mechanism incorporates a more condensed representation of the reactions of NMOC and is suitable for use in multi-cell Lagrangian and Eulerian AQS models. Under typical urban conditions, the two versions of the mechanism give very similar predictions for the concentrations of the key species involved in photochemical smog.

The approach used to model the complex mixture of NMOC with this mechanism is to use the chemical reactions of 12 common organic precursors as surrogates for actual reactions of hundreds of different compounds. A system of assigning individual organic compounds to the most appropriate surrogate species have been developed. Also, speciated ambient NMOC data from surface stations in 25 urban areas and from aircraft samples collected upwind of four urban areas have been analyzed to develop default NMOC speciation profiles for use with this mechanism.

Sensitivity analysis using surrogate species mechanism in the OZIPM/EKMA model is reported. This analysis investigates the relationships between model input parameters and the NMOC control requirement predictions. The input parameters included in the analysis are NMOC composition, NMOC/NO_x ratio, NMOC and ozone concentrations aloft, dilution rates, post-8 a.m. emission rates, future NO_x emission rates, present-day ozone concentrations, photolysis rates, and initial concentrations of peroxyacetylnitrate and nitrous acid.

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1. INTRODUCTION

This is the fourth volume in a series on a new atmospheric chemical mechanism for use in photochemical air quality simulation (AQS) models. The chemical mechanism is designed to predict the formation of ozone and other oxidants from emissions of nonmethane organic compounds (NMOC) and nitrogen oxides (NO_x) in urban areas. It is designed for use in models such as the OZIPM model (Hogo and Whitten 1986) and the Urban Airshed Model (Reynolds et al. 1973). These models are used to develop ozone control strategies for urban areas where ozone concentrations exceed the National Ambient Air Quality Standard.

The new mechanism was developed by updating and extending the Atkinson et al. (1982) and Lurmann et al. (1984, 1986) mechanisms based on the recommendations of Atkinson and Lloyd (1984) and NASA (1985). The mechanism employs the surrogate species approach to represent the reactions of NMOC in ambient air. The mechanism was extensively tested and refined using over 490 environmental chamber experiments from the University of North Carolina (UNC) and the University of California, Riverside (UCR) facilities. Two versions of the mechanism have been adapted for use in atmospheric simulation models. One version, referred to as the OZIPM mechanism, is designed for use in single cell AQS models, that can accommodate fairly large and detailed chemical mechanisms. The second version, referred to as the condensed mechanism, is designed for use in multi-cell AQS models that include more sophisticated treatment of transport processes and require smaller chemical mechanisms.

The technical basis for the new mechanism is fully documented in companion reports. The mechanism development, evaluation protocol, and preliminary evaluation results are described in Volumes I and II of a report entitled "Development and Testing of a Surrogate Species Chemical Reaction Mechanism" (Carter et al. 1986). The final mechanism evaluation results and the adaptation of the mechanism to atmospheric models are described in Volume I of this report.

The purpose of this report is to provide guidelines for using the new chemical mechanism in air quality models. Included in this report are

- instructions for implementing the mechanism in AQS models,

- sample problems that allow users to confirm that they have properly implemented the chemical mechanism, and

- instructions for speciating the NMOC into the organic compound classes used by the model.

The guidelines for implementation and NMOC speciation are provided in Sections 2 and 3 of the report, respectively. Computer-readable listings (files) of the mechanism are available from LRT, Inc. for a nominal cost. These files include sample problem input data for the OZIPM computer program.

2. IMPLEMENTATION OF THE MECHANISM

The chemical mechanisms developed in this research program can be implemented in almost all photochemical AQS models. The AQS models have different input data formats, numerical integration procedures, and capabilities for treating photolytic reaction rates. Some models are able to accommodate special rate constant and product coefficient expressions, whereas other models only accept rate data in standard format with constant product coefficients. Furthermore, most single cell models have the capability to read all of the mechanism data from an input file, whereas, most sophisticated multi-cell models require the chemistry to be implemented in "hard-wired" chemistry subroutines. Because of these difference, it is beyond the scope of this report to describe all the details of implementing the mechanism in different models. However, the general features that need to be considered in all implementations are described and sample input files for EPA's OZIPM model (Version 3) are provided.

The two versions of the new chemical mechanism are shown in Tables 2-1 through 2-4. Tables 2-1 and 2-3 list the chemical species that are included in the OZIPM and condensed mechanisms, respectively. Tables 2-2 and 2-4 show the reactions, the nonphotolytic rate constants at 298°K, and activation energies for the OZIPM and condensed mechanisms, respectively. These rate constants are appropriate for the lower troposphere where the atmospheric pressure is in the 700 to 1000 mb range. The first order rate constants are given in $minute^{-1}$ and $second^{-1}$ units. The second order rate constants are given in ppm^{-1} min^{-1} and cm^3 $molecules^{-1}$ sec^{-1} units. The third order rate constants are given in ppm^{-2} min^{-1} and cm^6 $molecules^{-2}$ sec^{-1} units. The organic classes and surrogate species used in the mechanism are shown in Tables 2-5 and 2-6.

2.1 Photolytic Reactions

The rates for the photolytic reactions depend on solar radiation intensity and its spectral distribution. Atmospheric radiation levels depend on the solar zenith angle, cloud cover, pollutant loadings, surface albedo, and elevation above the Earth's surface. The solar

TABLE 2-1

SAPRC/ERT OZIPM CHEMICAL MECHANISM SPECIES LIST

SPECIES	ABREVIATION
1. NITRIC OXIDE	NO
2. NITROGEN DIOXIDE	NO2
3. OZONE	O3
4. NITROUS ACID	HONO
5. NITRIC ACID	HNO3
6. PERNITRIC ACID	HNO4
7. NITROGEN PENTOXIDE	N2O5
8. NITROGEN TRIOXIDE	NO3
9. HYDROPEROXY RADICAL	HO2
10. HYDROGEN PEROXIDE	H2O2
11. CARBON MONOXIDE	CO
12. FORMALDEHYDE	HCHO
13. ACETALDEHYDE	ALD2
14. PROPIONALDEHYDE	RCHO
15. PEROXYACETYLNITRATE	PAN
16. PEROXYPROPIONYL NITRATE	PPN
17. TOTAL RO2 RADICALS	RO2
18. TOTAL RCO3 RADICALS	RCO3
19. ORGANIC PEROXIDE	ROOH
20. ACETONE	ACET
21. METHYL ETHYL KETONE	MEK
22. GLYOXAL	GLYX
23. GLYOXAL PAN	GPAN
24. METHYL GLYOXAL	MGLY
25. C4-C5 ALKANES	ALK4
26. >C5 ALKANES	ALK7
27. ALKYL NITRATE	ALKN
28. ETHENE	ETHE
29. PROPENE	PRPE
30. TRANS-2-BUTENE	TBUT
31. TOLUENE	TOLU
32. M-XYLENE	XYLE
33. 1,3,5 TRI-M-BENZENE	TMBZ
34. DICARBONYLS	DIAL
35. O-CRESOL	CRES
36. PHENOLS	PHEN
37. NITROPHENOL	NPHE
STEADY-STATE SPECIES	
38. OXYGEN - SINGLET D	O*SD
39. OXYGEN - ATOMIC	O
40. HYDROXYL RADICAL	OH

TABLE 2-1 (Continued)

SPECIES	ABREVIATION
41. ACETALDEHYDE RCO3	MCO3
42. PROPIONALDEHYDE RCO3	PCO3
43. GLYOXAL RCO3	GCO3
44. GENERAL RO2 #1	RO2R
45. GENERAL RO2 #2	R2O2
46. ALKYL NITRATE RO2	RO2N
47. PHENOL RO2	RO2P
48. BENZALDEHYDE N-RO2	BZN2
49. PHENOXY RADICAL	BZO
CONSTANT SPECIES	
50. WATER VAPOR	H2O

TABLE 2-2

SAPRC/ERT OZIPM CHEMICAL MECHANISM

	REACTION	MOLECULE-CC-SEC (298 K)	PPM-MIN (298 K)	EXPRESSION
1.	NO2 + HV ---> NO + O	RADIATION DEPENDENT		
2.	O ---> O3	8.12E+05	4.87E+07	1.10E+04*EXP(1282/T)
3.	O + NO2 ---> NO	9.30E-12	1.37E+04	
4.	O + NO2 ---> NO3	2.23E-12	3.29E+03	1.11E-13*EXP(894/T)
5.	NO + O3 ---> NO2	1.81E-14	2.68E+01	1.80E-12*EXP(-1370/T)
6.	NO2 + O3 ---> NO3	3.23E-17	4.77E-02	1.20E-13*EXP(-2450/T)
7.	NO + NO3 ---> 2.NO2	1.86E-11	2.75E+04	8.00E-12*EXP(252/T)
8.	NO + NO ---> 2.NO2	1.02E-19	1.50E-04	1.72E-20*EXP(529/T)
9.	NO2 + NO3 ---> N2O5	1.15E-12	1.71E+03	4.62E-13*EXP(273/T)
10.	N2O5 ---> NO2 + NO3	3.47E-02	2.08E+00	1.33E+15*EXP(-11379/T)
11.	N2O5 + H2O ---> 2.HNO3	1.00E-21	1.48E-06	
12.	NO2 + NO3 ---> NO + NO2	4.04E-16	5.98E-01	2.50E-14*EXP(-1229/T)
13.	NO3 + HV ---> NO	RADIATION DEPENDENT		
14.	NO3 + HV ---> NO2 + O	RADIATION DEPENDENT		
15.	O3 + HV ---> O	RADIATION DEPENDENT		
16.	O3 + HV ---> O*SD	RADIATION DEPENDENT		
17.	O*SD + H2O ---> 2.OH	2.20E-10	3.25E+05	
18.	O*SD ---> O	7.20E+08	4.32E+10	
19.	NO + OH ---> HONO	6.60E-12	9.75E+03	4.03E-13*EXP(833/T)
20.	HONO + HV ---> NO + OH	RADIATION DEPENDENT		
21.	NO2 + H2O ---> HONO - NO2 + HNO3	4.00E-24	5.91E-09	
22.	NO2 + OH ---> HNO3	1.13E-11	1.68E+04	9.57E-13*EXP(737/T)
23.	HNO3 + OH ---> NO3	1.28E-13	1.89E+02	9.40E-15*EXP(778/T)
24.	CO + OH ---> HO2	2.18E-13	3.22E+02	
25.	O3 + OH ---> HO2	6.78E-14	1.00E+02	1.69E-12*EXP(-942/T)
26.	NO + HO2 ---> NO2 + OH	8.28E-12	1.22E+04	3.70E-12*EXP(240/T)
27.	NO2 + HO2 ---> HNO4	1.37E-12	2.02E+03	1.02E-13*EXP(773/T)
28.	HNO4 ---> NO2 + HO2	8.22E-02	4.93E+00	4.35E+13*EXP(-10103/T)
29.	HNO4 + OH ---> NO2	4.00E-12	5.91E+03	
30.	O3 + HO2 ---> OH	2.01E-15	2.96E+00	1.40E-14*EXP(-579/T)
31.	HO2 + HO2 ---> H2O2	3.02E-12	4.46E+03	2.27E-13*EXP(771/T)
32.	HO2 + HO2 + H2O ---> H2O2	6.97E-30	2.54E-01	3.26E-34*EXP(2971/T)
33.	NO3 + HO2 ---> HNO3	3.02E-12	4.46E+03	2.27E-13*EXP(771/T)
34.	NO3 + HO2 + H2O ---> HNO3	6.97E-30	2.54E-01	3.26E-34*EXP(2971/T)
35.	H2O2 + HV ---> 2.OH	RADIATION DEPENDENT		
36.	H2O2 + OH ---> HO2	1.66E-12	2.45E+03	3.10E-12*EXP(-187/T)
37.	RO2 + NO ---> NO	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
38.	RCO3 + NO ---> NO	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)

TABLE 2-2 (Continued)

	REACTION		MOLECULE-CC-SEC (298 K)	PPM-MIN (298 K)	EXPRESSION
39.	RCO3 + NO2 ---> NO2		5.12E-12	7.57E+03	2.80E-12*EXP(180/T)
40.	RO2 + HO2 ---> HO2		3.00E-12	4.43E+03	
41.	RCO3 + HO2 ---> HO2		3.00E-12	4.43E+03	
42.	ROOH + HV ---> HO2 + OH		RADIATION DEPENDENT		
43.	RO2 + RO2 --->		1.00E-15	1.48E+00	
44.	RO2 + RCO3 --->		3.00E-12	4.43E+03	
45.	RCO3 + RCO3 --->		2.50E-12	3.69E+03	
46.	HCHO + HV ---> 2.HO2 + CO		RADIATION DEPENDENT		
47.	HCHO + HV ---> CO		RADIATION DEPENDENT		
48.	HCHO + OH ---> HO2 + CO		9.00E-12	1.33E+04	
49.	HCHO + NO3 ---> HNO3 + HO2 + CO		5.97E-16	8.82E-01	6.00E-13*EXP(-2060/T)
50.	HCHO + HO2 ---> RO2R + RO2		1.00E-14	1.48E+01	
51.	ALD2 + OH ---> MCO3 + RCO3		1.60E-11	2.36E+04	6.90E-12*EXP(250/T)
52.	ALD2 + HV ---> CO + HCHO + HO2 + RO2R + RO2		RADIATION DEPENDENT		
53.	ALD2 + NO3 ---> HNO3 + MCO3 + RCO3		2.50E-15	3.69E+00	3.00E-13*EXP(-1427/T)
54.	MCO3 + NO ---> NO2 + HCHO + RO2R + RO2		7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
55.	MCO3 + NO2 ---> PAN		5.12E-12	7.57E+03	2.80E-12*EXP(180/T)
56.	MCO3 + HO2 ---> ROOH + HCHO		3.00E-12	4.43E+03	
57.	MCO3 + RO2 ---> .5HO2 + HCHO + RO2		3.00E-12	4.43E+03	
58.	MCO3 + RCO3 ---> HO2 + HCHO + RCO3		2.50E-12	3.69E+03	
59.	PAN ---> MCO3 + NO2 + RCO3		3.68E-04	2.21E-02	2.00E+16*EXP(-13542/T)
60.	RCHO + OH ---> RCO3 + PCO3		1.98E-11	2.93E+04	8.50E-12*EXP(252/T)
61.	RCHO + HV ---> ALD2 + HO2 + CO + RO2R + RO2		RADIATION DEPENDENT		
62.	RCHO + NO3 ---> HNO3 + PCO3 + RCO3		2.46E-15	3.63E+00	3.00E-13*EXP(-1432/T)
63.	PCO3 + NO ---> NO2 + ALD2 + RO2R + RO2		7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
64.	PCO3 + NO2 ---> PPN		5.12E-12	7.57E+03	2.80E-12*EXP(180/T)
65.	PCO3 + HO2 ---> ROOH + ALD2		3.00E-12	4.43E+03	
66.	PCO3 + RO2 ---> .5HO2 + ALD2 + RO2		3.00E-12	4.43E+03	
67.	PCO3 + RCO3 ---> HO2 + ALD2 + RCO3		2.50E-12	3.69E+03	
68.	PPN ---> PCO3 + NO2 + RCO3		3.68E-04	2.21E-02	2.00E+16*EXP(-13542/T)
69.	ACET + HV ---> MCO3 + HCHO + RCO3 + RO2R + RO2		RADIATION DEPENDENT		
70.	ACET + OH ---> MGLY + RO2R + RO2		2.29E-13	3.39E+02	1.00E-11*EXP(-1125/T)
71.	MEK + HV ---> MCO3 + ALD2 + RCO3 + RO2R + RO2		RADIATION DEPENDENT		
72.	MEK + OH ---> 1.5R2O2 + 1.5RO2 + .5MCO3 + .5ALD2 + .5HCHO + .5PCO3 + RCO3		9.85E-13	1.46E+03	1.20E-11*EXP(-745/T)
73.	GLYX + HV ---> .13HCHO +1.87CO		RADIATION DEPENDENT		
74.	GLYX + OH ---> .63HO2 +1.26CO + .37GCO3 + .37RCO3		1.15E-11	1.70E+04	

TABLE 2-2 (Continued)

SAPRC/ERT OZIPM CHEMICAL MECHANISM

	REACTION	MOLECULE-CC-SEC (298 K)	PPM-MIN (298 K)	EXPRESSION
75.	GLYX + NO3 ---> HNO3 + .63HO2 +1.26CO + .37GCO3 + .37RCO3	6.01E-16	8.88E-01	6.00E-13*EXP(-2058/T)
76.	GCO3 + NO2 ---> GPAN	5.12E-12	7.57E+03	2.80E-12*EXP(180/T)
77.	GCO3 + NO ---> NO2 + HO2 + CO	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
78.	GPAN ---> NO2 + GCO3 + RCO3	3.68E-04	2.21E-02	2.00E+16*EXP(-13542/T)
		3.68E-04	2.21E-02	2.00E+16*EXP(-13542/T)
79.	GCO3 + HO2 ---> ROOH + CO	3.00E-12	4.43E+03	
80.	GCO3 + RO2 ---> .5HO2 + CO + RO2	3.00E-12	4.43E+03	
81.	GCO3 + RCO3 ---> HO2 + CO + RCO3	2.50E-12	3.69E+03	
82.	MGLY + HV ---> MCO3 + HO2 + CO + RCO3	RADIATION	DEPENDENT	
83.	MGLY + OH ---> MCO3 + CO + RCO3	1.70E-11	2.51E+04	
84.	MGLY + NO3 ---> HNO3 + MCO3 + CO + RCO3	2.50E-15	3.69E+00	3.00E-13*EXP(-1427/T)
85.	ALK4 + OH ---> B01*HCHO +B02*ALD2 +B03*RCHO +B04*ACET +B05*MEK +B06*RO2N +B07*RO2R +B08*R2O2 +B09*RO2	3.22E-12	4.76E+03	1.05E-11*EXP(-353/T)
		SEE TEXT		
86.	ALK7 + OH ---> B10*HCHO +B11*ALD2 +B12*RCHO +B13*ACET +B14*MEK +B15*RO2N +B16*RO2R +B17*R2O2 +B18*RO2	6.16E-12	9.11E+03	1.62E-11*EXP(-288/T)
		SEE TEXT		
87.	ALKN + OH ---> NO2 + .15MEK +1.05RCHO + .48ALD2 + .16HCHO +1.39R2O2 +1.39RO2	2.03E-12	3.00E+03	2.19E-11*EXP(-709/T)
88.	RO2N + NO ---> ALKN	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
89.	RO2N + HO2 ---> ROOH + MEK	3.00E-12	4.43E+03	
90.	RO2N + RO2 ---> RO2 + .5HO2 + MEK	1.00E-15	1.48E+00	
91.	RO2N + RCO3 ---> RCO3 + .5HO2 + MEK	3.00E-12	4.43E+03	
92.	R2O2 + NO ---> NO2	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
93.	R2O2 + HO2 ---> ROOH	3.00E-12	4.43E+03	
94.	R2O2 + RO2 ---> RO2	1.00E-15	1.48E+00	
95.	R2O2 + RCO3 ---> RCO3	3.00E-12	4.43E+03	
96.	RO2R + NO ---> NO2 + HO2	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
97.	RO2R + HO2 ---> ROOH	3.00E-12	4.43E+03	
98.	RO2R + RO2 ---> .5HO2 + RO2	1.00E-15	1.48E+00	
99.	RO2R + RCO3 ---> .5HO2 + RCO3	3.00E-12	4.43E+03	
100.	ETHE + OH ---> RO2R + RO2 +1.56HCHO + .22ALD2	8.54E-12	1.26E+04	2.15E-12*EXP(411/T)
101.	ETHE + O3 ---> HCHO + .12HO2 + .42CO	1.74E-18	2.57E-03	1.20E-14*EXP(-2634/T)
102.	ETHE + O ---> HCHO + HO2 + CO + RO2R + RO2	7.29E-13	1.08E+03	1.04E-11*EXP(-792/T)
103.	ETHE + NO3 ---> NO2 + 2.HCHO + R2O2 + RO2	1.10E-16	1.62E-01	2.00E-12*EXP(-2923/T)
104.	PRPE + OH ---> RO2R + HCHO + ALD2 + RO2	2.63E-11	3.89E+04	4.85E-12*EXP(504/T)
105.	PRPE + O3 ---> .65HCHO + .5ALD2 +.285CO + .060H +.165HO2 +.135RO2R +.135RO2	1.13E-17	1.67E-02	1.32E-14*EXP(-2105/T)

TABLE 2-2 (Continued)

	REACTION	MOLECULE-CC-SEC (298 K)	PPM-MIN (298 K)	EXPRESSION
106.	PRPE + O ---> .6ACET + .4HCHO + .2ALD2 + .2HO2 + .6RO2R + .4CO + .6RO2	3.98E-12	5.88E+03	1.18E-11*EXP(-324/T)
107.	PRPE + NO3 ---> NO2 + HCHO + ALD2 + R2O2 + RO2	7.57E-15	1.12E+01	5.00E-12*EXP(-1935/T)
108.	TBUT + OH ---> RO2R + 2.ALD2 + RO2	6.37E-11	9.42E+04	1.01E-11*EXP(549/T)
109.	TBUT + O3 ---> ALD2 + .15CO + .27RO2R + .12OH + .21HO2 + .27RO2 + .30HCHO	2.00E-16	2.96E-01	9.08E-15*EXP(-1137/T)
110.	TBUT + O ---> MEK + .4HO2	2.34E-11	3.45E+04	2.26E-11*EXP(10/T)
111.	TBUT + NO3 ---> NO2 + 2.ALD2 + R2O2 + RO2	3.79E-13	5.61E+02	1.00E-11*EXP(-975/T)
112.	TOLU + OH ---> .16CRES + .16HO2 + .84RO2R + .4DIAL + .84RO2 +.144MGLY +.114GLYX	6.19E-12	9.14E+03	2.10E-12*EXP(322/T)
113.	XYLE + OH ---> .17CRES + .17HO2 + .83RO2R + .83RO2 + .65DIAL +.316MGLY +.095GLYX	2.45E-11	3.62E+04	1.66E-11*EXP(116/T)
114.	TMBZ + OH ---> .17CRES + .17HO2 + .83RO2R + .83RO2 + .49DIAL + .86MGLY	6.20E-11	9.16E+04	
115.	DIAL + OH ---> PCO3 + RCO3	3.00E-11	4.43E+04	
116.	DIAL + HV ---> HO2 + CO + MCO3 + RCO3	RADIATION	DEPENDENT	
117.	CRES + OH ---> .2MGLY + .15RO2P + .85RO2R + RO2	4.00E-11	5.91E+04	
118.	CRES + NO3 ---> HNO3 + BZO	2.20E-11	3.25E+04	
119.	RO2P + NO ---> NPHE	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
120.	RO2P + HO2 ---> ROOH	3.00E-12	4.43E+03	
121.	RO2P + RO2 ---> .5HO2 + RO2	1.00E-15	1.48E+00	
122.	RO2P + RCO3 ---> .5HO2 + RCO3	3.00E-12	4.43E+03	
123.	BZO + NO2 ---> NPHE	1.50E-11	2.22E+04	
124.	BZO + HO2 ---> PHEN	3.00E-12	4.43E+03	
125.	BZO ---> PHEN	1.00E-03	6.00E-02	
126.	PHEN + OH ---> .2GLYX + .15RO2P + .85RO2R + RO2	2.80E-11	4.14E+04	
127.	PHEN + NO3 ---> HNO3 + BZO	3.80E-12	5.62E+03	
128.	NPHE + NO3 ---> HNO3 + BZN2	3.80E-12	5.62E+03	
129.	BZN2 + NO2 --->	1.50E-11	2.22E+04	
130.	BZN2 + HO2 ---> NPHE	3.00E-12	4.43E+03	
131.	BZN2 ---> NPHE	1.00E-03	6.00E-02	

TABLE 2-3

SAPRC/ERT CONDENSED CHEMICAL MECHANISM SPECIES LIST

	SPECIES	ABREVIATION
1.	NITRIC OXIDE	NO
2.	NITROGEN DIOXIDE	NO2
3.	OZONE	O3
4.	NITROUS ACID	HONO
5.	NITRIC ACID	HNO3
6.	PERNITRIC ACID	HNO4
7.	NITROGEN PENTOXIDE	N2O5
8.	NITROGEN TRIOXIDE	NO3
9.	HYDROPEROXY RADICAL	HO2
10.	CARBON MONOXIDE	CO
11.	FORMALDEHYDE	HCHO
12.	ACETALDEHYDE	ALD2
13.	METHYL ETHYL KETONE	MEK
14.	METHYL GLYOXAL	MGLY
15.	PEROXYACETYLNITRATE	PAN
16.	TOTAL RO2 RADICALS	RO2
17.	CH3CO3 RADICAL	MCO3
18.	ALKYL NITRATE	ALKN
19.	<C3 ALKANES	ALKA
20.	ETHENE	ETHE
21.	<C2 ALKENES	ALKE
22.	TOLUENE	TOLU
23.	HIGHER AROMATICS	AROM
24.	UNKNOWN DICARBONYLS	DIAL
25.	O-CRESOL	CRES
26.	NITROPHENOLS	NPHE
	STEADY STATE SPECIES	
27.	OXYGEN - SINGLET D	O*SD
28.	ATOMIC OXYGEN	O
29.	HYDROXAL RADICAL	OH
30.	GENERAL RO2 #1	RO2R
31.	GENERAL RO2 #2	R2O2
32.	ALKYL NITRATE RO2	RO2N
33.	PHENOL RO2	RO2P
34.	BENZALDEHYDE N-RO2	BZN2
35.	PHENOXY RADICAL	BZO
	CONSTANT SPECIES	
36.	WATER VAPOR	H2O

TABLE 2-4

SAPRC/ERT CONDENSED CHEMICAL MECHANISM

	REACTION									MOLECULE-CC-SEC (298 K)	PPM-MIN (298 K)	EXPRESSION
1.	NO2	+ HV		--->	NO	+	O			RADIATION DEPENDENT		
2.	O			--->	O3					7.75E+05	4.65E+07	1.05E+04*EXP(1282/T)
3.	O	+ NO2		--->	NO					9.30E-12	1.37E+04	
4.	O	+ NO2		--->	NO3					2.23E-12	3.29E+03	1.11E-13*EXP(894/T)
5.	NO	+ O3		--->	NO2					1.81E-14	2.68E+01	1.80E-12*EXP(-1370/T)
6.	NO2	+ O3		--->	NO3					3.23E-17	4.77E-02	1.20E-13*EXP(-2450/T)
7.	NO	+ NO3		--->	2.NO2					1.86E-11	2.75E+04	8.00E-12*EXP(252/T)
8.	NO	+ NO		--->	2.NO2					9.68E-20	1.43E-04	1.64E-20*EXP(529/T)
9.	NO2	+ NO3		--->	N2O5					1.15E-12	1.71E+03	4.62E-13*EXP(273/T)
10.	N2O5			--->	NO2	+	NO3			3.47E-02	2.08E+00	1.33E+15*EXP(-11379/T)
11.	N2O5	+ H2O		--->	2.HNO3					1.00E-21	1.48E-06	
12.	NO2	+ NO3		--->	NO	+	NO2			4.04E-16	5.98E-01	2.50E-14*EXP(-1229/T)
13.	NO3	+ HV		--->	NO					RADIATION DEPENDENT		
14.	NO3	+ HV		--->	NO2	+	O			RADIATION DEPENDENT		
15.	O3	+ HV		--->	O					RADIATION DEPENDENT		
16.	O3	+ HV		--->	O*SD					RADIATION DEPENDENT		
17.	O*SD	+ H2O		--->	2.OH					2.20E-10	3.25E+05	
18.	O*SD			--->	O					7.20E+08	4.32E+10	
19.	NO	+ OH		--->	HONO					6.60E-12	9.75E+03	4.03E-13*EXP(833/T)
20.	HONO	+ HV		--->	NO	+	OH			RADIATION DEPENDENT		
21.	NO2	+ H2O		--->	HONO	-	NO2	+	HNO3	4.00E-24	5.91E-09	
22.	NO2	+ OH		--->	HNO3					1.14E-11	1.68E+04	9.58E-13*EXP(737/T)
23.	HNO3	+ OH		--->	NO3					1.28E-13	1.89E+02	9.40E-15*EXP(778/T)
24.	CO	+ OH		--->	HO2					2.18E-13	3.22E+02	
25.	O3	+ OH		--->	HO2					6.78E-14	1.00E+02	1.60E-12*EXP(-942/T)
26.	NO	+ HO2		--->	NO2	+	OH			8.28E-12	1.22E+04	3.70E-12*EXP(240/T)
27.	NO2	+ HO2		--->	HNO4					1.37E-12	2.02E+03	1.02E-13*EXP(773/T)
28.	HNO4			--->	NO2	+	HO2			8.22E-02	4.93E+00	4.35E+13*EXP(-10103/T)
29.	HNO4	+ OH		--->	NO2					4.00E-12	5.91E+03	
30.	O3	+ HO2		--->	OH					2.01E-15	2.96E+00	1.40E-14*EXP(-579/T)
31.	HO2	+ HO2		--->						3.02E-12	4.46E+03	2.27E-13*EXP(771/T)
32.	HO2	+ HO2	+ H2O	--->						6.97E-30	2.54E-01	3.26E-34*EXP(2971/T)
33.	NO3	+ HO2		--->	HNO3					3.02E-12	4.46E+03	2.27E-13*EXP(771/T)
34.	NO3	+ HO2	+ H2O	--->	HNO3					6.97E-30	2.54E-01	3.26E-34*EXP(2971/T)
35.	RO2	+ NO		--->	NO					7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
36.	RO2	+ HO2		--->	HO2					3.00E-12	4.43E+03	
37.	RO2	+ RO2		--->						1.00E-15	1.48E+00	

TABLE 2-4 (Continued)

	REACTION	MOLECULE-CC-SEC (298 K)	PPM-MIN (298 K)	EXPRESSION
38.	RO2 + MCO3 ---> MCO3	3.00E-12	4.43E+03	
39.	HCHO + HV ---> 2.HO2 + CO	RADIATION DEPENDENT		
40.	HCHO + HV ---> CO	RADIATION DEPENDENT		
41.	HCHO + OH ---> HO2 + CO	9.00E-12	1.33E+04	
42.	HCHO + NO3 ---> HNO3 + HO2 + CO	5.97E-16	8.82E-01	6.00E-13*EXP(-2060/T)
43.	HCHO + HO2 ---> RO2R + RO2	1.00E-14	1.48E+01	
44.	ALD2 + OH ---> MCO3	1.60E-11	2.36E+04	6.90E-12*EXP(250/T)
45.	ALD2 + HV ---> CO + HCHO + HO2 + RO2R + RO2	RADIATION DEPENDENT		
46.	ALD2 + NO3 ---> HNO3 + MCO3	2.50E-15	3.69E+00	3.00E-13*EXP(-1427/T)
47.	MCO3 + NO ---> NO2 + HCHO + RO2R + RO2	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
48.	MCO3 + NO2 ---> PAN	5.12E-12	7.57E+03	2.80E-12*EXP(180/T)
49.	MCO3 + HO2 ---> HCHO	3.00E-12	4.43E+03	
50.	MCO3 + MCO3 ---> 2.HO2 + 2.HCHO	2.50E-12	3.69E+03	
51.	PAN ---> MCO3 + NO2	3.68E-04	2.21E-02	2.00E+16*EXP(-13542/T)
52.	MEK + HV ---> ALD2 + MCO3 + RO2R + RO2	RADIATION DEPENDENT		
53.	MEK + OH ---> 1.5RO2R + 1.5RO2 + MCO3 + .5ALD2 + .5HCHO	9.85E-13	1.46E+03	1.20E-11*EXP(-745/T)
54.	MGLY + HV ---> MCO3 + HO2 + CO	RADIATION DEPENDENT		
55.	MGLY + OH ---> MCO3 + CO	1.70E-11	2.51E+04	
56.	MGLY + NO3 ---> HNO3 + MCO3 + CO	2.50E-15	3.69E+00	3.00E-13*EXP(-1427/T)
57.	ALKA + OH ---> B01*HCHO +B02*ALD2 +B03*MEK +B04*RO2N +B05*RO2R +B06*R2O2 +B07*RO2	SEE TEXT		
58.	ALKN + OH ---> NO2 + .15MEK +1.53ALD2 + .16HCHO +1.39R2O2 +1.39RO2	2.03E-12	3.00E+03	2.19E-11*EXP(-709/T)
59.	RO2N + NO ---> ALKN	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
60.	RO2N + HO2 ---> MEK	3.00E-12	4.43E+03	
61.	RO2N + RO2 ---> RO2 + .5HO2 + MEK	1.00E-15	1.48E+00	
62.	RO2N + MCO3 ---> HCHO + HO2 + MEK	3.00E-12	4.43E+03	
63.	R2O2 + NO ---> NO2	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
64.	R2O2 + HO2 --->	3.00E-12	4.43E+03	
65.	R2O2 + RO2 ---> RO2	1.00E-15	1.48E+00	
66.	R2O2 MCO3 ---> HCHO + HO2	3.00E-12	4.43E+03	
67.	RO2R + NO ---> NO2 + HO2	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
68.	RO2R + HO2 --->	3.00E-12	4.43E+03	
69.	RO2R + RO2 ---> .5HO2 + RO2	1.00E-15	1.48E+00	
70.	RO2R + MCO3 ---> HCHO + HO2	3.00E-12	4.43E+03	
71.	ETHE + OH ---> RO2R + RO2 +1.56HCHO + .22ALD2	8.54E-12	1.26E+04	2.15E-12*EXP(411/T)
72.	ETHE + O3 ---> HCHO + .12HO2 + .42CO	1.74E-18	2.57E-03	1.20E-14*EXP(-2634/T)

TABLE 2-4 (Continued)

	REACTION	MOLECULE-CC-SEC (298 K)	PPM-MIN (298 K)	EXPRESSION
73.	ETHE + O ---> HCHO + HO2 + CO + R02R + RO2	7.29E-13	1.08E+03	1.04E-11*EXP(-792/T)
74.	ETHE + NO3 ---> NO2 + 2.HCHO + R2O2 + RO2	1.09E-16	1.61E-01	2.00E-12*EXP(-2925/T)
75.	ALKE + OH ---> B08*HCHO + B09*ALD2 + R02R + RO2	SEE TEXT		
76.	ALKE + O3 ---> B10*HCHO + B11*ALD2 + B12*R02R + B12*RO2 + B13*HO2 + B14*OH + B15*CO	SEE TEXT		
77.	ALKE + O ---> B16*CO + B17*MEK + B18*HCHO + B19*ALD2 + B20*HO2 + B21*R02R + B21*RO2	SEE TEXT		
78.	ALKE + NO3 ---> NO2 + B08*HCHO + B09*ALD2 + R2O2 + RO2	SEE TEXT		
79.	TOLJ + OH ---> .16CRES + .16HO2 + .84R02R + .4DIAL + .84RO2 + .144MGLY + .114HCHO + .114CO	6.19E-12	9.14E+03	2.10E-12*EXP(322/T)
80.	AROM + OH ---> .17CRES + .17HO2 + .83R02R + .83RO2 + B22*DIAL + B23*MGLY + B24*HCHO + B24*CO	SEE TEXT		
81.	DIAL + OH ---> MCO3	3.00E-11	4.43E+04	
82.	DIAL + HV ---> HO2 + CO + MCO3	RADIATION DEPENDENT		
83.	CRES + OH ---> .2MGLY + .15R02P + .85R02R + RO2	4.00E-11	5.91E+04	
84.	CRES + NO3 ---> HNO3 + BZO	2.20E-11	3.25E+04	
85.	RO2P + NO ---> NPHE	7.68E-12	1.14E+04	4.20E-12*EXP(180/T)
86.	RO2P + HO2 --->	3.00E-12	4.43E+03	
87.	RO2P + RO2 ---> .5HO2 + RO2	1.00E-15	1.48E+00	
88.	RO2P + MCO3 ---> HCHO + HO2	3.00E-12	4.43E+03	
89.	BZO + NO2 ---> NPHE	1.50E-11	2.22E+04	
90.	BZO + HO2 --->	3.00E-12	4.43E+03	
91.	BZO --->	1.00E-03	6.00E-02	
92.	NPHE + NO3 ---> HNO3 + BZN2	3.80E-12	5.62E+03	
93.	BZN2 + NO2 --->	1.50E-11	2.22E+04	
94.	BZN2 + HO2 ---> NPHE	3.00E-12	4.43E+03	
95.	BZN2 ---> NPHE	1.00E-03	6.00E-02	

TABLE 2-5

REPRESENTATION OF NMOC IN THE OZIPM MECHANISM

COMPOUND CLASS	SURROGATE SPECIES
ETHENE	ETHENE (ETHE)
TERMINAL ALKENES	PROPENE (PRPE)
INTERNAL ALKENES	TRANS-2-BUTENE (TBUT)
C4-C5 ALKANES	N-BUTANE* (ALK4) N-PENTANE* ISO-BUTANE* ISO-PENTANE*
C6+ ALKANES	N-HEXANE* (ALK7) N-HEPTANE* N-OCTANE* 2,3-DIMETHYLBUTANE* 2-METHYLPENTANE* 2,3-DIMETHYLPENTANE* ISO-OCTANE*
MONO-ALKYLBENZENES	TOLUENE (TOLU)
DI-ALKYLBENZENES	M-XYLENE (XYLE)
TRI-ALKYLBENZENES	MESITYLENE (TMBZ)
FORMALDEHYDE	FORMALDEHYDE (HCHO)
ACETALDEHYDE	ACETALDEHYDE (ALD2)
HIGHER ALDEHYDES	PROPIONALDEHYDE (RCHO)
HIGHER KETONES	METHYL ETHYL KETONE (MEK)

* Rate contants and product coefficient based on a mixture of these surrogate species.

TABLE 2-6

REPRESENTATION OF NMOC IN THE CONDENSED MECHANISM

COMPOUND CLASS	SURROGATE SPECIES
ETHENE	ETHENE (ETHE)
HIGHER ALKENES	PROPENE* (ALKE) TRANS-2-BUTENE*
>C3 ALKANES	N-BUTANE* (ALKA) N-PENTANE* ISO-BUTANE* ISO-PENTANE* N-HEXANE* N-HEPTANE* N-OCTANE* 2,3-DIMETHYLBUTANE* 2-METHYLPENTANE* 2,3-DIMETHYLPENTANE* ISO-OCTANE*
MONO-ALKYLBENZENES	TOLUENE (TOLU)
DI-& TRI-ALKYLBENZENES	M-XYLENE* (AROM) MESITYLENE*
FORMALDEHYDE	FORMALDEHYDE (HCHO)
HIGHER ALDEHYDES	ACETALDEHYDE (ALD2)
HIGHER KETONES	METHYL ETHYL KETONE (MEK)

* Rate contants and product coefficient based on a mixture of these surrogate species.

zenith angle, in turn, depends on geographic location, date, and time of day. In most atmospheric modeling applications, detailed solar intensity and spectral distribution data are not available so theoretical clear-sky actinic flux values, such as those reported by Peterson (1976), are used. In some model applications, the clear-sky values are adjusted to account for cloud cover. However, most of the adjustment methods are very approximate. Given the actinic fluxes, the photolytic reaction rates are calculated from the equation

$$K(z,j) = \sum_{w} I(w,z) \cdot A(w,j) \cdot Q(w,j)$$

where

K = photolytic rate of species j at solar zenith angle z,
I = actinic flux for wavelength increment w and solar zenith angle z,
A = absorption cross-section of species j for wavelength increment w, and
Q = quantum yield of species j for wavelength increment w.

In applying this equation, it is important to perform the summation for the smallest wavelength increment in I, A, or Q for which data are available.

Clear sky values for the photolytic reaction rates in the mechanism at zero elevation are shown in Table 2-7. These rates are based on the solar actinic flux, absorption cross-section, and quantum yield data shown in Appendix A. The ratios of other photolytic reactions rates to the NO_2 photolytic rate at zero elevation are shown in Table 2-8. These ratios are useful because the rates of other photolyic reactions are calculated from the NO_2 photolytic rate in many photochemical models. These ratios are, of course, dependent on the solar zenith angle. Values of the rates (and ratios) in between the zenith angles listed in the tables can be obtained by interpolation.

The solar radiation intensity increases with elevation above the surface. The clear-sky actinic flux typically increases 15% per 1000 meters (Peterson 1976). We recommend using elevation dependent

TABLE 2-7

ESTIMATED CLEAR SKY PHOTOLYTIC REACTION RATES (PER SECOND) AT THE EARTH'S SURFACE*

Reaction	Solar Zenith Angle									
	0	10	20	30	40	50	60	70	78	86
NO2 + hv --> NO + O	8.29E-03	8.22E-03	8.02E-03	7.66E-03	7.10E-03	6.26E-03	5.05E-03	3.32E-03	1.64E-03	3.51E-04
NO3 + hv --> NO + O2	1.87E-02	1.86E-02	1.83E-02	1.77E-02	1.70E-02	1.60E-02	1.43E-02	1.11E-02	6.65E-03	9.81E-04
NO3 + hv --> NO2 + O	1.70E-01	1.70E-01	1.70E-01	1.60E-01	1.50E-01	1.40E-01	1.30E-01	9.86E-02	5.82E-02	9.05E-03
O3 + hv --> O + O2	4.57E-04	4.55E-04	4.46E-04	4.29E-04	4.06E-04	3.75E-04	3.25E-04	2.47E-04	1.46E-04	2.32E-05
O3 + hv --> O*SD (270 K)	3.38E-05	3.27E-05	2.94E-05	2.41E-05	1.77E-05	1.11E-05	5.30E-06	1.59E-06	3.57E-07	4.30E-08
O3 + hv --> O*SD (300 K)	3.78E-05	3.66E-05	3.30E-05	2.72E-05	2.03E-05	1.29E-05	6.34E-06	1.99E-06	4.59E-07	5.42E-08
O3 + hv --> O*SD (330 K)	4.18E-05	4.06E-05	3.67E-05	3.05E-05	2.30E-05	1.49E-05	7.55E-06	2.48E-06	6.02E-07	7.02E-08
HONO + hv --> OH + NO	1.63E-03	1.61E-03	1.57E-03	1.50E-03	1.38E-03	1.21E-03	9.58E-04	6.14E-04	2.96E-04	6.61E-05
H2O2 + hv --> 2 OH	7.53E-06	7.43E-06	7.07E-06	6.47E-06	5.62E-06	4.50E-06	3.15E-06	1.70E-06	7.05E-07	1.34E-07
ROOH + hv --> OH + HO2	7.53E-06	7.43E-06	7.07E-06	6.47E-06	5.62E-06	4.50E-06	3.15E-06	1.70E-06	7.05E-07	1.34E-07
HCHO + hv --> HO2 + CO	3.02E-05	2.98E-05	2.83E-05	2.57E-05	2.21E-05	1.73E-05	1.18E-05	6.00E-06	2.32E-06	3.85E-07
HCHO + hv --> H2 + CO	4.63E-05	4.58E-05	4.41E-05	4.12E-05	3.68E-05	3.07E-05	2.28E-05	1.32E-05	5.85E-06	1.20E-06
ALD2 + hv --> CO + CH3O2	4.86E-06	4.76E-06	4.41E-06	3.84E-06	3.09E-06	2.21E-06	1.30E-06	5.40E-07	1.65E-07	2.10E-08
RCHO + hv --> CO + C2H5O2	9.84E-06	9.69E-06	9.17E-06	8.28E-06	7.05E-06	5.48E-06	3.66E-06	1.83E-06	6.98E-07	1.16E-07
ACET + hv --> HCHO + MCO3	1.11E-06	1.09E-06	1.02E-06	9.04E-07	7.50E-07	5.62E-07	3.56E-07	1.65E-07	5.81E-08	8.75E-09
MEK + hv --> ALD2 + MCO3	1.58E-06	1.55E-06	1.46E-06	1.29E-06	1.07E-06	8.03E-07	5.09E-07	2.36E-07	8.30E-08	1.25E-08
BCHO + hv --> Nonreactive	4.30E-05	4.26E-05	4.12E-05	3.89E-05	3.54E-05	3.04E-05	2.34E-05	1.45E-05	6.78E-06	1.49E-06
GLYX + hv --> HCHO + CO	6.46E-05	6.42E-05	6.31E-05	6.11E-05	5.80E-05	5.30E-05	4.53E-05	3.28E-05	1.78E-05	3.42E-06
MGLY + hv --> HO2 + MCO3	1.42E-04	1.42E-04	1.39E-04	1.35E-04	1.28E-04	1.17E-04	9.99E-05	7.19E-05	3.88E-05	7.52E-06
DIAL + hv --> HO2 + MCO3	5.29E-04	5.23E-04	5.04E-04	4.71E-04	4.23E-04	3.55E-04	2.65E-04	1.56E-04	7.03E-05	1.50E-05

* Based on Peterson (1976) Solar Actinic Fluxes

TABLE 2-8

RATIOS OF OTHER CLEAR SKY PHOTOLYTIC REACTION RATES TO THE NO2 PHOTOLYTIC RATE AT THE EARTH'S SURFACE*

Reaction	Solar Zenith Angle									
	0	10	20	30	40	50	60	70	78	86
NO3 + hv --> NO + O2	2.3	2.3	2.3	2.3	2.4	2.6	2.8	3.3	4.1	2.8
NO3 + hv --> NO2 + O	20.	20.	21.	21.	22.	23.	25.	30.	36.	26.
O3 + hv --> O + O2	5.52E-02	5.53E-02	5.56E-02	5.61E-02	5.71E-02	5.99E-02	6.45E-02	7.43E-02	8.90E-02	6.60E-02
O3 + hv --> O*SD 270 K	4.08E-03	3.98E-03	3.66E-03	3.14E-03	2.50E-03	1.77E-03	1.05E-03	4.80E-04	2.18E-04	1.22E-04
O3 + hv --> O*SD 300 K	4.56E-03	4.45E-03	4.12E-03	3.56E-03	2.86E-03	2.06E-03	1.26E-03	5.98E-04	2.80E-04	1.54E-04
O3 + hv --> O*SD 330 K	5.04E-03	4.93E-03	4.58E-03	3.98E-03	3.24E-03	2.36E-03	1.49E-03	7.48E-04	3.67E-04	2.00E-04
HONO + hv --> OH + NO	.20	.20	.20	.20	.19	.19	.19	.18	.18	.19
H2O2 + hv --> 2 OH	9.08E-04	9.03E-04	8.82E-04	8.45E-04	7.91E-04	7.18E-04	6.25E-04	5.12E-04	4.31E-04	3.83E-04
ROOH + hv --> OH + HO2	9.08E-04	9.03E-04	8.82E-04	8.45E-04	7.91E-04	7.18E-04	6.25E-04	5.12E-04	4.31E-04	3.83E-04
HCHO + hv --> 2 HO2 + CO	3.65E-03	3.62E-03	3.53E-03	3.36E-03	3.11E-03	2.77E-03	2.33E-03	1.81E-03	1.41E-03	1.10E-03
HCHO + hv --> H2 + CO	5.59E-03	5.57E-03	5.50E-03	5.38E-03	5.19E-03	4.91E-03	4.51E-03	3.97E-03	3.57E-03	3.43E-03
ALD2 + hv --> HCHO + CH3O2	5.87E-04	5.79E-04	5.51E-04	5.01E-04	4.36E-04	3.53E-04	2.58E-04	1.63E-04	1.01E-04	5.96E-05
RCHO + hv --> ALD2 + C2H5O2	1.19E-03	1.18E-03	1.14E-03	1.08E-03	9.94E-04	8.75E-04	7.26E-04	5.53E-04	4.27E-04	3.31E-04
ACET + hv --> HCHO + MCO3	1.34E-04	1.32E-04	1.27E-04	1.18E-04	1.06E-04	8.97E-05	7.05E-05	4.98E-05	3.55E-05	2.49E-05
MEK + hv --> ALD2 + MCO3	1.91E-04	1.89E-04	1.82E-04	1.69E-04	1 51E-04	1.28E-04	1.01E-04	7.11E-05	5.07E-05	3.56E-05
BCHO + hv --> Nonreactive	5.19E-03	5.18E-03	5.14E-03	5.09E-03	4.99E-03	4.85E-03	4.64E-03	4.36E-03	4.14E-03	4.23E-03
GLYX + hv --> HCHO + H2 + CO	7.79E-03	7.81E-03	7.87E-03	7.97E-03	8.17E-03	8.46E-03	8.97E-03	9.88E-03	1.09E-02	9.73E-03
MGLY + hv --> HO2 + MCO3	1.72E-02	1.72E-02	1.74E-02	1.76E-02	1.80E-02	1.87E-02	1.98E-02	2.17E-02	2.37E-02	2.14E-02
DIAL + hv --> HO2 + MCO3	6.38E-02	6.36E-02	6.29E-02	6.15E-02	5.95E-02	5.66E-02	5.25E-02	4.70E-02	4.29E-02	4.27E-02

photolysis rates in multi-layer AQS models. In single-cell models, photolytic rates appropriate for an elevation equal to one-half the maximum mixing depth are recommended.

2.2 Special Product Coefficients and Rate Constants

The product coefficients in the alkane reactions depend on temperature and pressure. The pressure dependency can be ignored in most urban-scale applications. However, the temperature dependency should not be ignored if the mechanism is going to be applied over a wide temperature range. The values of the coefficients in reactions 85 and 86 of the OZIPM mechanism (Table 2-2) between 270 and 330°K are shown below. Values at intermediate temperatures can be determined by linear interpolation or by using the computer routine that was developed for this purpose. A listing of the routine is given in Table 2-9.

	TEMPERATURE (K)						
COEFF.	270	280	290	300	310	320	330
B01	.197	.194	.192	.189	.189	.188	.188
B02	.168	.217	.266	.315	.404	.493	.582
B03	.115	.132	.149	.166	.192	.218	.244
B04	.351	.347	.343	.339	.343	.346	.350
B05	.489	.473	.458	.442	.384	.325	.267
B06	.114	.100	.087	.073	.065	.058	.050
B07	.886	.900	.913	.927	.935	.942	.950
B08	.446	.497	.548	.599	.668	.738	.807
B09	1.332	1.397	1.461	1.526	1.603	1.680	1.757
B10	.005	.011	.017	.023	.033	.044	.054
B11	.021	.025	.028	.032	.048	.065	.081
B12	.215	.226	.238	.249	.265	.280	.296
B13	.297	.316	.336	.355	.376	.398	.419
B14	.765	.804	.843	.882	.885	.888	.891
B15	.288	.255	.223	.190	.169	.147	.126
B16	.701	.737	.774	.810	.831	.852	.873
B17	.651	.713	.775	.837	.893	.948	1.004
B18	1.352	1.450	1.549	1.647	1.724	1.800	1.877

Several product coefficients and rate constants in the condensed mechanism (Table 2-4) depend on temperature and organic mixture composition. While the condensed mechanism can be used with the default composition assumptions, the recommended approach is for the user to

TABLE 2-9

EXAMPLE OF SPECIAL SUBROUTINE FOR THE OZIPM MECHANISM

```
      SUBROUTINE SPECIAL(TEMP,B)
C
C     THIS ROUTINE COMPUTES THE ALKANE PRODUCT COEFFICIENTS
C     FOR THE ERT/SAPRC OZIPM MECHANISM
C
C     INPUTS:
C        TEMP = TEMPERATURE (DEGREES K)
C     OUTPUTS:
C        B(J) = VARIABLE PRODUCT COEFFICIENTS FOR THE REACTIONS
C               OF ALKANES
C
      REAL B(18)
      B(01) = CT(TEMP,0.197,0.189,0.188)
      B(02) = CT(TEMP,0.168,0.315,0.582)
      B(03) = CT(TEMP,0.115,0.166,0.244)
      B(04) = CT(TEMP,0.351,0.339,0.350)
      B(05) = CT(TEMP,0.489,0.442.0.267)
      B(06) = CT(TEMP,0.114,0.073,0.050)
      B(07) = CT(TEMP,0.886,0.927,0.950)
      B(08) = CT(TEMP,0.446,0.599,0.807)
      B(09) = B(07) + B(08)
      B(10) = CT(TEMP,0.005,0.023,0.054)
      B(11) = CT(TEMP,0.021,0.032,0.081)
      B(12) = CT(TEMP,0.215,0.249,0.296)
      B(13) = CT(TEMP,0.297,0.355,0.419)
      B(14) = CT(TEMP,0.765,0.882,0.891)
      B(15) = CT(TEMP,0.288,0.190,0.126)
      B(16) = CT(TEMP,0.701,0.810,0.873)
      B(17) = CT(TEMP,0.651,0.837,1.004)
      B(18) = B(16) + B(17)
      RETURN
      END

      FUNCTION CT(TEMP,C1,C2,C3)
C.....LINEAR INTERPOLATION FOR 3 VALUE TABULATED FUNCTION
      REAL T(3)
      DATA T /270.,300.,330./
      CT = C1
      IF(TEMP.LE.T(1)) RETURN
      CT = C3
      IF(TEMP.GE.T(3)) RETURN
      IF(TEMP.LT.T(2)) THEN
      SLOPE = (C2-C1)/(T(2)-T(1))
      CT = C1 + SLOPE*(TEMP-T(1))
      ENDIF
      IF(TEMP.GE.T(2)) THEN
      SLOPE = (C3-C2)/(T(3)-T(2))
      CT = C2 + SLOPE*(TEMP-T(2))
      ENDIF
      RETURN
      END
```

estimate the average values for three composition fractions based on region-specific ambient air NMOC data or speciated emission inventory data. The lumped product coefficients and rate constants depend on the ratio of C4-C5 alkanes to >C3 alkanes (X), the ratio of terminal alkenes to >C2 alkenes (Y), and the ratio of di-alkylbenzenes to di- and tri-alkylbenzenes (Z), where X, Y, and Z are on a mole basis. These mole fractions are estimated from the corresponding carbon fractions (ie., X_c, Y_c, Z_c) as shown below:

$$X = (X_c/4.5) \; / \; (X_c/4.5 + (1.-X_c)/7.)$$

$$Y = (Y_c/3.0) \; / \; (Y_c/3.0 + (1.-Y_c)/4.)$$

$$Z = (Z_c/8.0) \; / \; (Z_c/8.0 + (1.-Z_c)/9.)$$

The lumped rate constants for reactions 57, 75-78, and 80 in Table 2-4 are then determined from the following expressions:

$$R57 = 1.053E\text{-}11*EXP(-354/T)*X + 1.62E\text{-}11*EXP(-289/T)*(1-X)$$

$$R75 = 4.850E\text{-}12*EXP(504/T)*Y + 1.01E\text{-}11*EXP(549/T)*(1-Y)$$

$$R76 = 1.320E\text{-}14*EXP(-2105/T)*Y + 9.08E\text{-}15*EXP(-1137/T)*(1-Y)$$

$$R77 = 1.180E\text{-}11*EXP(-324/T)*Y + 2.26E\text{-}11*EXP(10/T)*(1-Y)$$

$$R78 = 5.000E\text{-}12*EXP(-1935/T)*Y + 1.00E\text{-}11*EXP(-975/T)*(1-Y)$$

$$R80 = 1.660E\text{-}11*EXP(116/T)*Z + 6.20E\text{-}11*(1-Z)$$

The product coefficients for the same reactions are determined from the following expressions:

$$B01 = 0.197*X + 0.005*(1-X) \quad \text{at } 270°K$$
$$B02 = 0.282*X + 0.236*(1-X) \quad "$$
$$B03 = 0.489*X + 0.765*(1-X) \quad "$$
$$B04 = 0.114*X + 0.288*(1-X) \quad "$$
$$B05 = 0.886*X + 0.701*(1-X) \quad "$$
$$B06 = 0.446*X + 0.651*(1-X) \quad "$$
$$B07 = 1.332*X + 1.352*(1-X) \quad "$$

```
B01  =  0.189*X + 0.023*(1-X)  at 300°K
B02  =  0.481*X + 0.281*(1-X)      "
B03  =  0.442*X + 0.882*(1-X)      "
B04  =  0.073*X + 0.190*(1-X)      "
B05  =  0.927*X + 0.810*(1-X)      "
B06  =  0.599*X + 0.837*(1-X)      "
B07  =  1.526*X + 1.647*(1-X)      "


B01  =  0.188*X + 0.054*(1-X)  at 330°K
B02  =  0.826*X + 0.377*(1-X)      "
B03  =  0.267*X + 0.891*(1-X)      "
B04  =  0.050*X + 0.126*(1-X)      "
B05  =  0.950*X + 0.873*(1-X)      "
B06  =  0.807*X + 1.004*(1-X)      "
B07  =  1.757*X + 1.877*(1-X)      "


B08  =  Y
B09  =  Y + 2.00*(1-Y)
B10  =  0.64*Y
B11  =  0.50*Y + (1-Y)
B12  =  0.13*Y + 0.27*(1-Y)
B13  =  0.17*Y + 0.21*(1-Y)
B14  =  0.06*Y + 0.12*(1-Y)
B15  =  0.28*Y
B16  =  0.40*Y
B17  =  (1-Y)
B18  =  0.40*Y
B19  =  0.20*Y
B20  =  0.20*Y + 0.40*(1-Y)
321  =  0.60*Y


B22  =  0.650*Z + 0.49*(1-Z)
B23  =  0.316*Z + 0.86*(1-Z)
B24  =  0.095*Z
```

The expression for the coefficients in the alkane reaction (No. 57) are given at three temperatures. Values at intermediate temperatures can be obtained by linear interpolation. We have found it most convenient to implement a subroutine to calculate these rate constants and coefficients into the AQS model software. The routine we use for this purpose is shown in Table 2-10.

The default values of the carbons fractions are 0.43, 0.6, and 0.6 for X_c, Y_c, and Z_c, respectively. The default coefficients and rate constants (at 298°K) for the lumped reactions are shown below:

TABLE 2-10

EXAMPLE OF SPECIAL SUBROUTINE FOR THE CONDENSED MECHANISM

```
      SUBROUTINE SPECIAL(TEMP,F,B,R)
C
C     THIS IS THE FORTRAN77 SUBROUTINE TO COMPUTE THE VARIABLE PRODUCT
C     COEFFICIENTS AND SPECIAL RATE CONSTANTS FOR THE SAPRC/ERT
C     CONDENSED CHEMICAL MECHANISM.
C
C     INPUTS: TEMP = TEMPERATURE IN DEGRESS KELVIN
C        F(1) = XC = C4-C5 FRACTION OF ¶C3 ALKANES ON A CARBON BASIS
C        F(2) = YC = TERMINAL ALKENE FRACTION OF ¶C2 ALKENES ON A
C                    CARBON BASIS
C        F(3) = ZC = DI-ALKYLBENZENE FRACTION OF DI- & TRI-ALKYLBENZENES
C                    ON A CARBON BASIS
C
C     OUTPUTS:
C        B(J) = VARIABLE PRODUCT COEFFICIENTS FOR THE REACTIONS
C               OF ALKANES, HIGHER ALKENES, AND HIGHER AROMATICS
C
C        R(I) = RATE CONSTANTS FOR REACTIONS OF ALKANES, HIGHER
C               ALKENES, AND HIGHER AROMATICS
C
      REAL F(3), B(24), R(95)
C
C...COMPUTE THE FRACTIONS ON A MOLAR BASIS, WHERE
C     X = C4-C5 FRACTION OF >C3 ALKANES
C     Y = TERMINAL ALKENE FRACTION OF >C2 ALKENES
C     Z = TRI-ALKYLBENZENE  FRACTION OF DI- & TRI-ALKYLBENZENES
C
      X = (F(1)/4.5) / (F(1)/4.5 + (1.-F(1))/7.)
      Y = (F(2)/3. ) / (F(2)/3.  + (1.-F(2))/4.)
      Z = (F(3)/8. ) / (F(3)/8.  + (1.-F(3))/9.)
      XT = 1. - X
      YT = 1. - Y
      ZT = 1. - Z
C...COMPUTE COEFFICIENTS FOR ALKANES
      B(01) = CT(TEMP,0.197,0.189,0.188)*X + CT(TEMP,0.005,0.023,0.054)*XT
      B(02) = CT(TEMP,0.282,0.481,0.826)*X + CT(TEMP,0.236,0.281,0.377)*XT
      B(03) = CT(TEMP,0.489,0.442,0.267)*X + CT(TEMP,0.765,0.882,0.891)*XT
      B(04) = CT(TEMP,0.114,0.073,0.050)*X + CT(TEMP,0.288,0.190,0.126)*XT
      B(05) = CT(TEMP,0.886,0.927,0.950)*X + CT(TEMP,0.701,0.810,0.873)*XT
      B(06) = CT(TEMP,0.446,0.599,0.807)*X + CT(TEMP,0.651,0.837,1.004)*XT
      B(07) = B(05) + B(06)
C...COMPUTE COEFFICIENT FOR HIGHER ALKENES
      B(08) =      Y
      B(09) =      Y + 2.00*YT
      B(10) = 0.64*Y
      B(11) = 0.50*Y +      YT
      B(12) = 0.13*Y + 0.27*YT
      B(13) = 0.17*Y + 0.21*YT
      B(14) = 0.06*Y + 0.12*YT
      B(15) = 0.28*Y
      B(16) = 0.40*Y
```

TABLE 2-10 (Continued)

```
      B(17) =                YT
      B(18) = 0.40*Y
      B(19) = 0.20*Y
      B(20) = 0.20*Y + 0.40*YT
      B(21) = 0.60*Y
C...COMPUTE COEFFICENTS FOR HIGHER AROMATICS
      B(22) = 0.65*Z + 0.49*ZT
      B(23) =0.316*Z + 0.86*ZT
      B(24) =0.095*Z
C...REACTION RATE FOR ALKA + OH IN MOLECULE-CC-SEC UNITS
      R(57)  = 1.053E-11*EXP(  -354/T)*X  + 1.62E-11*EXP(  -289/T)*XT
C...REACTION RATE FOR ALKE + OH IN MOLECULE-CC-SEC UNITS
      R(75)  = 4.850E-12*EXP(   504/T)*Y  + 1.01E-11*EXP(   549/T)*YT
C...REACTION RATE FOR ALKE + O3 IN MOLECULE-CC-SEC UNITS
      R(76)  = 1.320E-14*EXP( -2105/T)*Y  + 9.08E-15*EXP( -1137/T)*YT
C...REACTION RATE FOR ALKE + O  IN MOLECULE-CC-SEC UNITS
      R(77)  = 1.180E-11*EXP(  -324/T)*Y  + 2.26E-11*EXP(    10/T)*YT
C...REACTION RATE FOR ALKE + NO3 IN MOLECULE-CC-SEC UNITS
      R(78)  = 5.000E-12*EXP( -1935/T)*Y  + 1.00E-11*EXP(  -975/T)*YT
C...REACTION RATE FOR AROM + OH IN MOLECULE-CC-SEC UNITS
      R(80)  = 1.660E-11*EXP(   116/T)*Z  + 6.20E-11*ZT
      RETURN
      END
C
      FUNCTION CT(TEMP,C1,C2,C3)
C.....LINEAR INTERPOLATION FOR 3 VALUE TABULATED FUNCTION
      REAL T(3)
      DATA T /270.,300.,330./
      CT = C1
      IF(TEMP.LE.T(1)) RETURN
      CT = C3
      IF(TEMP.GE.T(3)) RETURN
      IF(TEMP.LT.T(2)) THEN
      SLOPE = (C2-C1)/(T(2)-T(1))
      CT = C1 + SLOPE*(TEMP-T(1))
      ENDIF
      IF(TEMP.GE.T(2)) THEN
      SLOPE = (C3-C2)/(T(3)-T(2))
      CT = C2 + SLOPE*(TEMP-T(2))
      ENDIF
      RETURN
      END
```

ALKA + OH —> .112 HCHO +.380 ALD2 +.643 MEK +.131 RO2N
+.868 RO2R +.698 R2O2 +.157 RO2

k_{57} = 6740 ppm^{-1} min^{-1} (or 4.56E-12 cm^3 $molecule^{-1}$ sec^{-1})

ALKE + OH —> .667 HCHO +1.33 ALD2 + RO2R + RO2

k_{75} = 57300 ppm^{-1} min^{-1} (or 3.88E-11 cm^3 $molecule^{-1}$ sec^{-1})

ALKE + O3 —> .427 HCHO +.667 ALD2 +.177 RO2R +.177 RO2
+.183 HO2 + .08 OH +.187 CO

k_{76} = 0.110 ppm^{-1} min^{-1} (or 7.42E-17 cm^3 $molecule^{-1}$ sec^{-1})

ALKE + O —> .333 CO +.333 MEK +.267 HCHO +.133 ALD2
+.267 HO2 + .40 RO2R + .40 RO2

k_{77} = 15400 ppm^{-1} min^{-1} (or 1.04E-11 cm^3 $molecule^{-1}$ sec^{-1})

ALKE + NO3 —> NO2 +.667 HCHO +1.33 ALD2 + R2O2 + RO2

k_{78} = 194 ppm^{-1} min^{-1} (or 1.31E-13 cm^3 $molecule^{-1}$ sec^{-1})

AROM + OH --> .17 CRES + .17 HO2 + .83 RO2R + .83 RO2
+.59 DIAL +.518 MGLY +.597 HCHO +.597 CO

k_{80} = 56800 ppm^{-1} min^{-1} (or 3.84E-11 cm^3 $molecule^{-1}$ sec^{-1})

The default rate constant expressions are

k_{57} = 1.35E-11 * exp (-324/T) cm^3 $molecule^{-1}$ sec^{-1}

k_{75} = 6.80E-12 * exp (519/T) cm^3 $molecule^{-1}$ sec^{-1}

k_{76} = 2.93E-14 * exp (-1782/T) cm^3 $molecule^{-1}$ sec^{-1}

k_{77} = 2.13E-11 * exp (-213/T) cm^3 $molecule^{-1}$ sec^{-1}

$$k_{78} = 2.95E\text{-}11 * \exp(-1615/T)\ cm^3\ molecule^{-1}\ sec^{-1}$$

$$k_{80} = 2.97E\text{-}11 * \exp(77/T)\ cm^3\ molecule^{-1}\ sec^{-1}$$

2.3 Steady-State Approximations

Numerous species in the mechanism react so fast that their concentrations are essentially in steady-state under most atmospheric conditions. These species have large production and destruction rates, but small net rates of change of concentration. The computer memory and time requirements of AQS models can be reduced by calculating the concentrations of these species from algebraic equations based on the steady-state approximation rather than by numerical integration of their differential equations. However, not all kinetic solver software systems provide capabilities for treating species diagnostically (e.g. OZIPM and CHEMK).

The steady-state approximation assumes a system is at chemical equilibrium where the rate of change of concentration is zero. It is the state where the rate of chemical production (P) is equal to the rate of destruction (DC). With this assumption the species concentration (C) can be calculated from the simple linear algebraic equation (for species that do not react with themselves), as shown below.

$$dC/dt = P - DC = 0$$

$$C = P/D$$

The procedure for selecting the species for which this approximation is valid involves examining the characteristic reaction time (1/D) of the species over a range of conditions. In order for the approximation to be valid, the reaction time must be smaller than the typical time step size in the AQS model (~1 minute) under all plausible circumstances. We have examined the reaction time for a range of radiation, temperature, and concentrations including low NO_x conditions. Tables 2-11 and 2-12 list typical reaction times for daylight and nighttime conditions in urban and low NO_x environments, respectively, at 298°K. These characteristic

TABLE 2-11

CHARACTERISTIC REACTION TIME IN URBAN ENVIRONMENTS

SPECIES	REACTION TIME (MINUTES)* DAYLIGHT	NIGHTTIME
O*SD	2.E-11	2.E-11
O	2.E-08	2.E-08
OH	6.5E-4	4.E-04
BZO	0.002	5.E-04
BZN2	0.002	5.E-04
RCO3	0.003	0.002
MCO3	0.003	0.002
PCO3	0.003	0.002
GCO3	0.003	0.002
NO3	0.004	0.005
HO2	0.007	0.005
RO2	0.014	0.035
RO2P	0.014	0.035
RO2R	0.014	0.035
R2O2	0.014	0.035
RO2N	0.014	0.035
HNO4	0.2	0.2
NO	0.4	1.5
N2O5	0.5	0.5
NO2	2	40
O3	5	15
HONO	10	300
TBUT	23	130
DIAL	25	1,200
CRES	31	25
PAN	45	45
PPN	45	45
GPAN	45	45
TMBZ	58	4,500
MGLY	76	2,300
PHEN	88	140
PRPE	110	2,000
HCHO	140	8,000
GLYX	140	5,000
XYLE	150	11,000
RCHO	170	12,000
ALD2	210	16,000
NPHE	270	140
ETHE	390	11,000
TOLU	580	45,000
ALK7	590	45,000
H2O2	1,100	80,000
ALK4	1,100	86,000
ALKN	1,800	130,000
ROOH	2,300	150,000
MEK	2,700	240,000
ACET	7,800	800,000
CO	17,000	1,300,000
HNO3	28,000	2,200,000

TABLE 2-12

CHARACTERISTIC REACTION TIME IN LOW NO_x ENVIRONMENTS

	REACTION TIME (MINUTES)*	
SPECIES	DAYLIGHT	NIGHTTIME
O*SD	2.E-11	2.E-11
O	2.E-08	2.E-08
OH	2.E-03	2.E-03
BZO	0.08	0.07
BZN2	0.08	0.07
RCO3	0.2	0.2
MCO3	0.2	0.2
PCO3	0.2	0.2
GCO3	0.2	0.2
NO3	0.05	0.7
HO2	0.2	0.5
RO2	10	10
RO2P	10	10
RO2R	10	10
R2O2	10	10
RO2N	10	10
HNO4	0.2	0.2
NO	0.2	0.2
N2O5	0.5	0.5
NO2	120	60
O3	30	1,500
HONO	10	600
TBUT	23	19
DIAL	25	1,900
CRES	3	60
PAN	45	45
PPN	45	45
GPAN	45	45
TMBZ	58	3,000
MGLY	76	3,200
PHEN	18	110
PRPE	105	430
HCHO	130	6,500
GLYX	140	6,500
XYLE	145	7,500
RCHO	160	6,800
ALD2	210	8,000
NPHE	18	970
ETHE	370	2,700
TOLU	570	30,000
ALK7	580	30,000
H2O2	1,100	80,000
ALK4	1,100	57,000
ALKN	1,800	91,000
ROOH	2,300	300,000
MEK	2,700	180,000
ACET	7,800	700,000
CO	17,000	850,000
HNO3	28,000	1,450,000

reaction times indicate the steady-state approximation is valid for O*SD, O, OH, BZO, and BZN2 at all times.

The reactions times for RCO3, HO2, and RO2 indicate the approximation is valid under urban NO_x conditions. For low NOx conditions the approximation is marginally valid for RCO3 and HO2, and not valid for RO2 species. Since the mechanisms are invariably applied under low NO_x conditions, the steady-state species must be selected so as to avoid serious errors when these conditions occur. We have found, however, that if HO2 and the RO2 and RCO3 psuedo-species are integrated, the individual peroxy species (RO2R, R2O2, RO2P, and RO2N) and the acyl peroxy species (MCO3, PCO3, and GCO3 in the OZIPM mechanism) can be accurately calculated using the steady-state approximation (Carter et al. 1986).

The HNO4 and N2O5 reaction times at 298°K indicate the approximation is marginally valid, however, the lifetimes of these species are strongly dependent on temperature. For example, at 283°K (or 50°F) the reaction times of HNO4 and N2O5 are 1.2 and 3.6 minutes, respectively, which eliminates them as candidates for steady-state treatment in most photochemical model applications.

Concentrations of the NO3 radical can be accurately calculated from the approximation during daylight hours and whenever NO concentrations are greater than 1 ppb. However, the approximation becomes marginal for NO_3 when NO concentrations are low at night. Therefore, it is recommended that NO_3 be included as an integrated species.

If the mechanism is applied under conditions where steady-state treatment of HNO4, N2O5, and NO3 is valid and is used, the solution procedure should contain a nitrogen balance calculation (or nitrogen conservation constraint) to ensure that the approximation is not artificially introducing significant amounts of nitrogen to the system.

The diagnostic equations for the steady-state species in the OZIPM and condensed mechanisms are shown in Tables 2-13 and 2-14, respectively. These equations should be evaluated in the order shown because the concentrations of some steady-state species depend on the concentrations of other steady-state species. These equations should be evaluated each time chemical derivatives are calculated in the AQS model.

TABLE 2-13

DIAGNOSTIC EQUATIONS FOR THE STEADY-STATE SPECIES IN THE OZIPM MECHANISM

```
[O*SD] = R16*[O3] / (R17*[H2O] + R18)

[O]    = (R1*[NO2] + R14*[NO3] + R15*[O3] + R18*[O*SD] )/( R2 + R3*
         [NO2] + R4*[NO2] + R102*[ETHE] + R106*[PRPE] + R110*[TBUT])

[PCO3] = (R60*[RCHO]*[OH] + R62*[RCHO]*[NO3] + R68*[PPN]
         + 0.50*R72*[MEK*[OH] + R115*[OH]*[DIAL]) / (R63*[NO] +
         R64*[NO2] + R65*[HO2] + R66*[RO2] + R67*[RCO3])

[GCO3] = (.37*R74*[GLYX]*[OH] +.37*R75*[GLYX]*[NO3] + R78*[GPAN])/
         (R76*[NO2] + R77*[NO] + R79*[HO2] + R80*[RO2]
         + R81*[RCO3])

[RO2R] = (R50*[HCHO]*[HO2] + R52*[ALD2] + R54*[NO]*[MCO3] +
         R61*[RCHO] + R63*[NO]*[PCO3] + R69*[ACET] + R70*[ACET]
         *[OH] + R71*[MEK] + B07*R85*[OH]*[ALK4] + B16*R86*[OH]
         *[ALK7] + R100*[OH]*[ETHE] + R102*[ETHE]*[O] + R104*[OH]
         *[PRPE] + 0.13*R105*[O3]*[PRPE] + 0.60*R106*[PRPE]*[O] +
         R108*[OH]*[TBUT] + 0.27*R109*[O3]*[TBUT] + 0.84*R112*[OH]
         *[TOLU] + 0.83*R113*[OH]*[XYLE] + 0.83*R114*[OH]*[TMBZ] +
         0.85*R117*[OH]*[CRES] + 0.85*R126*[OH]*[PHEN]) /
         (R96*[NO] + R97*[HO2] + R98*[RO2] + R99*[RCO3])

[R2O2] = (1.50*R72*[MEK]*[OH] + B08*R85*[OH]*[ALK4] + B17*R86*
         [OH]*[ALK7] + 1.39*R87*[OH]*[ALKN] + R103*[NO3]*[ETHE]
         + R107*[NO3]*[PRPE] + R111*[NO3]*[TBUT]) /
         (R92*[NO] + R93*[HO2] + R94*[RO2] + R95*[RCO3])

[RO2N] = (B06*R85*[OH]*[ALK4] + B15*R86*[OH]*[ALK7]) /
         (R88*[NO] + R89*[HO2] + R90*[RO2] + R91*[RCO3])

[RO2P] = (0.14*R117*[OH]*[CRES] + 0.14*R126*[OH]*[PHEN]) /
         (R119*[NO] + R120*[HO2] + R121*[RO2] + R122*[RCO3])

[BZN2] = (R128*[NO3]*[NPHE]) / (R129*[NO2] + R130*[HO2] + R131)


[BZO]  = (R118*[NO3]*[CRES] + R127*[NO3]*[PHEN])/
         (R123*[NO2] + R124*[HO2] + R125)

[MCO3] = (R51*[ALD2]*[OH] + R53*[ALD2]*[NO3] + R59*[PAN] + R69
         *[ACET] + R71*[MEK] + 0.50*R72*[MEK]*[OH] + R82*[MGLY] +
         R83*[OH]*[MGLY] + R84*[MGLY]*[NO3] + R116*[DIAL]) / (R54
         *[NO] + R55*[NO2] + R56*[HO2] + R57*[RO2] + R58*[RCO3])
```

TABLE 2-14

DIAGNOSTIC EQUATIONS FOR THE STEADY-STATE SPECIES IN THE CONDENSED MECHANISM

```
[O*SD] = R16*[O3] / (R17*[H2O] + R18)

[O]    = (R1*[NO2] + R14*[NO3] + R15*[O3] + R18*[O*SD] /
         (R2 + R3*[NO2] + R4*[NO2] + R73*[ETHE] + R77*[ALKE])

[OH]   = (2.*R17*[O*SD]*[H2O] + R20*[HONO] + R26*[NO]*[HO2] +
         R30*[O3]*[HO2] + B14*R76*[O3]*[ALKE]) / (R19*[NO] +
         R22*[NO2] + R23*[HNO3] + R24*[CO] + R25*[O3] + R29*
         [HNO4] + R41*[HCHO] + R44*[ALD2] + R53*[MEK] + R55*
         [MGLY] + R57*[ALKA] + R58*[ALKN] + R71*[ETHE] + R75*
         [ALKE] + R79*[TOLU] + R80*[AROM] + R81*[DIAL] + R83*
         [CRES]

[RO2R] = (R43*[HO2]*[HCHO] + R45*[ALD2] + R47*[NO]*[MCO3] +
         R52*[MEK] + 1.50*R53*[MEK]*[OH] + B05*R57*[ALKA]*[OH]
         + R71*[ETHE]*[OH] + R73*[ETHE]*[O] + R75*[ALKE]*[OH]
         + B12*R76*[O3]*[ALKE] + B21*R77*[ALKE]*[O] + 0.84*R79
         *[TOLU]*[OH] + 0.83*R80*[AROM]*[OH] + 0.85*R83*[CRES]
         *[OH]) / (R67*[NO] + R68*[HO2] + R69*[RO2] + R70*[MCO3])

[R2O2] = (B06*R57*[ALKA]*[OH] + 1.39*R58*[ALKN]*[OH] + R74*[NO3]
         *[ETHE] + R78*[NO3]*[ALKE]) / (R63*[NO] + R64*[HO2] +
         R65*[RO2] + R66*[MCO3])

[RO2N] = B04*R57*[ALKA]*[OH] / (R59*[NO] + R60*[HO2] + R61*[RO2]
         + R62*[MCO3])

[RO2P] = 0.14*R83*[CRES]*[OH] / (R85*[NO] + R86*[HO2] + R87*[RO2]
         + R88*[MCO3])

[BZN2] = R92*[NO3]*[NPHE] / (R93*[NO2] + R94*[HO2] + R95)

[BZO]  = R84*[NO3]*[CRES] / (R89*[NO2] + R90*[HO2] + R91)
```

2.4 Sample Problems

Four sample problems have been generated to facilitate verification of proper mechanism implementation. The first two cases are simple initial value kinetic problems that should be easy to reproduce. Constant photolytic rates and temperature are used. The emissions, dilution, and deposition rates are zero in these examples. Tables 2-15 and 2-16 summarize the inputs and outputs for Example No. 1 which employs the OZIPM mechanism. Tables 2-17 and 2-18 summarize the inputs and outputs for Example No. 2 which employs the condensed chemical mechanism.

These solutions were computed using the LSODE numerical integration procedure (Hindmarsh 1980) with a maximum step size of five minutes. Relative and absolute error control tolerances of 0.01 and 1.E-7 ppm were used. All species except water vapor were integrated (ie., no steady-state approximations). The user should verify that his solutions compare well with these solutions for each hour of the simulation. Solutions using the recommended steady-state approximations should also compare well with those shown for all of the key species.

Two sample problems using the OZIPM computer program and the 131-step mechanism are provided in Tables 2-19 and 2-20. Each table shows all of the inputs and outputs for the simulation. The examples are relatively complex photochemical box model calculations. Diurnally varying solar radiation, emission injection, dilution and entrainment of O_3 and NMOC from aloft are included. The OZIPM input data formats are described by Hugo and Whitten (1986) and, therefore, are not repeated here. Example No. 3, shown in Table 2-19, is an OZIPM "CALC" run whose output consists of concentrations as a function of time for a single set of initial concentrations. Example No. 4, shown in Table 2-20, is an OZIPM "EKMA" run where the VOC control requirement is calculated for a specific set of input data.

The chemical mechanism input to OZIPM is identical to that shown in Table 2-2 except for three minor changes. First, a water vapor concentration of 20,000 ppm (the recommended default value) has been incorporated into the rate constants for reactions 11, 17, 21, 32, and 34 instead of having OZIPM integrate the water vapor concentration. The rate constants should be adjusted to the actual water vapor concentration

for a particular application using OZIPM's RATE option. These rate constants are calculated from the following expressions:

$$K_{11} = 1.48E\text{-}06 * [H2O]$$

$$K_{17} = 3.25E{+}05 * [H2O]$$

$$K_{21} = 5.91E\text{-}09 * [H2O]$$

$$K_{32} = K_{34} = 1.19E\text{-}05 * [H2O] * EXP(2971/T)$$

Second, since OZIPM can not accommodate temperature dependent product coefficients, product coefficients appropriate for 300°K were input for reactions 85 and 86 in these examples. The user should input product coefficients for these reactions that reflect the average temperature (within ~5°C) in the simulation.

Third, a dummy reaction (No. 132) for nonreactive hydrocarbons (NRHC) has been included so that the sum of the concentrations of the individual NMOC classes equals the NMOC concentration. The reaction is needed so that the program recognizes NRHC as a species. The reaction is not essential for using the mechanism in OZIPM.

TABLE 2-15

INPUT PARAMETERS FOR TEST PROBLEM #1

Initial Concentrations (ppm):

NO	.075
NO2	.025
ALK4	.04667
ALK7	.040
ETHE	.015
PRPE	.020
TBUT	.010
TOLU	.02286
XYLE	.0075
TMBZ	.00444
HCHO	.030
ALD2	.010
CO	1.0
O3	.00001
H2O	20000.

Temperature: 298°K

Dilution Rate: 0

Emission Rates: 0

Deposition Rates: 0

Photolytic Reaction Rates (per min):

NO2	5.000E-01
NO3 to NO	1.130E+00
NO3 to NO2	1.020E+01
O3 to O	2.760E-02
O3 to O*SD	2.280E-03
HONO	9.800E-02
H2O2	4.540E-04
ROOH	4.540E-04
HCHO to HO2	1.825E-03
HCHO to H2	2.795E-03
ALD2	2.935E-04
RCHO	5.950E-04
ACET	6.700E-05
MEK	9.550E-05
GLYX	3.895E-03
MGLY	8.600E-03
DIAL	3.190E-02

TABLE 2-15 (Continued)

Product Coefficients:

B01	.190
B02	.305
B03	.163
B04	.340
B05	.445
B06	.0757
B07	.924
B08	.589
B09	1.51
B10	.0218
B11	.0313
B12	.247
B13	.351
B14	.874
B15	.197
B16	.803
B17	.825
B18	1.63

TABLE 2-16

TEST PROBLEM #1 - CONSTANT SOLAR RADIATION - 131 REACTION MECHANISM

TIME (MIN)	NO	NO2	O3	HONO	HNO3	HNO4	N2O5	NO3	OH	HO2
	H2O2	CO	HCHO	ALD2	RCHO	PAN	PPN	RO2	RCO3	ROOH
	ACET	MEK	GLYX	GPAN	MGLY	ALK4	ALK7	ALKN	ETHE	PRPE
	TBUT	TOLU	XYLE	TMBZ	DIAL	CRES	PHEN	NPHE	O*SD	O
	MCO3	PCO3	GCO3	RO2R	R2O2	RO2N	RO2P	BZN2	BZO	H2O
	CONCENTRATION (PPM)									
30.000	4.309E-02	5.044E-02	2.098E-02	1.141E-03	3.734E-03	4.191E-05	1.604E-06	4.125E-08	2.327E-07	2.049E-06
	5.511E-07	1.006E+00	3.217E-02	2.146E-02	6.582E-04	9.442E-04	8.413E-05	1.613E-06	2.641E-07	2.408E-07
	1.157E-03	2.363E-03	2.337E-04	1.389E-06	1.825E-03	4.540E-02	3.794E-02	4.979E-04	1.393E-02	1.586E-02
	5.231E-03	2.168E-02	6.074E-03	2.602E-03	1.363E-03	6.197E-04	4.006E-10	2.273E-05	9.625E-16	5.302E-10
	2.399E-07	2.382E-08	4.269E-10	1.411E-06	1.994E-07	4.001E-08	2.429E-09	4.776E-12	7.416E-10	2.000E+04
60.000	2.173E-02	6.175E-02	5.083E-02	6.574E-04	1.037E-02	8.243E-05	1.142E-05	2.334E-07	2.034E-07	3.273E-06
	2.567E-06	1.015E+00	3.427E-02	2.750E-02	1.240E-03	3.824E-03	3.757E-04	2.313E-06	4.594E-07	1.089E-06
	2.392E-03	4.857E-03	4.119E-04	7.911E-06	2.514E-03	4.400E-02	3.574E-02	1.019E-03	1.279E-02	1.208E-02
	2.058E-03	2.042E-02	4.795E-03	1.430E-03	1.439E-03	8.450E-04	5.046E-09	1.577E-04	2.332E-15	6.643E-10
	4.173E-07	4.110E-08	9.819E-10	1.970E-06	3.363E-07	6.578E-08	5.760E-09	1.511E-10	4.684E-09	2.000E+04
90.000	1.292E-02	5.956E-02	8.218E-02	3.790E-04	1.700E-02	1.148E-04	2.821E-05	5.923E-07	1.936E-07	4.719E-06
	6.981E-06	1.023E+00	3.452E-02	2.900E-02	1.646E-03	7.251E-03	7.120E-04	3.143E-06	6.731E-07	2.845E-06
	3.452E-03	6.970E-03	5.116E-04	1.784E-05	2.494E-03	4.279E-02	3.387E-02	1.457E-03	1.181E-02	9.287E-03
	6.496E-04	1.935E-02	3.873E-03	8.331E-04	1.168E-03	6.942E-04	1.899E-08	4.783E-04	3.770E-15	6.610E-10
	6.111E-07	6.030E-08	1.701E-09	2.611E-06	5.244E-07	1.005E-07	7.606E-09	1.205E-09	1.012E-08	2.000E+04
120.000	8.305E-03	5.306E-02	1.126E-01	2.593E-04	2.336E-02	1.461E-04	4.649E-05	1.094E-06	2.013E-07	6.749E-06
	1.594E-05	1.031E+00	3.377E-02	2.845E-02	1.961E-03	1.072E-02	1.073E-03	4.406E-06	9.703E-07	6.330E-06
	4.460E-03	8.957E-03	5.720E-04	3.029E-05	2.246E-03	4.160E-02	3.210E-02	1.865E-03	1.088E-02	7.031E-03
	1.554E-04	1.833E-02	3.129E-03	4.854E-04	9.478E-04	4.132E-04	3.771E-08	8.452E-04	5.163E-15	6.128E-10
	8.768E-07	9.068E-08	2.806E-09	3.575E-06	8.230E-07	1.546E-07	7.416E-09	4.428E-09	1.247E-08	2.000E+04
150.000	5.516E-03	4.482E-02	1.424E-01	1.934E-04	2.942E-02	1.800E-04	6.214E-05	1.722E-06	2.210E-07	9.830E-06
	3.464E-05	1.039E+00	3.246E-02	2.694E-02	2.220E-03	1.420E-02	1.488E-03	6.426E-06	1.415E-06	1.360E-05
	5.488E-03	1.096E-02	6.099E-04	4.550E-05	1.934E-03	4.037E-02	3.031E-02	2.271E-03	9.950E-03	5.157E-03
	2.620E-05	1.730E-02	2.489E-03	2.719E-04	8.029E-04	2.107E-04	5.065E-08	1.033E-03	6.534E-15	5.466E-10
	1.269E-06	1.413E-07	4.605E-09	5.098E-06	1.321E-06	2.425E-07	6.147E-09	1.005E-08	1.186E-08	2.000E+04

TABLE 2-16 (Continued)

TIME (MIN)	NO	NO2	O3	HONO	HNO3	HNO4	N2O5	NO3	OH	HO2
	H2O2	CO	HCHO	ALD2	RCHO	PAN	PPN	RO2	RCO3	ROOH
	ACET	MEK	GLYX	GPAN	MGLY	ALK4	ALK7	ALKN	ETHE	PRPE
	TBUT	TOLU	XYLE	TMBZ	DIAL	CRES	PHEN	NPHE	O*SD	O
	MCO3	PCO3	GCO3	RO2R	R2O2	RO2N	RO2P	BZN2	BZO	H2O
	CONCENTRATION (PPM)									
180.000	3.596E-03	3.587E-02	1.722E-01	1.468E-04	3.509E-02	2.180E-04	7.086E-05	2.447E-06	2.502E-07	1.487E-05
	7.595E-05	1.046E+00	3.075E-02	2.488E-02	2.433E-03	1.777E-02	1.992E-03	9.903E-06	2.125E-06	2.988E-05
	6.576E-03	1.305E-02	6.319E-04	6.403E-05	1.624E-03	3.904E-02	2.843E-02	2.689E-03	8.993E-03	3.621E-03
	2.888E-06	1.622E-02	1.929E-03	1.424E-04	7.076E-04	1.194E-04	5.623E-08	9.981E-04	7.900E-15	4.730E-10
	1.887E-06	2.303E-07	7.699E-09	7.677E-06	2.219E-06	3.971E-07	6.050E-09	1.724E-08	1.196E-08	2.000E+04
210.000	2.219E-03	2.666E-02	2.021E-01	1.081E-04	4.022E-02	2.588E-04	6.916E-05	3.205E-06	2.878E-07	2.376E-05
	1.764E-04	1.052E+00	2.872E-02	2.244E-02	2.602E-03	2.144E-02	2.616E-03	1.640E-05	3.374E-06	7.052E-05
	7.747E-03	1.527E-02	6.407E-04	8.644E-05	1.348E-03	3.757E-02	2.642E-02	3.123E-03	8.007E-03	2.407E-03
	1.886E-07	1.507E-02	1.441E-03	6.787E-05	6.390E-04	8.254E-05	6.449E-08	8.372E-04	9.268E-15	3.968E-10
	2.960E-06	4.006E-07	1.350E-08	1.241E-05	3.982E-06	6.913E-07	7.777E-09	2.549E-08	1.454E-08	2.000E+04
240.000	1.239E-03	1.778E-02	2.312E-01	7.277E-05	4.447E-02	2.876E-04	5.523E-05	3.824E-06	3.225E-07	3.957E-05
	4.480E-04	1.058E+00	2.636E-02	1.978E-02	2.718E-03	2.516E-02	3.375E-03	2.929E-05	5.804E-06	1.860E-04
	8.995E-03	1.759E-02	6.363E-04	1.128E-04	1.112E-03	3.596E-02	2.430E-02	3.564E-03	7.013E-03	1.509E-03
	7.149E-09	1.386E-02	1.033E-03	2.915E-05	5.784E-04	6.413E-05	9.250E-08	6.512E-04	1.061E-14	3.235E-10
	5.025E-06	7.546E-07	2.534E-08	2.168E-05	7.591E-06	1.273E-06	1.200E-08	3.544E-08	2.022E-08	2.000E+04
270.000	6.121E-04	1.033E-02	2.567E-01	4.123E-05	4.745E-02	2.603E-04	3.258E-05	3.862E-06	3.176E-07	6.166E-05
	1.165E-03	1.063E+00	2.382E-02	1.725E-02	2.773E-03	2.852E-02	4.193E-03	5.295E-05	1.085E-05	5.268E-04
	1.022E-02	1.982E-02	6.166E-04	1.400E-04	9.168E-04	3.433E-02	2.223E-02	3.968E-03	6.085E-03	9.121E-04
	1.552E-10	1.268E-02	7.259E-04	1.187E-05	5.045E-04	5.302E-05	1.699E-07	5.013E-04	1.177E-14	2.625E-10
	9.285E-06	1.514E-06	5.034E-08	3.879E-05	1.414E-05	2.284E-06	1.925E-08	4.745E-08	2.908E-08	2.000E+04
300.000	2.879E-04	5.508E-03	2.738E-01	1.982E-05	4.905E-02	1.732E-04	1.405E-05	3.110E-06	2.675E-07	7.665E-05
	2.543E-03	1.067E+00	2.150E-02	1.532E-02	2.772E-03	3.079E-02	4.858E-03	8.554E-05	2.070E-05	1.365E-03
	1.124E-02	2.165E-02	5.819E-04	1.612E-04	7.596E-04	3.294E-02	2.054E-02	4.263E-03	5.343E-03	5.732E-04
	1.000E-30	1.171E-02	5.314E-04	5.451E-06	4.117E-04	4.763E-05	3.266E-07	4.105E-04	1.256E-14	2.233E-10
	1.763E-05	3.010E-06	9.897E-08	6.305E-05	2.246E-05	3.506E-06	2.854E-08	5.852E-08	3.935E-08	2.000E+04

TABLE 2-16 (Continued)

TIME (MIN)	NO	NO2	O3	HONO	HNO3	HNO4	N2O5	NO3	OH	HO2
	H2O2	CO	HCHO	ALD2	RCHO	PAN	PPN	RO2	RCO3	ROOH
	ACET	MEK	GLYX	GPAN	MGLY	ALK4	ALK7	ALKN	ETHE	PRPE
	TBUT	TOLU	XYLE	TMBZ	DIAL	CRES	PHEN	NPHE	O*SD	O
	MCO3	CO3	GCO3	RO2R	R2O2	RO2N	RO2P	BZN2	BZO	H2O
	CONCENTRATION (PPM)									
330.000	1.420E-04	2.975E-03	2.836E-01	8.912E-06	4.987E-02	9.854E-05	5.233E-06	2.147E-06	2.217E-07	8.065E-05
	4.236E-03	1.071E+00	1.979E-02	1.401E-02	2.742E-03	3.184E-02	5.278E-03	1.220E-04	3.744E-05	2.787E-03
	1.203E-02	2.307E-02	5.407E-04	1.737E-04	6.320E-04	3.182E-02	1.922E-02	4.450E-03	4.770E-03	3.748E-04
	1.000E-30	1.095E-02	4.081E-04	2.784E-06	3.247E-04	4.832E-05	5.642E-07	3.643E-04	1.301E-14	2.031E-10
	3.186E-05	5.608E-06	1.823E-07	9.072E-05	3.127E-05	4.744E-06	4.161E-08	6.618E-08	5.091E-08	2.000E+04
360.000	9.455E-05	2.083E-03	2.887E-01	5.105E-06	5.034E-02	6.869E-05	2.808E-06	1.661E-06	2.079E-07	8.056E-05
	5.947E-03	1.074E+00	1.882E-02	1.311E-02	2.698E-03	3.182E-02	5.482E-03	1.428E-04	5.117E-05	4.720E-03
	1.268E-02	2.426E-02	4.995E-04	1.786E-04	5.335E-04	3.087E-02	1.814E-02	4.562E-03	4.305E-03	2.532E-04
	1.000E-30	1.033E-02	3.240E-04	1.551E-06	2.655E-04	5.215E-05	8.599E-07	3.465E-04	1.324E-14	1.969E-10
	4.353E-05	7.916E-06	2.534E-07	1.059E-04	3.686E-05	5.454E-06	5.449E-08	6.933E-08	6.057E-08	2.000E+04
390.000	8.302E-05	1.866E-03	2.922E-01	4.130E-06	5.071E-02	6.148E-05	2.325E-06	1.543E-06	2.115E-07	8.061E-05
	7.607E-03	1.077E+00	1.822E-02	1.239E-02	2.646E-03	3.133E-02	5.592E-03	1.478E-04	5.554E-05	6.853E-03
	1.329E-02	2.536E-02	4.615E-04	1.797E-04	4.608E-04	2.996E-02	1.713E-02	4.642E-03	3.889E-03	1.713E-04
	1.000E-30	9.756E-03	2.581E-04	8.718E-07	2.331E-04	5.362E-05	1.123E-06	3.393E-04	1.340E-14	1.968E-10
	4.709E-05	8.879E-06	2.786E-07	1.087E-04	3.911E-05	5.647E-06	6.126E-08	7.031E-08	6.465E-08	2.000E+04
420.000	8.006E-05	1.814E-03	2.951E-01	3.960E-06	5.106E-02	5.993E-05	2.250E-06	1.535E-06	2.196E-07	8.077E-05
	9.217E-03	1.079E+00	1.770E-02	1.175E-02	2.588E-03	3.071E-02	5.682E-03	1.490E-04	5.669E-05	9.014E-03
	1.389E-02	2.641E-02	4.275E-04	1.794E-04	4.087E-04	2.905E-02	1.615E-02	4.708E-03	3.506E-03	1.159E-04
	1.000E-30	9.197E-03	2.048E-04	4.905E-07	2.150E-04	5.241E-05	1.291E-06	3.339E-04	1.354E-14	1.981E-10
	4.780E-05	9.344E-06	2.865E-07	1.085E-04	4.047E-05	5.694E-06	6.376E-08	7.085E-08	6.466E-08	2.000E+04
450.000	7.820E-05	1.784E-03	2.979E-01	3.931E-06	5.141E-02	5.911E-05	2.225E-06	1.544E-06	2.284E-07	8.101E-05
	1.079E-02	1.082E+00	1.717E-02	1.114E-02	2.525E-03	3.008E-02	5.772E-03	1.491E-04	5.677E-05	1.116E-02
	1.447E-02	2.744E-02	3.967E-04	1.784E-04	3.699E-04	2.813E-02	1.519E-02	4.766E-03	3.148E-03	7.683E-05
	1.000E-30	8.649E-03	1.605E-04	2.645E-07	2.018E-04	5.019E-05	1.376E-06	3.274E-04	1.366E-14	1.994E-10
	4.759E-05	9.653E-06	2.884E-07	1.075E-04	4.153E-05	5.688E-06	6.449E-08	7.102E-08	6.335E-08	2.000E+04

TABLE 2-16 (Continued)

TIME (MIN)	NO	NO2	O3	HONO	HNO3	HNO4	N2O5	NO3	OH	HO2
	H2O2	CO	HCHO	ALD2	RCHO	PAN	PPN	RO2	RCO3	ROOH
	ACET	MEK	GLYX	GPAN	MGLY	ALK4	ALK7	ALKN	ETHE	PRPE
	TBUT	TOLU	XYLE	TMBZ	DIAL	CRES	PHEN	NPHE	O*SD	O
	MCO3	PCO3	GCO3	RO2R	R2O2	RO2N	RO2P	BZN2	BZO	H2O
	CONCENTRATION (PPM)									
480.000	7.661E-05	1.758E-03	3.004E-01	3.929E-06	5.176E-02	5.845E-05	2.210E-06	1.556E-06	2.374E-07	8.128E-05
	1.231E-02	1.084E+00	1.664E-02	1.058E-02	2.457E-03	2.946E-02	5.864E-03	1.489E-04	5.677E-05	1.329E-02
	1.505E-02	2.842E-02	3.687E-04	1.769E-04	3.412E-04	2.721E-02	1.426E-02	4.816E-03	2.816E-03	5.036E-05
	1.000E-30	8.114E-03	1.246E-04	1.393E-07	1.908E-04	4.772E-05	1.397E-06	3.191E-04	1.378E-14	2.007E-10
	4.730E-05	9.951E-06	2.890E-07	1.064E-04	4.249E-05	5.659E-06	6.454E-08	7.079E-08	6.160E-08	2.000E+04

TABLE 2-17

INPUT PARAMETERS FOR TEST PROBLEM #2

Initial Concentrations (ppm):

NO	.075
NO2	.025
ALKA	.0827
ETHE	.015
ALKE	.0294
TBUT	.010
TOLU	.02286
AROM	.01190
HCHO	.030
ALD2	.010
CO	1.0
O3	.00001
H2O	20000.

Temperature: 298°K

Dilution Rate: 0

Emission Rates: 0

Deposition Rates: 0

Photolytic Reaction Rates (per min):

NO2		5.000E-01
NO3	to NO	1.130E+00
NO3	to NO2	1.020E+01
O3	to O	2.760E-02
O3	to O*SD	2.280E-03
HONO		9.800E-02
H2O2		4.540E-04
ROOH		4.540E-04
HCHO	to HO2	1.825E-03
HCHO	to H2	2.795E-03
ALD2		2.935E-04
RCHO		5.950E-04
ACET		6.700E-05
MEK		9.550E-05
GLYX		3.895E-03
MGLY		8.600E-03
DIAL		3.190E-02

TABLE 2-17

INPUT PARAMETERS FOR TEST PROBLEM #2

Initial Concentrations (ppm):

NO	.075
NO2	.025
ALKA	.0827
ETHE	.015
ALKE	.0294
TBUT	.010
TOLU	.02286
AROM	.01190
HCHO	.030
ALD2	.010
CO	1.0
O3	.00001
H2O	20000.

Temperature: 298°K

Dilution Rate: 0

Emission Rates: 0

Deposition Rates: 0

Photolytic Reaction Rates (per min):

NO2	5.000E-01
NO3 to NO	1.130E+00
NO3 to NO2	1.020E+01
O3 to O	2.760E-02
O3 to O*SD	2.280E-03
HONO	9.800E-02
H2O2	4.540E-04
ROOH	4.540E-04
HCHO to HO2	1.825E-03
HCHO to H2	2.795E-03
ALD2	2.935E-04
RCHO	5.950E-04
ACET	6.700E-05
MEK	9.550E-05
GLYX	3.895E-03
MGLY	8.600E-03
DIAL	3.190E-02

TABLE 2-17 (Continued)

Composition:

X_C = .4286 Carbon Basis
Y_C = .6000 " "
Z_C = .6000 " "

Special Rate Constants:

R57	6.74E+03	per ppm-min
R75	5.70E+04	" "
R76	1.10E-01	" "
R77	1.54E+04	" "
R78	1.94E+02	" "
R80	5.68E+04	" "

Product Coefficients:

B01	.112
B02	.380
B03	.643
B04	.131
B05	.868
B06	.698
B07	1.57
B08	.667
B09	1.33
B10	.427
B11	.667
B12	.177
B13	.183
B14	.080
B15	.187
B16	.267
B17	.333
B18	.267
B19	.133
B20	.267
B21	.400
B22	.590
B23	.518
B24	.0597

TABLE 2-18

TEST PROBLEM #2 - CONSTANT SOLAR RADIATION - 95 REACTION MECHANISM

TIME (MIN)	NO	NO2	O3	HONO	HNO3	HNO4	N2O5	NO3	OH	HO2
	CO	HCHO	ALD2	PAN	RO2	MCO3	MEK	MGLY	ALKA	ALKN
	ETHE	ALKE	TOLU	AROM	DIAL	CRES	NPHE	O*SD	O	RO2R
	R2O2	RO2N	RO2P	BZN2	BZO	H2O				
	CONCENTRATION (PPM)									
30.000	4.262E-02	5.082E-02	2.134E-02	1.172E-03	3.857E-03	4.523E-05	1.674E-06	4.275E-08	2.435E-07	2.194E-06
	1.007E+00	3.417E-02	2.091E-02	1.031E-03	1.697E-06	2.664E-07	2.089E-03	1.630E-03	7.944E-02	4.253E-04
	1.390E-02	2.012E-02	2.165E-02	8.473E-03	1.488E-03	6.441E-04	2.412E-05	9.789E-16	5.597E-10	1.505E-06
	1.893E-07	3.544E-08	2.683E-09	5.142E-12	7.947E-10	2.000E+04				
60.000	2.066E-02	6.204E-02	5.350E-02	6.750E-04	1.102E-02	9.579E-05	1.267E-05	2.578E-07	2.212E-07	3.786E-06
	1.016E+00	3.735E-02	2.797E-02	4.409E-03	2.607E-06	4.915E-07	4.401E-03	2.410E-03	7.578E-02	8.919E-04
	1.269E-02	1.193E-02	2.031E-02	5.698E-03	1.601E-03	8.875E-04	1.772E-04	2.454E-15	7.008E-10	2.257E-06
	3.426E-07	6.343E-08	6.943E-09	1.871E-10	5.407E-09	2.000E+04				
90.000	1.184E-02	5.871E-02	8.743E-02	3.876E-04	1.831E-02	1.356E-04	3.117E-05	6.652E-07	2.167E-07	5.665E-06
	1.026E+00	3.768E-02	3.060E-02	8.645E-03	3.633E-06	7.579E-07	6.436E-03	2.504E-03	7.252E-02	1.299E-03
	1.162E-02	6.487E-03	1.913E-02	3.932E-03	1.301E-03	7.081E-04	5.440E-04	4.011E-15	6.866E-10	3.061E-06
	5.622E-07	1.032E-07	9.412E-09	1.582E-09	1.178E-08	2.000E+04				
120.000	7.477E-03	5.075E-02	1.195E-01	2.624E-04	2.525E-02	1.687E-04	4.976E-05	1.220E-06	2.275E-07	8.134E-06
	1.035E+00	3.634E-02	3.038E-02	1.305E-02	5.048E-06	1.132E-06	8.388E-03	2.310E-03	6.934E-02	1.686E-03
	1.061E-02	3.203E-03	1.800E-02	2.714E-03	1.035E-03	3.999E-04	9.308E-04	5.484E-15	6.217E-10	4.137E-06
	9.010E-07	1.646E-07	8.869E-09	5.661E-09	1.411E-08	2.000E+04				
150.000	4.803E-03	4.149E-02	1.504E-01	1.890E-04	3.170E-02	2.007E-04	6.335E-05	1.895E-06	2.495E-07	1.184E-05
	1.043E+00	3.416E-02	2.856E-02	1.746E-02	7.322E-06	1.692E-06	1.036E-02	2.015E-03	6.609E-02	2.073E-03
	9.593E-03	1.349E-03	1.687E-02	1.810E-03	8.380E-04	1.956E-04	1.095E-03	6.900E-15	5.420E-10	5.846E-06
	1.468E-06	2.676E-07	7.394E-09	1.267E-08	1.310E-08	2.000E+04				

TABLE 2-18 (Continued)

TIME (MIN)	NO	NO2	O3	HONO	HNO3	HNO4	N2O5	NO3	OH	HO2
	CO	HCHO	ALD2	PAN	RO2	MCO3	MEK	MGLY	ALKA	ALKN
	ETHE	ALKE	TOLU	AROM	DIAL	CRES	NPHE	O*SD	O	RO2R
	R2O2	RO2N	RO2P	BZN2	BZO	H2O				
	CONCENTRATION (PPM)									
180.000	3.017E-03	3.190E-02	1.807E-01	1.389E-04	3.754E-02	2.380E-04	6.802E-05	2.639E-06	2.847E-07	1.828E-05
	1.051E+00	3.152E-02	2.573E-02	2.186E-02	1.159E-05	2.609E-06	1.243E-02	1.688E-03	6.263E-02	2.473E-03
	8.564E-03	4.880E-04	1.568E-02	1.150E-03	7.001E-04	1.108E-04	1.016E-03	8.288E-15	4.583E-10	9.047E-06
	2.539E-06	4.610E-07	7.615E-09	2.128E-08	1.346E-08	2.000E+04				
210.000	1.765E-03	2.246E-02	2.108E-01	9.818E-05	4.264E-02	2.794E-04	6.140E-05	3.372E-06	3.304E-07	3.047E-05
	1.057E+00	2.866E-02	2.249E-02	2.631E-02	2.040E-05	4.288E-06	1.466E-02	1.371E-03	5.885E-02	2.893E-03
	7.508E-03	1.479E-04	1.441E-02	6.804E-04	6.002E-04	7.692E-05	8.232E-04	9.670E-15	3.761E-10	1.563E-05
	4.764E-06	8.595E-07	1.043E-08	3.128E-08	1.697E-08	2.000E+04				
240.000	9.101E-04	1.396E-02	2.395E-01	6.135E-05	4.661E-02	2.941E-04	4.336E-05	3.816E-06	3.614E-07	5.155E-05
	1.063E+00	2.572E-02	1.929E-02	3.065E-02	3.847E-05	7.685E-06	1.697E-02	1.084E-03	5.483E-02	3.315E-03
	6.464E-03	3.704E-05	1.310E-02	3.746E-04	5.154E-04	5.958E-05	6.269E-04	1.099E-14	3.031E-10	2.920E-05
	9.258E-06	1.656E-06	1.680E-08	4.339E-08	2.387E-08	2.000E+04				
270.000	4.303E-04	7.692E-03	2.623E-01	3.144E-05	4.911E-02	2.302E-04	2.210E-05	3.505E-06	3.276E-07	7.299E-05
	1.067E+00	2.298E-02	1.667E-02	3.412E-02	6.719E-05	1.449E-05	1.909E-02	8.444E-04	5.109E-02	3.674E-03
	5.554E-03	8.366E-06	1.190E-02	2.059E-04	4.243E-04	4.943E-05	4.825E-04	1.203E-14	2.502E-10	5.131E-05
	1.586E-05	2.810E-06	2.536E-08	5.563E-08	3.296E-08	2.000E+04				
300.000	2.107E-04	4.187E-03	2.765E-01	1.444E-05	5.040E-02	1.412E-04	9.119E-06	2.661E-06	2.697E-07	8.216E-05
	1.071E+00	2.089E-02	1.482E-02	3.607E-02	1.005E-04	2.636E-05	2.076E-02	6.606E-04	4.810E-02	3.919E-03
	4.858E-03	1.879E-06	1.096E-02	1.232E-04	3.342E-04	4.563E-05	3.992E-04	1.268E-14	2.214E-10	7.777E-05
	2.270E-05	3.991E-06	3.537E-08	6.405E-08	4.240E-08	2.000E+04				
330.000	1.305E-04	2.762E-03	2.842E-01	7.816E-06	5.107E-02	9.464E-05	4.628E-06	2.056E-06	2.421E-07	8.360E-05
	1.074E+00	1.966E-02	1.350E-02	3.656E-02	1.253E-04	3.864E-05	2.207E-02	5.271E-04	4.572E-02	4.070E-03
	4.325E-03	5.129E-07	1.024E-02	8.088E-05	2.688E-04	4.643E-05	3.592E-04	1.304E-14	2.108E-10	9.752E-05
	2.770E-05	4.839E-06	4.580E-08	6.726E-08	5.033E-08	2.000E+04				

TABLE 2-18 (Continued)

TIME (MIN)	NO	NO2	O3	HONO	HNO3	HNO4	N2O5	NO3	OH	HO2
	CO	HCHO	ALD2	PAN	RO2	MCO3	MEK	MGLY	ALKA	ALKN
	ETHE	ALKE	TOLU	AROM	DIAL	CRES	NPHE	O*SD	O	RO2R
	R2O2	RO2N	RO2P	BZN2	BZO	H2O				
	CONCENTRATION (PPM)									
360.000	1.050E-04	2.294E-03	2.894E-01	5.600E-06	5.157E-02	7.865E-05	3.399E-06	1.831E-06	2.393E-07	8.379E-05
	1.077E+00	1.897E-02	1.242E-02	3.627E-02	1.360E-04	4.508E-05	2.326E-02	4.278E-04	4.356E-02	4.180E-03
	3.864E-03	1.278E-07	9.585E-03	5.375E-05	2.295E-04	4.729E-05	3.369E-04	1.328E-14	2.091E-10	1.058E-04
	3.014E-05	5.235E-06	5.300E-08	6.755E-08	5.489E-08	2.000E+04				
390.000	9.886E-05	2.190E-03	2.937E-01	5.124E-06	5.201E-02	7.512E-05	3.205E-06	1.811E-06	2.470E-07	8.384E-05
	1.079E+00	1.845E-02	1.146E-02	3.567E-02	1.382E-04	4.613E-05	2.438E-02	3.558E-04	4.147E-02	4.271E-03
	3.446E-03	3.186E-08	8.968E-03	3.553E-05	2.083E-04	4.613E-05	3.214E-04	1.347E-14	2.106E-10	1.072E-04
	3.094E-05	5.345E-06	5.548E-08	6.673E-08	5.546E-08	2.000E+04				
420.000	9.682E-05	2.165E-03	2.975E-01	5.080E-06	5.245E-02	7.426E-05	3.221E-06	1.842E-06	2.573E-07	8.387E-05
	1.081E+00	1.792E-02	1.060E-02	3.500E-02	1.383E-04	4.574E-05	2.547E-02	3.030E-04	3.941E-02	4.351E-03
	3.062E-03	7.484E-09	8.369E-03	2.311E-05	1.951E-04	4.383E-05	3.069E-04	1.365E-14	2.128E-10	1.069E-04
	3.127E-05	5.369E-06	5.573E-08	6.557E-08	5.421E-08	2.000E+04				
450.000	9.552E-05	2.152E-03	3.012E-01	5.125E-06	5.289E-02	7.384E-05	3.270E-06	1.881E-06	2.681E-07	8.389E-05
	1.083E+00	1.735E-02	9.834E-03	3.433E-02	1.377E-04	4.513E-05	2.652E-02	2.639E-04	3.737E-02	4.424E-03
	2.709E-03	1.700E-09	7.787E-03	1.476E-05	1.848E-04	4.127E-05	2.922E-04	1.382E-14	2.150E-10	1.063E-04
	3.143E-05	5.363E-06	5.528E-08	6.413E-08	5.244E-08	2.000E+04				
480.000	9.427E-05	2.139E-03	3.046E-01	5.180E-06	5.333E-02	7.339E-05	3.316E-06	1.920E-06	2.792E-07	8.391E-05
	1.085E+00	1.676E-02	9.141E-03	3.368E-02	1.370E-04	4.456E-05	2.752E-02	2.341E-04	3.536E-02	4.487E-03
	2.386E-03	3.828E-10	7.224E-03	9.253E-06	1.754E-04	3.875E-05	2.771E-04	1.397E-14	2.171E-10	1.054E-04
	3.150E-05	5.337E-06	5.461E-08	6.245E-08	5.056E-08	2.000E+04				

TABLE 2-19. EXAMPLE #3

```
****************************************
*                                      *
*   OZONE ISOPLETH PLOTTING PACKAGE    *
*      WITH OPTIONAL MECHANISMS        *
*                                      *
*              O Z I P M               *
*                                      *
*             VERSION 3.1              *
*                                      *
*           SEPTEMBER, 1985            *
*                                      *
****************************************
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THE INPUTS FOR THIS RUN ARE

```
TITL
      TEST PROBLEM #3 - OZIPM "CALC" RUN - 131 REACTION MECHANISM
MECH            132.       17.       13.        0.       303.
        1.       13.       14.       15.       16.       20.       35.
       42.       46.       47.       52.       61.       69.       71.
       73.       82.      114.
ALK4       ALK7       ETHE       PRPE       TBUT       TOLU       XYLE
TMBZ       HCHO       ALD2       RCHO       MEK        NRHC
 4.5        7.0        2.0        3.0        4.0        7.0        8.0
 9.0        1.0        2.0        3.0        4.0        1.0
NO2        HV      1  1.NO       1. O                          1.00E 00     0.
O                  2  1.O3                                     4.87E+07 -1282.
O       NO2        3  1.NO                                     1.37E+04     0.
O       NO2        4  1.NO3                                    3.29E+03  -894.
NO      O3         5  1.NO2                                    2.68E+01  1370.
NO2     O3         6  1.NO3                                    4.77E-02  2450.
NO      NO3        7  2.NO2                                    2.75E+04  -252.
NO      NO         8  2.NO2                                    1.50E-04  -529.
NO2     NO3        9  1.N2O5                                   1.71E+03  -273.
N2O5               10  1.NO2      1. NO3                      2.08E+00 11379.
N2O5               11  2.HNO3                                  3.00E-02     0.
NO2     NO3        12  1.NO       1. NO2                      5.98E-01  1229.
NO3        HV      13  1.NO                                    1.00E 00     0.
NO3        HV      14  1.NO2      1. O                        1.00E 00     0.
O3         HV      15  1.O                                     1.00E 00     0.
O3         HV      16  1.O*SD                                  1.00E 00     0.
O*SD               17  2.OH                                    6.50E+09     0.
O*SD               18  1.O                                     4.32E+10     0.
NO      OH         19  1.HONO                                  9.75E+03  -833.
HONO       HV      20  1.NO       1. OH                       1.00E 00     0.
NO2                21  1.HONO    -1. NO2       1. HNO3       1.17E-04     0.
NO2     OH         22  1.HNO3                                  1.68E+04  -737.
HNO3    OH         23  1.NO3                                   1.89E+02  -778.
CO      OH         24  1.HO2                                   3.22E+02     0.
O3      OH         25  1.HO2                                   1.00E+02   942.
NO      HO2        26  1.NO2      1. OH                       1.22E+04  -240.
NO2     HO2        27  1.HNO4                                  2.02E+03  -773.
HNO4               28  1.NO2      1. HO2                      4.93E+00 10103.
HNO4    OH         29  1.NO2                                   5.91E+03     0.
O3      HO2        30  1.OH                                    2.96E+00   579.
HO2     HO2        31  1.H2O2                                  4.46E+03  -771.
HO2     HO2        32  1.H2O2                                  5.08E+03 -2971.
NO3     HO2        33  1.HNO3                                  4.46E+03  -771.
NO3     HO2        34  1.HNO3                                  5.08E+03 -2971.
H2O2       HV      35  2.OH                                    1.00E 00     0.
H2O2    OH         36  1.HO2                                   2.45E+03   187.
RO2     NO         37  1.NO                                    1.14E+04  -180.
RCO3    NO         38  1.NO                                    1.14E+04  -180.
RCO3    NO2        39  1.NO2                                   7.57E+03  -180.
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TABLE 2-19 (CONTINUED)

THE INPUTS FOR THIS RUN ARE

```
RO2   HO2          40   1.HO2                                    4.43E+03     0.
RCO3  HO2          41   1.HO2                                    4.43E+03     0.
ROOH      HV       42   1.HO2        1. OH                       1.00E 00     0.
RO2   RO2          43                                            1.48E+00     0.
RO2   RCO3         44                                            4.43E+03     0.
RCO3  RCO3         45                                            3.69E+03     0.
HCHO      HV       46   2.HO2        1. CO                       1.00E 00     0.
HCHO      HV       47   1.CO                                     1.00E 00     0.
HCHO  OH           48   1.HO2        1. CO                       1.33E+04     0.
HCHO  NO3          49   1.HNO3       1. HO2       1. CO          8.82E-01  2060.
HCHO  HO2          50   1.RO2R       1. RO2                      1.48E+01     0.
ALD2  OH           51   1.MCO3       1. RCO3                     2.36E+04  -250.
ALD2      HV       52   1.CO  *      1. HCHO      1. HO2         1.00E 00     0.
   1. RO2R      1. RO2
ALD2  NO3          53   1.HNO3       1. MCO3      1. RCO3        3.69E+00  1427.
MCO3  NO           54   1.NO2 *      1. HCHO      1. RO2R        1.14E+04  -180.
   1. RO2
MCO3  NO2          55   1.PAN                                    7.57E+03  -180.
MCO3  HO2          56   1.ROOH       1. HCHO                     4.43E+03     0.
MCO3  RO2          57   .5HO2        1. HCHO      1. RO2         4.43E+03     0.
MCO3  RCO3         58   1.HO2        1. HCHO      1. RCO3        3.69E+03     0.
PAN                59   1.MCO3       1. NO2       1. RCO3        2.21E-02 13542.
RCHO  OH           60   1.RCO3       1. PCO3                     2.93E+04  -252.
RCHO      HV       61   1.ALD2*      1. HO2       1. CO          1.00E 00     0.
   1. RO2R      1. RO2
RCHO  NO3          62   1.HNO3       1. PCO3      1. RCO3        3.63E+00  1432.
PCO3  NO           63   1.NO2 *      1. ALD2      1. RO2R        1.14E+04  -180.
   1. RO2
PCO3  NO2          64   1.PPN                                    7.57E+03  -180.
PCO3  HO2          65   1.ROOH       1. ALD2                     4.43E+03     0.
PCO3  RO2          66   .5HO2        1. ALD2      1. RO2         4.43E+03     0.
PCO3  RCO3         67   1.HO2        1. ALD2      1. RCO3        3.69E+03     0.
PPN                68   1.PCO3       1. NO2       1. RCO3        2.21E-02 13542.
ACET      HV       69   1.MCO3*      1. HCHO      1. RCO3        1.00E 00     0.
   1. RO2R      1. RO2
ACET  OH           70   1.MGLY       1. RO2R      1. RO2         3.39E+02  1125.
MEK       HV       71   1.MCO3*      1. ALD2      1. RCO3        1.00E 00     0.
   1. RO2R      1. RO2
MEK   OH           72  1.5RO2R*    1.5 RO2       .5 MCO3        1.46E+03   745.
   .5 ALD2      .5 HCHO      .5 PCO3      1. RCO3
GLYX      HV       73  .13HCHO   1.87 CO                        1.00E 00     0.
GLYX  OH           74  .63HO2 *  1.26 CO       .37 GCO3         1.70E+04     0.
  .37 RCO3
GLYX  NO3          75   1.HNO3*    .63 HO2     1.26 CO          8.88E-01  2058.
  .37 GCO3     .37 RCO3
GCO3  NO2          76   1.GPAN                                   7.57E+03  -180.
GCO3  NO           77   1.NO2        1. HO2       1. CO          1.14E+04  -180.
GPAN               78   1.GCO3       1. NO2       1. RCO3        2.21E-02 13542.
GCO3  HO2          79   1.ROOH       1. CO                       4.43E+03     0.
GCO3  RO2          80   .5HO2        1. CO        1. RO2         4.43E+03     0.
```

THE INPUTS FOR THIS RUN ARE

```
GCO3  RCO3      81   1.HO2      1. CO       1. RCO3    3.69E+03     0.
MGLY      HV    82   1.MCO3*    1. HO2      1. CO      1.00E 00     0.
   1. RCO3
MGLY  OH        83   1.MCO3     1. CO       1. RCO3    2.51E+04     0.
MGLY  NO3       84   1.HNO3*    1. MCO3     1. CO      3.69E+00  1427.
   1. RCO3
ALK4  OH        85  .19HCHO*   .31 ALD2    .17 RCHO    4.76E+03   353.
  .34 ACET    .44 MEK     .07 RO2N    .93 RO2R     .6 R2O2    1.6 RO2
ALK7  OH        86  .02HCHO*   .03 ALD2    .25 RCHO    9.11E+03   288.
  .36 ACET    .88 MEK     .18 RO2N    .82 RO2R    .84 R2O2   1.84 RO2
ALKN  OH        87   1.NO2 *   .15 MEK    1.05 RCHO    3.00E+03   709.
  .48 ALD2    .16 HCHO   1.39 R2O2   1.39 RO2
RO2N  NO        88   1.ALKN                           1.14E+04  -180.
RO2N  HO2       89   1.ROOH     1. MEK                4.43E+03     0.
RO2N  RO2       90   1.RO2       .5 HO2      1. MEK    1.48E+00     0.
RO2N  RCO3      91   1.RCO3      .5 HO2      1. MEK    4.43E+03     0.
R2O2  NO        92   1.NO2                            1.14E+04  -180.
R2O2  HO2       93   1.ROOH                           4.43E+03     0.
R2O2  RO2       94   1.RO2                            1.48E+00     0.
R2O2  RCO3      95   1.RCO3                           4.43E+03     0.
RO2R  NO        96   1.NO2      1. HO2                1.14E+04  -180.
RO2R  HO2       97   1.ROOH                           4.43E+03     0.
RO2R  RO2       98   .5HO2      1. RO2                1.48E+00     0.
RO2R  RCO3      99   .5HO2      1. RCO3               4.43E+03     0.
ETHE  OH       100   1.RO2R*    1. RO2    1.56 HCHO   1.26E+04  -411.
  .22 ALD2
ETHE  O3       101   1.HCHO     .12 HO2     .42 CO     2.57E-03  2634.
ETHE  O        102   1.HCHO*    1. HO2      1. CO      1.08E+03   792.
   1. RO2R     1. RO2
ETHE  NO3      103   1.NO2 *    2. HCHO     1. R2O2    1.62E-01  2923.
   1. RO2
PRPE  OH       104   1.RO2R*    1. HCHO     1. ALD2    3.89E+04  -504.
   1. RO2
PRPE  O3       105  .64HCHO*    .5 ALD2     .28 CO     1.67E-02  2105.
  .06 OH      .17 HO2      .13 RO2R    .13 RO2
PRPE  O        106   .6ACET*    .4 HCHO     .2 ALD2    5.88E+03   324.
   .2 HO2      .6 RO2R     .4 CO       .6 RO2
PRPE  NO3      107   1.NO2 *    1. HCHO     1. ALD2    1.12E+01  1935.
   1. R2O2     1. RO2
TBUT  OH       108   1.RO2R     2. ALD2     1. RO2     9.42E+04  -549.
TBUT  O3       109   1.ALD2*    .15 CO      .27 RO2R   2.96E-01  1137.
  .12 OH      .21 HO2      .27 RO2     .30 HCHO
TBUT  O        110   1.MEK       .4 HO2                3.45E+04   -10.
TBUT  NO3      111   1.NO2 *    2. ALD2     1. R2O2    5.61E+02   975.
   1. RO2
TOLU  OH       112  .16CRES*   .16 HO2     .84 RO2R    9.14E+03  -322.
   .4 DIAL    .84 RO2     .144 MGLY   .114 GLYX
DIAL  OH       113   1.PCO3     1. RCO3               4.43E+04     0.
DIAL      HV   114   1.HO2 *    1. CO       1. MCO3    1.00E 00     0.
   1. RCO3
```

TABLE 2-19 (CONTINUED)

THE INPUTS FOR THIS RUN ARE

```
XYLE  OH       115  .17CRES*   .17 HO2     .83 RO2R    3.62E+04  -116.
  .83 RO2     .65 DIAL   .316 MGLY   .095 GLYX
TMBZ  OH       116  .17CRES*   .17 HO2     .83 RO2R    9.16E+04     0.
  .83 RO2     .49 DIAL    .86 MGLY
CRES  OH       117   .2MGLY*   .15 RO2P    .85 RO2R    5.91E+04     0.
   1. RO2
CRES  NO3      118   1.HNO3     1. BZO                  3.25E+04     0.
RO2P  NO       119   1.NPHE                             1.14E+04  -180.
RO2P  HO2      120   1.ROOH                             4.43E+03     0.
RO2P  RO2      121   .5HO2      1. RO2                  1.48E+00     0.
RO2P  RCO3     122   .5HO2      1. RCO3                 4.43E+03     0.
BZO   NO2      123   1.NPHE                             2.22E+04     0.
BZO   HO2      124   1.PHEN                             4.43E+03     0.
BZO            125   1.PHEN                             6.00E-02     0.
PHEN  OH       126   .2GLYX*   .15 RO2P    .85 RO2R    4.14E+04     0.
   1. RO2
PHEN  NO3      127   1.HNO3     1. BZO                  5.62E+03     0.
NPHE  NO3      128   1.HNO3     1. BZN2                 5.62E+03     0.
BZN2  NO2      129                                      2.22E+04     0.
BZN2  HO2      130   1.NPHE                             4.43E+03     0.
BZN2           131   1.NPHE                             6.00E-02     0.
NRHC           132   1.NRHC                             1.00E-10     0.
ZENITH          17.
1.          1.0        1.0        1.0        1.0        1.0        1.0
   1.0      1.0        1.0        1.0
13.         2.3        2.3        2.3        2.3        2.4        2.6
   2.8      3.3        4.1        2.8
14.         20.        20.        21.        21.        22.        23.
   25.      30.        36.        26.
15.      5.52E-02   5.53E-02   5.56E-02   5.61E-02   5.71E-02   5.99E-02
  6.45E-02 7.43E-02   8.90E-02   6.60E-02
16.      4.56E-03   4.45E-03   4.12E-03   3.56E-03   2.86E-03   2.06E-03
  1.26E-03 5.98E-04   2.80E-04   1.54E-04
20.         .20        .20        .20        .20        .19        .19
   .19      .18        .18        .19
35.      9.08E-04   9.03E-04   8.82E-04   8.45E-04   7.91E-04   7.18E-04
  6.25E-04 5.12E-04   4.31E-04   3.83E-04
42.      9.08E-04   9.03E-04   8.82E-04   8.45E-04   7.91E-04   7.18E-04
  6.25E-04 5.12E-04   4.31E-04   3.83E-04
46.      3.65E-03   3.62E-03   3.53E-03   3.36E-03   3.11E-03   2.77E-03
  2.33E-03 1.81E-03   1.41E-03   1.10E-03
47.      5.59E-03   5.57E-03   5.50E-03   5.38E-03   5.19E-03   4.91E-03
  4.51E-03 3.97E-03   3.57E-03   3.43E-03
52.      5.87E-04   5.79E-04   5.51E-04   5.01E-04   4.36E-04   3.53E-04
  2.58E-04 1.63E-04   1.01E-04   5.98E-05
61.      1.19E-03   1.18E-03   1.14E-03   1.08E-03   9.94E-04   8.75E-04
  7.26E-04 5.53E-04   4.27E-04   3.31E-04
69.      1.34E-04   1.32E-04   1.27E-04   1.18E-04   1.06E-04   8.97E-05
  7.05E-05 4.98E-05   3.55E-05   2.49E-05
71.      1.91E-04   1.89E-04   1.82E-04   1.69E-04   1.51E-04   1.28E-04
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TABLE 2-19 (CONTINUED)

THE INPUTS FOR THIS RUN ARE

```
  1.01E-04  7.11E-05  5.07E-05  3.56E-05
73.         7.79E-03  7.81E-03  7.87E-03  7.97E-03  8.17E-03  8.46E-03
  8.97E-03  9.88E-03  1.09E-02  9.73E-03
82.         1.72E-02  1.72E-02  1.74E-02  1.76E-02  1.80E-02  1.87E-02
  1.98E-02  2.17E-02  2.37E-02  2.14E-02
114.        6.38E-02  6.36E-02  6.29E-02  6.15E-02  5.95E-02  5.66E-02
  5.25E-02  4.70E-02  4.29E-02  4.27E-02
PLAC          34.057    118.24       8.0      1986.       6.0       21.
LOS ANGELES, CA
DILU              250.      1500.      800.      1400.
REAC               13.       .25
      .210       .280       .030       .060       .040       .160       .060
      .040       .030       .020       .000       .000       .070
INIT               2.
CO         HONO
1.00       .0005
EMIS              -4.       .15        .10        .10        .05
       .25       .167       .167       .083
TRAN                         .080      -13.       -13.
      .001       .210       .180       .015       .030       .005       .070
      .040       .020       .050       .030       .000       .000       .350
      .050       .210       .180       .015       .030       .005       .070
      .040       .020       .050       .030       .000       .000       .350
SPEC               2.
O3         NO2
CALC            2.00       0.20         1.
```

TABLE 2-19 (CONTINUED)

	THE REACTIONS										RATE CONSTANT	ACT. ENERGY(K)
1	NO2			=		NO	+	O			1.000E+00	0.000E-01
2	O			=		O3					4.870E+07	-1.282E+03
3	O	+	NO2	=		NO					1.370E+04	0.000E-01
4	O	+	NO2	=		NO3					3.290E+03	-8.940E+02
5	NO	+	O3	=		NO2					2.680E+01	1.370E+03
6	NO2	+	O3	=		NO3					4.770E-02	2.450E+03
7	NO	+	NO3	=	2	NO2					2.750E+04	-2.520E+02
8	NO	+	NO	=	2	NO2					1.500E-04	-5.290E+02
9	NO2	+	NO3	=		N2O5					1.710E+03	-2.730E+02
10	N2O5			=		NO2	+	NO3			2.080E+00	1.138E+04
11	N2O5			=	2	HNO3					3.000E-02	0.000E-01
12	NO2	+	NO3	=		NO	+	NO2			5.980E-01	1.229E+03
13	NO3			=		NO					1.000E+00	0.000E-01
14	NO3			=		NO2	+	O			1.000E+00	0.000E-01
15	O3			=		O					1.000E+00	0.000E-01
16	O3			=		O*SD					1.000E+00	0.000E-01
17	O*SD			=	2	OH					6.500E+09	0.000E-01
18	O*SD			=		O					4.320E+10	0.000E-01
19	NO	+	OH	=		HONO					9.750E+03	-8.330E+02
20	HONO			=		NO	+	OH			1.000E+00	0.000E-01
21	NO2			=		HONO	-	NO2	+	HNO3	1.170E-04	0.000E-01
22	NO2	+	OH	=		HNO3					1.680E+04	-7.370E+02
23	HNO3	+	OH	=		NO3					1.890E+02	-7.780E+02
24	CO	+	OH	=		HO2					3.220E+02	0.000E-01
25	O3	+	OH	=		HO2					1.000E+02	9.420E+02
26	NO	+	HO2	=		NO2	+	OH			1.220E+04	-2.400E+02
27	NO2	+	HO2	=		HNO4					2.020E+03	-7.730E+02
28	HNO4			=		NO2	+	HO2			4.930E+00	1.010E+04
29	HNO4	+	OH	=		NO2					5.910E+03	0.000E-01
30	O3	+	HO2	=		OH					2.960E+00	5.790E+02
31	HO2	+	HO2	=		H2O2					4.460E+03	-7.710E+02
32	HO2	+	HO2	=		H2O2					5.080E+03	-2.971E+03
33	NO3	+	HO2	=		HNO3					4.460E+03	-7.710E+02
34	NO3	+	HO2	=		HNO3					5.080E+03	-2.971E+03
35	H2O2			=	2	OH					1.000E+00	0.000E-01
36	H2O2	+	OH	=		HO2					2.450E+03	1.870E+02
37	RO2	+	NO	=		NO					1.140E+04	-1.800E+02
38	RCO3	+	NO	=		NO					1.140E+04	-1.800E+02
39	RCO3	+	NO2	=		NO2					7.570E+03	-1.800E+02
40	RO2	+	HO2	=		HO2					4.430E+03	0.000E-01
41	RCO3	+	HO2	=		HO2					4.430E+03	0.000E-01
42	ROOH			=		HO2	+	OH			1.000E+00	0.000E-01
43	RO2	+	RO2	=							1.480E+00	0.000E-01
44	RO2	+	RCO3	=							4.430E+03	0.000E-01
45	RCO3	+	RCO3	=							3.690E+03	0.000E-01
46	HCHO			=	2	HO2	+	CO			1.000E+00	0.000E-01
47	HCHO			=		CO					1.000E+00	0.000E-01
48	HCHO	+	OH	=		HO2	+	CO			1.330E+04	0.000E-01
49	HCHO	+	NO3	=		HNO3	+	HO2	+	CO	8.820E-01	2.060E+03
50	HCHO	+	HO2	=		RO2R	+	RO2			1.480E+01	0.000E-01

TABLE 2-19 (CONTINUED)

	THE REACTIONS														RATE CONSTANT	ACT. ENERGY(K)
51	ALD2	+	OH	=		MCO3	+	RCO3							2.360E+04	-2.500E+02
52	ALD2			=		CO	+	HCHO	+	HO2	+	RO2R			1.000E+00	0.000E-01
				+		RO2										
53	ALD2	+	NO3	=		HNO3	+	MCO3	+	RCO3					3.690E+00	1.427E+03
54	MCO3	+	NO	=		NO2	+	HCHO	+	RO2R	+	RO2			1.140E+04	-1.800E+02
55	MCO3	+	NO2	=		PAN									7.570E+03	-1.800E+02
56	MCO3	+	HO2	=		ROOH	+	HCHO							4.430E+03	0.000E-01
57	MCO3	+	RO2	=	0.5	HO2	+	HCHO	+	RO2					4.430E+03	0.000E-01
58	MCO3	+	RCO3	=		HO2	+	HCHO	+	RCO3					3.690E+03	0.000E-01
59	PAN			=		MCO3	+	NO2	+	RCO3					2.210E-02	1.354E+04
60	RCHO	+	OH	=		RCO3	+	PCO3							2.930E+04	-2.520E+02
61	RCHO			=		ALD2	+	HO2	+	CO	+	RO2R			1.000E+00	0.000E-01
				+		RO2										
62	RCHO	+	NO3	=		HNO3	+	PCO3	+	RCO3					3.630E+00	1.432E+03
63	PCO3	+	NO	=		NO2	+	ALD2	+	RO2R	+	RO2			1.140E+04	-1.800E+02
64	PCO3	+	NO2	=		PPN									7.570E+03	-1.800E+02
65	PCO3	+	HO2	=		ROOH	+	ALD2							4.430E+03	0.000E-01
66	PCO3	+	RO2	=	0.5	HO2	+	ALD2	+	RO2					4.430E+03	0.000E-01
67	PCO3	+	RCO3	=		HO2	+	ALD2	+	RCO3					3.690E+03	0.000E-01
68	PPN			=		PCO3	+	NO2	+	RCO3					2.210E-02	1.354E+04
69	ACET			=		MCO3	+	HCHO	+	RCO3	+	RO2R			1.000E+00	0.000E-01
				+		RO2										
70	ACET	+	OH	=		MGLY	+	RO2R	+	RO2					3.390E+02	1.125E+03
71	MEK			=		MCO3	+	ALD2	+	RCO3	+	RO2R			1.000E+00	0.000E-01
				+		RO2										
72	MEK	+	OH	=	1.5	RO2R	+	1.5	RO2	+	0.5	MCO3	+	0.5	ALD2	1.460E+03	7.450E+02
				+	0.5	HCHO	+	0.5	PCO3	+		RCO3				
73	GLYX			=	0.13	HCHO	+	1.87	CO						1.000E+00	0.000E-01
74	GLYX	+	OH	=	0.63	HO2	+	1.26	CO	+	0.37	GCO3	+	0.37	RCO3	1.700E+04	0.000E-01
75	GLYX	+	NO3	=		HNO3	+	0.63	HO2	+	1.26	CO	+	0.37	GCO3	8.880E-01	2.058E+03
				+	0.37	RCO3										
76	GCO3	+	NO2	=		GPAN									7.570E+03	-1.800E+02
77	GCO3	+	NO	=		NO2	+	HO2	+	CO					1.140E+04	-1.800E+02
78	GPAN			=		GCO3	+	NO2	+	RCO3					2.210E-02	1.354E+04
79	GCO3	+	HO2	=		ROOH	+	CO							4.430E+03	0.000E-01
80	GCO3	+	RO2	=	0.5	HO2	+	CO	+	RO2					4.430E+03	0.000E-01
81	GCO3	+	RCO3	=		HO2	+	CO	+	RCO3					3.690E+03	0.000E-01
82	MGLY			=		MCO3	+	HO2	+	CO	+	RCO3			1.000E+00	0.000E-01
83	MGLY	+	OH	=		MCO3	+	CO	+	RCO3					2.510E+04	0.000E-01
84	MGLY	+	NO3	=		HNO3	+	MCO3	+	CO	+	RCO3			3.690E+00	1.427E+03
85	ALK4	+	OH	=	0.19	HCHO	+	0.31	ALD2	+	0.17	RCHO	+	0.34	ACET	4.760E+03	3.530E+02
				+	0.44	MEK	+	0.07	RO2N	+	0.93	RO2R	+	0.60	R2O2		
				+	1.6	RO2										
86	ALK7	+	OH	=	. 2	HCHO	+	. 3	ALD2	+	0.25	RCHO	+	0.36	ACET	9.110E+03	2.880E+02
				+	0.88	MEK	+	0.18	RO2N	+	0.82	RO2R	+	0.84	R2O2		
				+	1.84	RO2										
87	ALKN	+	OH	=		NO2	+	0.15	MEK	+	1. 5	RCHO	+	0.48	ALD2	3.000E+03	7.090E+02
				+	0.16	HCHO	+	1.39	R2O2	+	1.39	RO2				
88	RO2N	+	NO	=		ALKN										1.140E+04	-1.800E+02
89	RO2N	+	HO2	=		ROOH	+		MEK							4.430E+03	0.000E-01

TABLE 2-19 (CONTINUED)

THE REACTIONS														RATE CONSTANT	ACT. ENERGY(K)
90	RO2N	+	RO2	=		RO2	+	0.5	HO2	+		MEK		1.480E+00	0.000E-01
91	RO2N	+	RCO3	=		RCO3	+	0.5	HO2	+		MEK		4.430E+03	0.000E-01
92	R2O2	+	NO	=		NO2								1.140E+04	-1.800E+02
93	R2O2	+	HO2	=		ROOH								4.430E+03	0.000E-01
94	R2O2	+	RO2	=		RO2								1.480E+00	0.000E-01
95	R2O2	+	RCO3	=		RCO3								4.430E+03	0.000E-01
96	RO2R	+	NO	=		NO2	+		HO2					1.140E+04	-1.800E+02
97	RO2R	+	HO2	=		ROOH								4.430E+03	0.000E-01
98	RO2R	+	RO2	=	0.5	HO2	+		RO2					1.480E+00	0.000E-01
99	RO2R	+	RCO3	=	0.5	HO2	+		RCO3					4.430E+03	0.000E-01
100	ETHE	+	OH	=		RO2R	+		RO2	+	1.56	HCHO	+ 0.22 ALD2	1.260E+04	-4.110E+02
101	ETHE	+	O3	=		HCHO	+	0.12	HO2	+	0.42	CO		2.570E-03	2.634E+03
102	ETHE	+	O	=		HCHO	+		HO2	+		CO	+ RO2R	1.080E+03	7.920E+02
				+		RO2									
103	ETHE	+	NO3	=		NO2	+	2	HCHO	+		R2O2	+ RO2	1.620E-01	2.923E+03
104	PRPE	+	OH	=		RO2R	+		HCHO	+		ALD2	+ RO2	3.890E+04	-5.040E+02
105	PRPE	+	O3	=	0.64	HCHO	+	0.5	ALD2	+	0.28	CO	+ .6 OH	1.670E-02	2.105E+03
				+	0.17	HO2	+	0.13	RO2R	+	0.13	RO2			
106	PRPE	+	O	=	0.6	ACET	+	0.4	HCHO	+	0.2	ALD2	+ 0.2 HO2	5.880E+03	3.240E+02
				+	0.6	RO2R	+	0.4	CO	+	0.6	RO2			
107	PRPE	+	NO3	=		NO2	+		HCHO	+		ALD2	+ R2O2	1.120E+01	1.935E+03
				+		RO2									
108	TBUT	+	OH	=		RO2R	+	2	ALD2	+		RO2		9.420E+04	-5.490E+02
109	TBUT	+	O3	=		ALD2	+	0.15	CO	+	0.27	RO2R	+ 0.12 OH	2.960E-01	1.137E+03
				+	0.21	HO2	+	0.27	RO2	+	0.3	HCHO			
110	TBUT	+	O	=		MEK	+	0.4	HO2					3.450E+04	-1.000E+01
111	TBUT	+	NO3	=		NO2	+	2	ALD2	+		R2O2	+ RO2	5.610E+02	9.750E+02
112	TOLU	+	OH	=	0.16	CRES	+	0.16	HO2	+	0.84	RO2R	+ 0.4 DIAL	9.140E+03	-3.220E+02
				+	0.84	RO2	+	0.144	MGLY	+	0.114	GLYX			
113	DIAL	+	OH	=		PCO3	+		RCO3					4.430E+04	0.000E-01
114	DIAL			=		HO2	+		CO	+		MCO3	+ RCO3	1.000E+00	0.000E-01
115	XYLE	+	OH	=	0.17	CRES	+	0.17	HO2	+	0.83	RO2R	+ 0.83 RO2	3.620E+04	-1.160E+02
				+	0.65	DIAL	+	0.316	MGLY	+	.95	GLYX			
116	TMBZ	+	OH	=	0.17	CRES	+	0.17	HO2	+	0.83	RO2R	+ 0.83 RO2	9.160E+04	0.000E-01
				+	0.49	DIAL	+	0.86	MGLY						
117	CRES	+	OH	=	0.2	MGLY	+	0.15	RO2P	+	0.85	RO2R	+ RO2	5.910E+04	0.000E-01
118	CRES	+	NO3	=		HNO3	+		BZO					3.250E+04	0.000E-01
119	RO2P	+	NO	=		NPHE								1.140E+04	-1.800E+02
120	RO2P	+	HO2	=		ROOH								4.430E+03	0.000E-01
121	RO2P	+	RO2	=	0.5	HO2	+		RO2					1.480E+00	0.000E-01
122	RO2P	+	RCO3	=	0.5	HO2	+		RCO3					4.430E+03	0.000E-01
123	BZO	+	NO2	=		NPHE								2.220E+04	0.000E-01
124	BZO	+	HO2	=		PHEN								4.430E+03	0.000E-01
125	BZO			=		PHEN								6.000E-02	0.000E-01
126	PHEN	+	OH	=	0.2	GLYX	+	0.15	RO2P	+	0.85	RO2R	+ RO2	4.140E+04	0.000E-01
127	PHEN	+	NO3	=		HNO3	+		BZO					5.620E+03	0.000E-01
128	NPHE	+	NO3	=		HNO3	+		BZN2					5.620E+03	0.000E-01
129	BZN2	+	NO2	=										2.220E+04	0.000E-01
130	BZN2	+	HO2	=		NPHE								4.430E+03	0.000E-01
131	BZN2			=		NPHE								6.000E-02	0.000E-01
132	NRHC			=		NRHC								1.000E-10	0.000E-01

TABLE 2-19 (CONTINUED)

THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION NO.	SPECIES	ZENITH ANGLE (DEG) 0	10	20	30	40	50	60	70	78	86
1	NO2	6.00E-01	5.95E-01	5.86E-01	5.64E-01	5.32E-01	4.85E-01	4.09E-01	2.88E-01	1.55E-01	3.49E-02
13	NO3	1.38E+00	1.37E+00	1.35E+00	1.30E+00	1.28E+00	1.26E+00	1.14E+00	9.51E-01	6.36E-01	9.77E-02
14	NO3	1.20E+01	1.19E+01	1.23E+01	1.18E+01	1.17E+01	1.12E+01	1.02E+01	8.65E+00	5.59E+00	9.07E-01
15	O3	3.31E-02	3.29E-02	3.26E-02	3.16E-02	3.04E-02	2.91E-02	2.64E-02	2.14E-02	1.38E-02	2.30E-03
16	O3	2.74E-03	2.65E-03	2.41E-03	2.01E-03	1.52E-03	9.99E-04	5.15E-04	1.72E-04	4.35E-05	5.37E-06
20	HONO	1.20E-01	1.19E-01	1.17E-01	1.13E-01	1.01E-01	9.22E-02	7.77E-02	5.19E-02	2.79E-02	6.63E-03
35	H2O2	5.45E-04	5.37E-04	5.16E-04	4.77E-04	4.21E-04	3.48E-04	2.55E-04	1.48E-04	6.69E-05	1.34E-05
42	ROOH	5.45E-04	5.37E-04	5.16E-04	4.77E-04	4.21E-04	3.48E-04	2.55E-04	1.48E-04	6.69E-05	1.34E-05
46	HCHO	2.19E-03	2.15E-03	2.07E-03	1.90E-03	1.65E-03	1.34E-03	9.52E-04	5.22E-04	2.19E-04	3.84E-05
47	HCHO	3.35E-03	3.32E-03	3.22E-03	3.04E-03	2.76E-03	2.38E-03	1.84E-03	1.14E-03	5.54E-04	1.20E-04
52	ALD2	3.52E-04	3.45E-04	3.23E-04	2.83E-04	2.32E-04	1.71E-04	1.05E-04	4.70E-05	1.57E-05	2.09E-06
61	RCHO	7.14E-04	7.02E-04	6.68E-04	6.09E-04	5.29E-04	4.24E-04	2.97E-04	1.59E-04	6.63E-05	1.16E-05
69	ACET	8.04E-05	7.86E-05	7.44E-05	6.66E-05	5.64E-05	4.35E-05	2.88E-05	1.44E-05	5.51E-06	8.69E-07
71	MEK	1.15E-04	1.12E-04	1.07E-04	9.53E-05	8.03E-05	6.21E-05	4.13E-05	2.05E-05	7.87E-06	1.24E-06
73	GLYX	4.67E-03	4.65E-03	4.61E-03	4.50E-03	4.34E-03	4.10E-03	3.67E-03	2.85E-03	1.69E-03	3.40E-04
82	MGLY	1.03E-02	1.02E-02	1.02E-02	9.93E-03	9.57E-03	9.07E-03	8.09E-03	6.25E-03	3.68E-03	7.47E-04
114	DIAL	3.83E-02	3.79E-02	3.68E-02	3.47E-02	3.16E-02	2.75E-02	2.15E-02	1.35E-02	6.66E-03	1.49E-03

TABLE 2-19 (CONTINUED)

TEST PROBLEM #3 - OZIPM "CALC" RUN - 131 REACTION MECHANISM

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

LOS ANGELES, CA

LATITUDE 34.057

LONGITUDE 118.240

TIME ZONE 8.0

DATE 6 21 1986

TIME 800 TO 1800 LOCAL DAYLIGHT TIME

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS	INITIAL	250.	FINAL	1500.
TIMING	START	800.	STOP	1400.

MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME	800	900	1000	1100	1200	1300	1400
HEIGHT	250.0	482.5	774.7	1048.7	1251.5	1394.8	1500.0

REACTIVITY

EMISSIONS	ALK4 FRACTION	.210	ALK7 FRACTION	.280	ETHE FRACTION	.030
EMISSIONS	PRPE FRACTION	.060	TBUT FRACTION	.040	TOLU FRACTION	.160
EMISSIONS	XYLE FRACTION	.060	TMBZ FRACTION	.040	HCHO FRACTION	.030
EMISSIONS	ALD2 FRACTION	.020	RCHO FRACTION	.000	MEK FRACTION	.000
EMISSIONS	NRHC FRACTION	.070				

TABLE 2-19 (CONTINUED)

SURFACE LAYER	ALK4 FRACTION	.210	ALK7 FRACTION	.180	ETHE FRACTION	.015		
SURFACE LAYER	PRPE FRACTION	.030	TBUT FRACTION	.005	TOLU FRACTION	.070		
SURFACE LAYER	XYLE FRACTION	.040	TMBZ FRACTION	.020	HCHO FRACTION	.050		
SURFACE LAYER	ALD2 FRACTION	.030	RCHO FRACTION	.000	MEK FRACTION	.000		
SURFACE LAYER	NRHC FRACTION	.350						
ALOFT	ALK4 FRACTION	.210	ALK7 FRACTION	.180	ETHE FRACTION	.015		
ALOFT	PRPE FRACTION	.030	TBUT FRACTION	.005	TOLU FRACTION	.070		
ALOFT	XYLE FRACTION	.040	TMBZ FRACTION	.020	HCHO FRACTION	.050		
ALOFT	ALD2 FRACTION	.030	RCHO FRACTION	.000	MEK FRACTION	.000		
ALOFT	NRHC FRACTION	.350						
NO2/NOX	.250							

TRANSPORTED CONCENTRATIONS

SURFACE LAYER	OZONE	.000	HYDROCARBON	.001	NOX	.000 PPM
SURFACE LAYER	CO	1.000	HONO	.001		
ALOFT	OZONE	.080	HYDROCARBON	.050	NOX	.000 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES	HOUR	1	2	3	4
VOC	FRACTION	.150	.100	.100	.050
NOX	FRACTION	.250	.167	.167	.083

TABLE 2-19 (CONTINUED)

TEST PROBLEM #3 - OZIPM "CALC" RUN - 131 REACTION MECHANISM

INITIAL CONCENTRATIONS

CO	HONO
1.000E+00	5.000E-04

THE ERROR TOLERANCE IS 3.000E-03

THE TEMPERATURE USED IS 3.030E+02

THE MIXING HEIGHT IS 2.50E+02

THE RATE CONSTANTS USED WERE

3.661E-01	4.536E+07	1.370E+04	3.131E+03	2.891E+01	5.463E-02	2.712E+04	1.457E-04	1.684E+03	3.906E+00
3.000E-02	6.401E-01	1.059E+00	9.614E+00	2.437E-02	3.523E-04	6.500E+09	4.320E+10	9.310E+03	6.815E-02
1.170E-04	1.613E+04	1.810E+02	3.220E+02	1.054E+02	1.204E+04	1.935E+03	8.626E+00	5.910E+03	3.056E+00
4.274E+03	4.309E+03	4.274E+03	4.309E+03	2.123E-04	2.476E+03	1.129E+04	1.129E+04	7.495E+03	4.430E+03
4.430E+03	2.123E-04	1.480E+00	4.430E+03	3.690E+03	7.771E-04	1.575E-03	1.330E+04	9.886E-01	1.480E+01
2.328E+04	7.983E-05	3.993E+00	1.129E+04	7.495E+03	4.430E+03	4.430E+03	3.690E+03	4.678E-02	2.889E+04
2.402E-04	3.930E+00	1.129E+04	7.495E+03	4.430E+03	4.430E+03	3.690E+03	4.678E-02	2.269E-05	3.608E+02
3.248E-05	1.521E+03	3.381E-03	1.700E+04	9.952E-01	7.495E+03	1.129E+04	4.678E-02	4.430E+03	4.430E+03
3.690E+03	7.459E-03	2.510E+04	3.993E+00	4.854E+03	9.256E+03	3.120E+03	1.129E+04	4.430E+03	1.480E+00
4.430E+03	1.129E+04	4.430E+03	1.480E+00	4.430E+03	1.129E+04	4.430E+03	1.480E+00	4.430E+03	1.232E+04
2.974E-03	1.128E+03	1.905E-01	3.783E+04	1.876E-02	5.986E+03	1.247E+01	9.138E+04	3.152E-01	3.448E+04
5.921E+02	8.978E+03	4.430E+04	1.845E-02	3.597E+04	9.160E+04	5.910E+04	3.250E+04	1.129E+04	4.430E+03
1.480E+00	4.430E+03	2.220E+04	4.430E+03	6.000E-02	4.140E+04	5.620E+03	5.620E+03	2.220E+04	4.430E+03
6.000E-02	1.000E-10								

THE PHOTOLYSIS REACTIONS ARE

1	13	14	15	16	20	35	42	46
47	52	61	69	71	73	82	114	

THE PHOTOLYTIC RATE CONSTANTS ARE

3.661E-01	1.059E+00	9.614E+00	2.437E-02	3.523E-04	6.815E-02	2.123E-04	2.123E-04	7.771E-04
1.575E-03	7.983E-05	2.402E-04	2.269E-05	3.248E-05	3.381E-03	7.459E-03	1.845E-02	

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
800.	2.00100	10.00501	.20000	.25000	.00000	.05000

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
8.000E+02	5.000E-02	1.500E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	5.000E-04
1.000E-10	1.000E+00	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	6.005E-02	0.000E-01	2.002E-02
	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	0.000E-01	9.338E-02	0.000E-01	0.000E-01	8.003E-02	0.000E-01	3.001E-02	4.001E-02	2.000E-02	4.572E-02
	0.000E-01	0.000E-01	1.500E-02	8.891E-03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.403E-01
NET RATES	-1.886E-02	1.736E-02	1.831E-02	9.431E-04	0.000E-01	0.000E-01	5.850E-06	0.000E-01	3.408E-05	-3.412E-05
	-1.165E-02	9.492E-05	0.000E-01	0.000E-01	1.598E-06	0.000E-01	0.000E-01	-6.681E-04	1.598E-06	-1.787E-04
	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	0.000E-01	-8.400E-04	0.000E-01	0.000E-01	-7.282E-04	0.000E-01	-2.743E-04	-3.658E-04	-1.851E-04	-4.189E-04
	0.000E-01	0.000E-01	-1.364E-04	-8.128E-05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-1.098E-03

THE REACTION RATES ARE

1.83E-02 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 3.28E-06 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 3.41E-05 5.85E-06 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 4.67E-05 9.46E-05 0.00E-01 0.00E-01 0.00E-01 0.00E-01 1.60E-06 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01
0.00E-01 0.00E-01 0.00E-01 0.00E-01 0.00E-01 1.40E-11

THE PHOTOLYTIC RATE CONSTANTS ARE

3.661E-01 1.059E+00 9.614E+00 2.437E-02 3.523E-04 6.815E-02 2.123E-04 2.123E-04 7.771E-04
1.575E-03 7.983E-05 2.402E-04 2.269E-05 3.248E-05 3.381E-03 7.459E-03 1.845E-02

THE CURRENT MIXING HEIGHT IS 250.00
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 64.10

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
900.	1.12006	9.60915	.11656	.72542	.04239	.08456

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
9.000E+02	8.456E-02	3.201E-02	9.147E-10	4.239E-02	2.103E-07	7.461E-06	7.925E-03	7.907E-16	1.537E-07	7.324E-04
1.000E+01	5.201E-01	2.134E-06	4.022E-05	7.164E-07	1.685E-06	2.903E-07	3.497E-07	3.968E-02	1.426E-06	2.802E-02
	2.663E-07	2.007E-03	9.809E-04	2.355E-08	1.730E-04	1.754E-03	2.247E-03	3.528E-03	3.279E-04	4.684E-10
	3.225E-06	5.407E-02	3.931E-08	2.167E-07	4.456E-02	6.780E-04	1.624E-02	1.773E-02	4.385E-03	2.540E-02
	7.682E-04	1.559E-03	6.905E-03	2.745E-03	2.898E-09	2.808E-09	1.057E-04	2.561E-09	6.566E-11	9.101E-02
NET RATES	-2.606E-04	-8.199E-04	-1.678E-04	1.097E-03	4.385E-06	5.097E-07	1.498E-04	-8.626E-07	-6.792E-07	-1.741E-05
	-4.658E-03	-1.265E-06	1.821E-06	3.176E-08	-4.447E-07	7.953E-08	1.523E-08	-2.244E-04	-7.183E-07	-1.900E-05
	3.223E-08	5.578E-05	8.974E-06	4.528E-08	5.190E-06	1.976E-05	1.728E-06	3.916E-05	2.324E-06	1.913E-09
	1.153E-07	-4.338E-04	4.060E-08	2.327E-07	-3.905E-04	7.425E-06	-1.520E-04	-2.390E-04	-1.408E-04	-2.236E-04
	-8.611E-07	-9.007E-06	-8.563E-05	-5.432E-05	9.137E-11	-2.166E-08	5.187E-06	1.513E-10	1.702E-09	-5.511E-04

THE REACTION RATES ARE

4.01E-02 4.15E-02 1.06E-06 2.42E-07 3.92E-02 1.96E-04 1.82E-04 1.49E-07 2.99E-05 2.91E-05 2.24E-07 1.14E-08 2.63E-07 2.32E-06
1.22E-03 3.84E-05 5.14E-06 3.42E-05 4.58E-05 6.61E-05 9.89E-06 2.10E-04 2.21E-07 2.58E-05 6.87E-07 8.22E-04 3.49E-04 3.47E-04
3.65E-08 2.76E-07 1.95E-08 1.96E-08 1.92E-09 1.93E-09 2.39E-10 2.73E-10 6.09E-04 1.05E-04 1.84E-04 1.59E-08 2.74E-09 1.17E-10
4.20E-12 2.17E-09 3.11E-10 5.08E-05 9.12E-05 8.11E-05 8.25E-09 1.25E-06 1.00E-04 4.47E-06 2.35E-08 9.62E-05 1.69E-04 2.52E-09
1.99E-09 2.85E-10 9.39E-05 4.36E-06 3.95E-07 8.10E-10 8.51E-06 1.49E-05 2.23E-10 1.76E-10 2.52E-11 8.09E-06 7.19E-08 9.73E-08
2.06E-07 8.25E-07 1.33E-06 8.57E-07 6.86E-11 2.97E-07 1.69E-07 1.51E-07 4.43E-12 3.50E-12 5.02E-13 2.01E-05 8.67E-06 1.89E-09
4.04E-05 6.34E-05 3.25E-07 1.42E-05 3.72E-10 9.80E-14 5.05E-11 7.83E-05 2.05E-09 5.40E-13 2.79E-10 5.15E-04 1.35E-08 3.56E-12
1.83E-09 3.08E-05 2.05E-06 1.68E-08 6.51E-10 1.03E-04 1.41E-05 9.71E-08 4.65E-08 6.16E-05 5.86E-05 1.38E-07 5.46E-07 3.51E-05
1.06E-05 4.14E-05 3.82E-05 3.87E-05 6.98E-06 5.25E-06 1.05E-06 2.74E-11 7.23E-15 3.73E-12 5.27E-06 2.65E-11 1.68E-10 1.63E-11
3.03E-12 1.25E-07 1.23E-07 6.21E-13 3.94E-12 9.10E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

4.739E-01 1.250E+00 1.103E+01 2.875E-02 9.066E-04 9.032E-02 3.331E-04 3.331E-04 1.279E-03
2.298E-03 1.595E-04 4.031E-04 4.097E-05 5.851E-05 4.045E-03 8.943E-03 2.652E-02

THE CURRENT MIXING HEIGHT IS 482.50
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 51.79

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1000.	.72683	10.51088	.06915	.84094	.09256	.05815

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.000E+03	5.815E-02	1.100E-02	7.493E-10	9.256E-02	9.006E-07	2.221E-05	1.499E-02	2.889E-15	1.863E-07	2.659E-04
1.000E+01	3.401E-01	4.334E-06	5.644E-05	4.912E-06	3.165E-06	7.430E-07	2.322E-06	2.921E-02	2.585E-06	2.307E-02
	6.779E-07	4.803E-03	1.274E-03	6.340E-08	4.395E-04	2.594E-03	1.791E-03	5.167E-03	3.782E-04	1.706E-09
	1.108E-05	3.619E-02	8.747E-08	4.872E-07	2.849E-02	9.874E-04	9.969E-03	8.272E-03	5.040E-04	1.620E-02
	3.953E-04	9.141E-04	3.523E-03	8.984E-04	5.082E-09	8.793E-09	5.223E-04	1.964E-08	2.097E-09	6.822E-02
NET RATES	-9.622E-04	4.023E-04	1.470E-05	1.187E-03	-1.875E-06	6.534E-07	1.012E-04	2.950E-08	-1.475E-05	-2.861E-06
	-1.911E-03	4.975E-06	4.852E-07	1.256E-07	8.920E-06	1.317E-06	5.926E-08	-1.337E-04	7.060E-06	-1.123E-04
	1.116E-06	4.018E-05	2.786E-06	1.949E-07	4.272E-06	1.199E-05	-1.138E-05	2.293E-05	7.694E-08	6.216E-09
	1.547E-07	-1.982E-04	2.722E-07	1.566E-06	-1.794E-04	3.996E-06	-7.060E-05	-1.008E-04	-1.562E-05	-1.025E-04
	-7.484E-06	-8.788E-06	-3.638E-05	-1.556E-05	2.174E-08	2.175E-07	6.012E-06	3.204E-10	-6.413E-08	-2.478E-04

THE REACTION RATES ARE

3.11E-02 3.40E-02 5.97E-07 1.36E-07 2.94E-02 2.94E-04 2.69E-04 1.76E-08 8.82E-05 8.68E-05 6.66E-07 3.35E-08 1.15E-06 1.05E-05
2.82E-03 1.44E-04 1.88E-05 1.25E-04 1.91E-05 2.70E-05 6.80E-06 1.75E-04 5.06E-07 2.04E-05 1.82E-06 5.74E-04 4.88E-04 4.87E-04
6.21E-08 1.23E-06 8.03E-08 8.10E-08 1.67E-08 1.68E-08 2.08E-09 2.27E-09 3.93E-04 9.22E-05 3.24E-04 6.08E-08 1.43E-08 9.85E-10
1.48E-11 1.04E-08 2.04E-09 4.88E-05 8.12E-05 7.24E-05 2.60E-08 1.87E-06 1.00E-04 5.43E-06 8.30E-08 8.42E-05 2.95E-04 1.30E-08
9.51E-09 1.86E-09 2.25E-04 6.86E-06 6.81E-07 4.51E-09 7.87E-06 2.76E-05 1.22E-09 8.89E-10 1.74E-10 2.06E-05 1.48E-07 1.74E-07
4.20E-07 1.46E-06 1.65E-06 1.20E-06 3.39E-10 7.44E-07 2.12E-07 5.18E-07 3.28E-11 2.39E-11 4.68E-12 1.72E-05 8.37E-06 6.44E-09
3.27E-05 4.91E-05 5.74E-07 1.09E-05 1.68E-09 4.10E-13 2.88E-10 6.05E-05 9.35E-09 2.28E-12 1.60E-09 3.21E-04 4.96E-08 1.21E-11
8.51E-09 2.29E-05 2.74E-06 8.43E-09 1.71E-09 5.83E-05 1.44E-05 3.71E-08 9.29E-08 8.58E-06 1.47E-05 1.30E-08 2.69E-07 2.71E-05
7.54E-06 2.91E-05 2.36E-05 1.53E-05 4.35E-06 1.16E-05 6.31E-07 9.76E-11 2.38E-14 1.67E-11 1.14E-05 1.69E-10 5.28E-10 1.51E-10
9.94E-11 2.64E-06 2.71E-06 4.03E-11 1.26E-10 6.82E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

5.340E-01 1.277E+00 1.171E+01 3.044E-02 1.552E-03 1.017E-01 4.244E-04 4.244E-04 1.670E-03
2.779E-03 2.352E-04 5.341E-04 5.706E-05 8.130E-05 4.356E-03 9.596E-03 3.185E-02

THE CURRENT MIXING HEIGHT IS 774.73
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 39.40

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1100.	.54572	12.44048	.04387	.87349	.12965	.03832

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.100E+03	3.832E-02	5.550E-03	5.797E-10	1.296E-01	1.575E-06	2.576E-05	2.103E-02	5.572E-15	2.704E-07	1.647E-04
1.000E+01	2.654E-01	8.260E-06	7.096E-05	2.175E-05	6.136E-06	1.550E-06	1.052E-05	2.337E-02	4.873E-06	1.737E-02
	1.386E-06	7.086E-03	1.432E-03	1.585E-07	7.636E-04	3.454E-03	1.234E-03	6.792E-03	3.817E-04	4.934E-09
	2.308E-05	2.784E-02	1.890E-07	1.068E-06	2.072E-02	1.285E-03	6.870E-03	4.057E-03	1.267E-04	1.178E-02
	1.579E-04	6.025E-04	1.944E-03	3.304E-04	6.111E-09	9.447E-09	6.607E-04	3.173E-08	6.885E-09	5.840E-02
NET RATES	-2.615E-04	-9.502E-05	4.117E-06	5.885E-04	-8.691E-07	1.332E-07	1.061E-04	-3.842E-09	-1.549E-06	-1.096E-06
	-7.741E-04	8.057E-07	6.379E-08	4.775E-07	1.305E-06	3.228E-07	2.360E-07	-7.693E-05	1.002E-06	-8.254E-05
	2.277E-07	3.965E-05	2.761E-06	9.242E-08	6.871E-06	1.736E-05	-7.477E-06	3.254E-05	1.148E-07	2.808E-09
	2.493E-07	-1.062E-04	4.652E-08	2.619E-07	-1.024E-04	5.856E-06	-4.145E-05	-5.322E-05	-2.776E-06	-5.810E-05
	-2.028E-06	-3.110E-06	-2.094E-05	-6.397E-06	-4.423E-09	4.490E-08	5.512E-08	1.557E-10	-1.079E-08	-1.146E-04

THE REACTION RATES ARE

2.19E-02 2.63E-02 3.04E-07 6.95E-08 2.08E-02 2.71E-04 2.37E-04 4.49E-09 1.02E-04 1.01E-04 7.73E-07 3.86E-08 2.06E-06 1.89E-05
4.14E-03 2.77E-04 3.62E-05 2.41E-04 1.40E-05 1.89E-05 4.48E-06 1.67E-04 1.03E-06 2.31E-05 3.69E-06 5.52E-04 6.13E-04 6.12E-04
1.13E-07 3.27E-06 2.92E-07 2.94E-07 5.56E-08 5.60E-08 1.07E-08 1.46E-08 3.84E-04 9.71E-05 4.45E-04 2.25E-07 5.67E-08 5.15E-09
5.57E-11 4.21E-08 8.86E-09 4.56E-05 7.24E-05 8.40E-05 3.64E-08 2.86E-06 1.09E-04 5.13E-06 1.09E-07 8.68E-05 3.98E-04 5.07E-08
3.77E-08 7.93E-09 3.32E-04 1.12E-05 9.00E-07 8.86E-09 9.92E-06 4.55E-05 5.80E-09 4.31E-09 9.06E-10 3.57E-05 2.39E-07 3.37E-07
6.72E-07 2.79E-06 1.73E-06 1.75E-06 5.98E-10 1.42E-06 3.09E-07 1.08E-06 1.81E-10 1.34E-10 2.82E-11 1.24E-05 8.37E-06 7.76E-09
3.65E-05 5.19E-05 1.08E-06 1.18E-05 6.92E-09 1.72E-12 1.30E-09 6.69E-05 3.91E-08 9.70E-12 7.33E-09 3.05E-04 1.78E-07 4.43E-11
3.35E-08 2.29E-05 2.65E-06 4.49E-09 2.06E-09 4.15E-05 9.87E-06 1.41E-08 7.96E-08 3.13E-06 5.18E-06 2.53E-09 1.18E-07 2.86E-05
7.22E-06 2.13E-05 1.89E-05 8.18E-06 2.52E-06 8.08E-06 3.83E-07 2.24E-10 5.55E-14 4.20E-11 8.04E-06 3.46E-10 5.67E-10 3.55E-10
2.81E-10 5.85E-06 5.86E-06 2.52E-10 4.13E-10 5.84E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

5.715E-01 1.311E+00 1.199E+01 3.197E-02 2.136E-03 1.149E-01 4.899E-04 4.899E-04 1.953E-03
3.098E-03 2.954E-04 6.282E-04 6.908E-05 9.901E-05 4.534E-03 1.002E-02 3.541E-02

THE CURRENT MIXING HEIGHT IS 1048.69
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 27.15

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1200.	.43031	17.89621	.02404	.90144	.16968	.02168

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.200E+03	2.168E-02	2.370E-03	4.135E-10	1.697E-01	2.406E-06	2.234E-05	2.758E-02	8.637E-15	4.261E-07	1.079E-04
2.500E+00	2.368E-01	1.957E-05	9.504E-05	1.021E-04	1.522E-05	3.829E-06	5.160E-05	1.915E-02	1.164E-05	1.263E-02
	3.307E-06	9.875E-03	1.569E-03	5.056E-07	1.387E-03	4.769E-03	8.412E-04	9.206E-03	3.810E-04	1.644E-08
	4.469E-05	2.240E-02	5.248E-07	3.041E-06	1.529E-02	1.711E-03	4.672E-03	1.625E-03	1.706E-05	8.710E-03
	8.602E-05	4.530E-04	9.119E-04	8.007E-05	1.210E-08	1.397E-08	5.831E-04	4.696E-08	1.638E-08	5.327E-02
NET RATES	-2.938E-04	-4.599E-05	7.668E-08	7.185E-04	3.271E-09	-1.641E-07	1.037E-04	3.492E-09	1.158E-07	-1.032E-06
	-3.054E-04	1.372E-07	6.126E-07	2.895E-06	2.176E-07	-7.376E-08	1.508E-06	-7.703E-05	1.686E-07	-8.390E-05
	-6.039E-08	5.300E-05	1.396E-06	-1.303E-08	1.415E-05	2.561E-05	-6.433E-06	4.612E-05	-2.579E-07	-4.266E-10
	4.787E-07	-9.157E-05	7.139E-09	4.206E-08	-9.193E-05	7.904E-06	-3.658E-05	-3.395E-05	-1.498E-06	-5.184E-05
	-8.470E-07	-2.551E-06	-1.547E-05	-3.055E-06	1.449E-10	-2.363E-10	-2.148E-06	4.807E-10	-9.021E-10	-8.068E-05

THE REACTION RATES ARE

1.28E-02 1.88E-02 1.23E-07 2.81E-08 1.16E-02 2.01E-04 1.55E-04 8.18E-10 8.78E-05 8.73E-05 6.70E-07 3.34E-08 3.27E-06 2.93E-05
5.56E-03 4.29E-04 5.61E-05 3.73E-04 9.40E-06 1.27E-05 2.54E-06 1.49E-04 2.13E-06 3.25E-05 7.62E-06 5.58E-04 8.21E-04 8.20E-04
2.39E-07 1.01E-05 1.64E-06 1.65E-06 2.01E-07 2.03E-07 5.38E-08 1.08E-07 4.07E-04 1.02E-04 6.22E-04 1.32E-06 3.32E-07 2.72E-08
3.43E-10 2.58E-07 5.41E-08 4.04E-05 6.26E-05 1.09E-04 4.55E-08 5.54E-06 1.25E-04 4.21E-06 1.21E-07 8.85E-05 5.37E-04 2.87E-07
2.23E-07 4.67E-08 4.62E-04 1.93E-05 1.07E-06 1.48E-08 1.35E-05 8.21E-05 4.38E-08 3.41E-08 7.14E-09 6.49E-05 3.65E-07 7.33E-07
1.01E-06 5.97E-06 1.76E-06 2.76E-06 9.12E-10 2.67E-06 4.40E-07 2.09E-06 1.42E-09 1.11E-09 2.32E-10 8.60E-06 9.00E-06 8.08E-09
4.63E-05 6.03E-05 2.27E-06 1.40E-05 4.55E-08 1.18E-11 8.90E-09 8.13E-05 2.64E-07 6.85E-11 5.16E-08 3.11E-04 1.01E-06 2.62E-10
1.97E-07 2.45E-05 2.36E-06 2.18E-09 2.14E-09 2.62E-05 5.17E-06 4.02E-09 4.87E-08 6.64E-07 9.12E-07 2.43E-10 2.43E-08 3.33E-05
8.55E-06 1.69E-05 1.40E-05 3.13E-06 2.17E-06 6.73E-06 3.24E-07 1.05E-09 2.73E-13 2.05E-10 6.72E-06 1.21E-09 8.38E-10 8.28E-10
6.35E-10 7.88E-06 7.88E-06 1.42E-09 9.83E-10 5.33E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

5.906E-01 1.359E+00 1.219E+01 3.275E-02 2.530E-03 1.179E-01 5.271E-04 5.271E-04 2.112E-03
3.268E-03 3.338E-04 6.846E-04 7.648E-05 1.096E-04 4.631E-03 1.022E-02 3.736E-02

THE CURRENT MIXING HEIGHT IS 1251.47
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 15.97

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1300.	.33500	42.37859	.00790	.92735	.20912	.00733

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TM8Z	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.300E+03	7.331E-03	5.743E-04	2.590E-10	2.091E-01	2.586E-06	8.179E-06	3.187E-02	1.110E-14	5.944E-07	4.209E-05
1.000E+01	2.249E-01	5.921E-05	9.736E-05	8.729E-04	5.656E-05	1.464E-05	5.129E-04	1.445E-02	4.220E-05	7.955E-03
	1.206E-05	1.292E-02	1.528E-03	2.512E-06	2.473E-03	6.444E-03	5.000E-04	1.210E-02	3.343E-04	8.069E-08
	7.989E-05	1.747E-02	2.026F-06	1.230E-05	1.038E-02	2.163E-03	2.790E-03	4.054E-04	8.708E-07	5.940E-03
	5.419E-05	2.980E-04	2.879E-04	8.419E-06	4.199E-08	2.797E-08	4.393E-04	1.453E-07	3.918E-08	4.965E-02
NET RATES	-1.732E-04	-1.886E-05	5.443E-08	5.218E-04	1.066E-07	-2.693E-07	3.456E-05	2.491E-08	2.660E-07	-1.030E-06
	-1.380E-04	9.784E-07	-3.208E-07	2.707E-05	4.798E-07	-2.377E-06	1.766E-05	-7.411E-05	4.207E-07	-6.384E-05
	-1.892E-06	3.956E-05	-2.482E-06	-4.807E-07	1.878E-05	2.650E-05	-4.637E-06	4.391E-05	-1.216E-06	-1.470E-08
	5.806E-07	-7.228E-05	9.519E-09	4.925E-08	-7.022E-05	5.993E-06	-2.565E-05	-1.058E-05	-1.703E-08	-3.956E-05
	-3.403E-07	-2.642E-06	-6.211E-06	-3.101E-07	9.334E-11	-3.771E-09	-2.183E-06	3.117E-09	-4.419E-09	-4.644E-05

THE REACTION RATES ARE

4.36E-03 1.17E-02 2.60E-08 5.95E-09 3.47E-03 8.37E-05 4.03E-05 4.80E-11 3.19E-05 3.19E-05 2.45E-07 1.21E-08 3.54E-06 3.08E-05
6.88E-03 5.52E-04 7.22E-05 4.80E-04 3.18E-06 5.01E-06 8.58E-07 7.03E-05 3.43E-06 4.30E-05 1.31E-05 4.09E-04 8.40E-04 8.40E-04
3.42E-07 3.78E-05 1.50E-05 1.51E-05 6.54E-07 6.60E-07 4.68E-07 1.28E-06 3.67E-04 9.49E-05 8.04E-04 1.48E-05 3.84E-06 2.75E-07
4.73E-09 3.67E-06 7.91E-07 3.11E-05 4.78E-05 1.14E-04 3.69E-08 1.27E-05 1.10E-04 2.73E-06 8.22E-08 7.82E-05 6.62E-04 3.16E-06
3.02E-06 6.51E-07 6.04E-04 2.62E-05 1.07E-06 1.55E-08 1.63E-05 1.38E-04 6.59E-07 6.29E-07 1.36E-07 1.16E-04 5.05E-07 1.38E-06
1.36E-06 1.09E-05 1.55E-06 3.38E-06 8.60E-10 4.43E-06 5.23E-07 3.74E-06 2.12E-08 2.02E-08 4.36E-09 5.12E-06 7.46E-06 5.16E-09
5.04E-05 5.71E-05 4.01E-06 1.31E-05 5.31E-07 1.70E-10 1.31E-07 7.97E-05 3.23E-06 1.03E-09 7.97E-07 2.74E-04 1.11E-05 3.53E-09
2.74E-06 2.04E-05 1.73E-06 8.15E-10 1.37E-09 9.12E-06 1.59E-06 6.29E-10 1.31E-08 4.73E-08 5.74E-08 7.78E-12 1.33E-09 3.17E-05
7.85E-06 1.13E-05 6.16E-06 4.58E-07 1.90E-06 4.55E-06 2.72E-07 1.10E-08 3.52E-12 2.72E-09 4.55E-06 7.34E-09 1.68E-09 3.58E-09
2.11E-09 6.38E-06 6.38E-06 1.03E-08 2.35E-09 4.97E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

5.948E-01 1.368E+00 1.193E+01 3.290E-02 2.638E-03 1.189E-01 5.366E-04 5.366E-04 2.151E-03
3.311E-03 3.437E-04 7.008E-04 7.838E-05 1.122E-04 4.647E-03 1.023E-02 3.781E-02

THE CURRENT MIXING HEIGHT IS 1394.76
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 10.68

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1400.	.27925	100.37181	.00278	.93821	.22455	.00261

TIME INTERVAL										
	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.400E+03	2.610E-03	1.719E-04	2.067E-10	2.245E-01	1.517E-06	1.842E-06	3.203E-02	1.121E-14	4.824E-07	1.111E-05
9.628E+00	2.180E-01	7.554E-05	4.332E-05	3.227E-03	1.100E-04	4.023E-05	2.712E-03	1.150E-02	8.405E-05	5.686E-03
	3.244E-05	1.298E-02	1.334E-03	7.810E-06	2.989E-03	7.531E-03	3.082E-04	1.381E-02	2.549E-04	2.410E-07
	9.327E-05	1.417E-02	3.526E-06	2.238E-05	7.365E-03	2.309E-03	1.746E-03	1.204E-04	5.700E-07	4.237E-03
	4.305E-05	1.703E-04	1.046E-04	3.066E-06	7.873E-08	3.785E-08	3.504E-04	3.882E-07	5.329E-08	4.747E-02
NET RATES	-5.159E-05	-3.280E-05	-8.171E-07	1.223E-04	1.441E-06	-5.824E-07	-8.607E-06	-2.515E-08	6.124E-06	-2.396E-07
	-9.893E-05	-1.535E-06	7.740E-06	4.014E-05	-8.403E-06	-4.663E-05	4.618E-05	-2.783E-05	-5.414E-06	-2.281E-05
	-3.776E-05	1.427E-05	-3.358E-06	-8.395E-06	9.908E-06	1.355E-05	-2.306E-06	2.014E-05	-1.263E-06	-2.790E-07
	2.557E-07	-4.525E-05	-4.127E-07	-2.568E-06	-3.909E-05	1.010E-06	-1.294E-05	-2.320E-06	-2.772E-09	-2.217E-05
	-1.261E-07	-1.553E-06	-1.666E-06	-2.516E-08	-7.986E-09	-8.252E-08	-9.783E-07	3.481E-09	-1.210E-07	-3.059E-05

THE REACTION RATES ARE

1.54E-03 9.38E-03 7.39E-09 1.69E-09 1.12E-03 3.20E-05 7.07E-06 4.30E-12 6.67E-06 7.20E-06 5.53E-08 2.54E-09 2.06E-06 1.86E-05
7.34E-03 5.57E-04 7.29E-05 4.84E-04 7.72E-07 1.31E-06 3.05E-07 2.03E-05 2.80E-06 3.39E-05 1.14E-05 1.56E-04 3.82E-04 3.74E-04
1.23E-07 5.18E-05 2.44E-05 2.46E-05 4.90E-07 4.94E-07 1.69E-06 3.85E-06 2.13E-04 7.81E-05 7.87E-04 3.68E-05 1.35E-05 1.42E-05
1.79E-08 1.96E-05 5.97E-06 2.41E-05 3.74E-05 7.38E-05 1.73E-08 1.29E-05 6.38E-05 1.87E-06 3.44E-08 6.29E-05 6.35E-04 1.09E-05
1.58E-05 4.82E-06 6.07E-04 1.86E-05 9.04E-07 7.95E-09 1.52E-05 1.53E-04 2.61E-06 3.81E-06 1.16E-06 1.40E-04 5.69E-07 1.31E-06
1.50E-06 1.01E-05 1.18E-06 2.09E-06 3.85E-10 4.71E-06 4.68E-07 4.36E-06 8.06E-08 1.17E-07 3.58E-08 3.15E-06 3.73E-06 1.87E-09
3.32E-05 3.29E-05 3.47E-06 6.84E-06 1.18E-06 5.74E-10 6.28E-07 4.34E-05 7.49E-06 3.64E-09 3.99E-06 1.63E-04 2.81E-05 1.37E-08
1.50E-05 1.04E-05 1.17E-06 4.07E-10 5.05E-10 2.20E-06 5.07E-07 1.49E-10 2.28E-09 2.51E-08 4.03E-08 4.06E-12 5.12E-10 1.84E-05
3.64E-06 6.33E-06 1.81E-06 1.35E-07 1.23E-06 2.12E-06 1.53E-07 2.63E-08 1.28E-11 1.40E-08 2.19E-06 1.27E-08 2.27E-09 7.75E-09
3.31E-09 2.99E-06 3.09E-06 1.78E-08 3.20E-09 4.75E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

5.886E-01 1.355E+00 1.226E+01 3.267E-02 2.481E-03 1.176E-01 5.227E-04 5.227E-04 2.093E-03
3.249E-03 3.292E-04 6.774E-04 7.561E-05 1.083E-04 4.623E-03 1.021E-02 3.715E-02

THE CURRENT MIXING HEIGHT IS 1500.00
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 17.79

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1500.	.25520	122.61586	.00208	.94395	.23705	.00196

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.500E+03	1.965E-03	1.166E-04	1.999E-10	2.370E-01	1.416E-06	1.192E-06	3.315E-02	9.727E-15	4.466E-07	6.507E-06
1.000E+01	2.244E-01	7.279E-05	3.209E-05	5.642E-03	1.115E-04	4.692E-05	5.721E-03	1.048E-02	8.605E-05	4.925E-03
	3.719E-05	1.208E-02	1.202E-03	9.919E-06	3.110E-03	8.603E-03	2.244E-04	1.545E-02	2.000E-04	2.851E-07
	9.159E-05	1.240E-02	3.333E-06	2.207E-05	5.729E-03	2.411E-03	1.205E-03	3.670E-05	5.469E-09	3.321E-03
	3.347E-05	1.172E-04	4.150E-05	3.637E-07	7.268E-08	3.514E-08	3.064E-04	4.960E-07	5.551E-08	4.747E-02
NET RATES	-3.449E-06	-1.215E-06	8.188E-07	1.749E-04	2.784E-08	-4.876E-09	1.669E-05	1.686E-07	1.986E-09	-2.313E-08
	9.760E-05	5.694E-08	-1.446E-07	3.653E-05	-1.454E-07	-1.273E-06	4.850E-05	-1.437E-05	-6.910E-08	-9.462E-06
	-9.657E-07	-1.743E-05	-2.237E-06	-3.505E-07	5.620E-07	1.570E-05	-1.045E-06	2.296E-05	-8.363E-07	-8.903E-09
	-8.674E-08	-2.689E-05	-1.067E-08	-6.540E-08	-2.368E-05	1.029E-06	-7.476E-06	-7.840E-07	-6.365E-10	-1.332E-05
	-1.777E-07	-6.398E-07	-6.667E-07	-1.488E-08	-3.572E-10	-1.712E-09	-7.893E-07	3.225E-10	-3.103E-09	0.000E-01

THE REACTION RATES ARE

1.11E-03 9.07E-03 5.38E-09 1.23E-09 7.99E-04 2.54E-05 4.48E-06 1.98E-12 4.69E-06 4.66E-06 3.58E-08 1.78E-09 1.84E-06 1.68E-05
7.52E-03 4.84E-04 6.32E-05 4.20E-04 4.85E-07 7.38E-07 2.30E-07 1.42E-05 2.68E-06 3.23E-05 1.12E-05 1.02E-04 2.77E-04 2.77E-04
8.47E-08 5.27E-05 2.26E-05 2.28E-05 4.41E-07 4.44E-07 2.71E-06 6.24E-06 1.47E-04 6.18E-05 6.91E-04 3.60E-05 1.51E-05 2.75E-06
1.84E-08 2.32E-05 8.12E-06 2.00E-05 3.20E-05 6.22E-05 1.47E-08 1.13E-05 5.12E-05 1.41E-06 2.79E-08 4.90E-05 5.48E-04 1.20E-05
1.84E-05 6.44E-06 5.65E-04 1.55E-05 7.38E-07 6.69E-09 1.31E-05 1.46E-04 3.20E-06 4.90E-06 1.72E-06 1.45E-04 5.78E-07 1.39E-06
1.49E-06 1.05E-05 9.01E-07 1.52E-06 2.82E-10 4.20E-06 3.75E-07 4.28E-06 9.19E-08 1.41E-07 4.94E-08 2.23E-06 2.52E-06 1.27E-09
2.69E-05 2.37E-05 3.36E-06 4.39E-06 1.07E-06 5.50E-10 6.93E-07 2.91E-05 7.12E-06 3.64E-09 4.59E-06 1.13E-04 2.77E-05 1.42E-08
1.79E-05 6.63E-06 8.49E-07 2.72E-10 3.25E-10 6.20E-07 1.63E-07 4.39E-11 6.48E-10 2.23E-10 4.09E-10 3.77E-14 4.59E-12 1.33E-05
2.32E-06 4.09E-06 6.67E-07 1.49E-08 8.83E-07 1.54E-06 9.57E-08 2.34E-08 1.20E-11 1.51E-08 1.53E-06 1.13E-08 2.11E-09 9.17E-09
3.95E-09 2.44E-06 2.42E-06 1.79E-08 3.33E-09 4.75E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

5.660E-01 1.301E+00 1.188E+01 3.173E-02 2.040E-03 1.134E-01 4.800E-04 4.800E-04 1.910E-03
3.051E-03 2.858E-04 6.141E-04 6.720E-05 9.626E-05 4.506E-03 9.952E-03 3.488E-02

THE CURRENT MIXING HEIGHT IS 1500.00
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 29.31

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1600.	.23663	115.05038	.00206	.94781	.24676	.00195

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.600E+03	1.949E-03	1.073E-04	1.933E-10	2.468E-01	1.542E-06	1.286E-06	3.411E-02	6.978E-15	3.883E-07	6.235E-06
1.000E+01	2.297E-01	6.449E-05	2.821E-05	7.542E-03	9.536E-05	4.341E-05	8.359E-03	9.661E-03	7.488E-05	4.485E-03
	3.391E-05	1.095E-02	1.071E-03	9.660E-06	3.050E-03	9.420E-03	1.774E-04	1.656E-02	1.552E-04	2.559E-07
	8.315E-05	1.093E-02	2.588E-06	1.785E-05	4.514E-03	2.441E-03	8.418E-04	1.143E-05	0.000E-01	2.635E-03
	2.281E-05	8.762E-05	1.722E-05	4.822E-08	4.721E-08	2.631E-08	2.502E-04	4.327E-07	4.976E-08	4.747E-02
NET RATES	-3.547E-06	4.481E-06	1.748E-05	1.202E-04	-3.145E-09	2.186E-09	1.433E-05	8.010E-06	3.660E-08	-3.643E-09
	7.392E-05	2.646E-07	-9.107E-08	2.535E-05	-2.071E-07	-2.400E-07	3.633E-05	-1.200E-05	-1.336E-07	-5.375E-06
	-1.330E-07	-1.700E-05	-1.909E-06	-1.155E-07	-1.554E-06	1.101E-05	-5.920E-07	1.396E-05	-6.225E-07	-1.580E-09
	-1.515E-07	-2.060E-05	-9.095E-09	-6.425E-08	-1.622E-05	1.774E-07	-4.644E-06	-2.211E-07	0.000E-01	-9.186E-06
	-1.555E-07	-3.971E-07	-2.405E-07	-1.715E-09	-2.274E-10	-8.783E-10	-9.553E-07	-1.612E-09	-2.155E-09	0.000E-01

THE REACTION RATES ARE

1.02E-03 8.77E-03 5.16E-09 1.18E-09 7.66E-04 2.63E-05 4.49E-06 1.68E-12 5.06E-06 5.02E-06 3.86E-08 1.92E-09 1.97E-06 1.80E-05
7.44E-03 3.55E-04 4.54E-05 3.01E-04 3.88E-07 6.20E-07 2.28E-07 1.22E-05 2.40E-06 2.87E-05 1.01E-05 8.33E-05 2.43E-04 2.43E-04
6.47E-08 4.86E-05 1.78E-05 1.79E-05 4.25E-07 4.29E-07 3.09E-06 7.25E-06 1.16E-04 5.26E-05 6.34E-04 2.72E-05 1.24E-05 3.43E-06
1.35E-08 1.83E-05 6.95E-06 1.55E-05 2.62E-05 4.99E-05 1.47E-08 9.22E-06 4.05E-05 9.99E-07 2.76E-08 4.11E-05 4.95E-04 9.69E-06
1.43E-05 5.43E-06 5.12E-04 1.20E-05 5.50E-07 6.49E-09 1.17E-05 1.41E-04 2.76E-06 4.08E-06 1.55E-06 1.43E-04 5.13E-07 1.32E-06
1.28E-06 9.78E-06 6.69E-07 1.02E-06 2.38E-10 3.74E-06 3.10E-07 3.89E-06 7.31E-08 1.08E-07 4.10E-08 1.69E-06 1.73E-06 1.09E-09
2.06E-05 1.62E-05 2.96E-06 3.13E-06 7.39E-07 3.65E-10 4.98E-07 2.16E-05 5.10E-06 2.52E-09 3.43E-06 9.07E-05 2.14E-05 1.06E-08
1.44E-05 4.03E-06 6.18E-07 1.84E-10 2.47E-10 1.68E-07 5.29E-08 1.32E-11 2.20E-10 0.00E-01 0.00E-01 0.00E-01 0.00E-01 9.19E-06
1.51E-06 2.72E-06 2.40E-07 1.72E-09 5.23E-07 1.14E-06 5.72E-08 1.35E-08 6.66E-12 9.08E-09 1.14E-06 7.52E-09 1.58E-09 6.96E-09
3.75E-09 2.17E-06 2.15E-06 1.42E-08 2.99E-09 4.75E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

5.255E-01 1.276E+00 1.165E+01 3.016E-02 1.438E-03 9.941E-02 4.102E-04 4.102E-04 1.609E-03
2.707E-03 2.227E-04 5.134E-04 5.447E-05 7.757E-05 4.313E-03 9.507E-03 3.106E-02

THE CURRENT MIXING HEIGHT IS 1500.00
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 41.61

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1700.	.22497	102.38159	.00220	.95294	.25397	.00209

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.700E+03	2.094E-03	1.034E-04	1.838E-10	2.540E-01	1.821E-06	1.630E-06	3.486E-02	4.062E-15	2.961E-07	6.075E-06
1.000E+01	2.332E-01	5.331E-05	2.506E-05	8.644E-03	7.590E-05	3.737E-05	1.000E-02	9.133E-03	6.095E-05	4.275E-03
	2.894E-05	1.004E-02	9.802E-04	8.517E-06	2.916E-03	9.916E-03	1.497E-04	1.714E-02	1.257E-04	2.105E-07
	7.406E-05	9.968E-03	1.839E-06	1.310E-05	3.791E-03	2.440E-03	6.416E-04	4.659E-06	0.000E-01	2.224E-03
	1.432E-05	7.007E-05	9.052E-06	1.374E-08	2.448E-08	1.836E-08	1.918E-04	3.274E-07	4.215E-08	4.747E-02
NET RATES	3.931E-06	-3.175E-07	5.730E-06	1.100E-04	5.007E-08	7.901E-09	1.218E-05	1.550E-08	5.814E-08	-2.476E-09
	5.217E-05	-2.121E-07	-1.815E-07	1.535E-05	-3.765E-07	-4.957E-08	2.369E-05	-7.337E-06	-2.749E-07	-2.558E-06
	2.301E-09	-1.548E-05	-1.362E-06	-5.356E-08	-2.764E-06	7.179E-06	-4.340E-07	7.879E-06	-4.475E-07	4.140E-10
	-1.613E-07	-1.433E-05	-1.259E-08	-8.883E-08	-1.039E-05	-1.074E-07	-2.825E-06	-7.450E-08	0.000E-01	-5.914E-06
	-1.355E-07	-2.629E-07	-9.642E-08	-3.726E-10	-2.148E-10	-8.216E-09	-1.068E-06	-1.926E-09	-8.776E-09	0.000E-01

THE REACTION RATES ARE

9.61E-04 8.34E-03 5.27E-09 1.20E-09 7.59E-04 2.91E-05 5.11E-06 1.56E-12 6.42E-06 6.37E-06 4.89E-08 2.44E-09 2.24E-06 1.98E-05
7.19E-03 2.02E-04 2.64E-05 1.75E-04 2.85E-07 5.33E-07 2.45E-07 1.00E-05 1.87E-06 2.22E-05 7.92E-06 6.64E-05 2.16E-04 2.16E-04
4.39E-08 4.14E-05 1.21E-05 1.22E-05 4.15E-07 4.18E-07 2.71E-06 6.34E-06 8.86E-05 4.36E-05 5.87E-04 1.79E-05 8.83E-06 3.14E-06
8.53E-09 1.26E-05 5.15E-06 1.09E-05 2.00E-05 3.60E-05 1.64E-08 7.21E-06 2.95E-05 6.20E-07 3.11E-08 3.38E-05 4.54E-04 6.83E-06
9.73E-06 3.99E-06 4.70E-04 8.39E-06 3.68E-07 7.01E-09 9.94E-06 1.34E-04 2.01E-06 2.86E-06 1.17E-06 1.36E-04 3.74E-07 1.06E-06
9.25E-07 7.72E-06 4.98E-07 6.33E-07 2.28E-10 3.30E-06 2.46E-07 3.46E-06 4.97E-08 7.08E-08 2.90E-08 1.31E-06 1.11E-06 1.09E-09
1.43E-05 1.04E-05 2.25E-06 2.15E-06 4.34E-07 2.07E-10 3.05E-07 1.53E-05 3.09E-06 1.47E-09 2.17E-06 7.11E-05 1.44E-05 6.85E-09
1.01E-05 2.34E-06 4.85E-07 1.33E-10 2.23E-10 5.22E-08 2.22E-08 5.13E-12 1.06E-10 0.00E-01 0.00E-01 0.00E-01 0.00E-01 5.91E-06
9.19E-07 1.77E-06 9.64E-08 3.73E-10 2.51E-07 8.47E-07 2.86E-08 5.78E-09 2.75E-12 4.05E-09 8.54E-07 4.34E-09 1.10E-09 4.01E-09
3.35E-09 1.96E-06 1.96E-06 9.95E-09 2.53E-09 4.75E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

4.588E-01 1.231E+00 1.085E+01 2.830E-02 7.950E-04 8.767E-02 3.136E-04 3.136E-04 1.196E-03
2.187E-03 1.449E-04 3.757E-04 3.776E-05 5.399E-05 3.964E-03 8.761E-03 2.529E-02

THE CURRENT MIXING HEIGHT IS 1500.00
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 54.00

TABLE 2-19 (CONTINUED)

TIME (LDT)	NMOC TOTAL	NMOC/ NOX	NOX TOTAL	NO2 FRACTION	O3 (INSTANT)	NO2 (INSTANT)
1800.	.21773	87.53822	.00249	.96344	.25964	.00240

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HNO3	O*SD	OH	HONO
	CO	HO2	HNO4	H2O2	RO2	RCO3	ROOH	HCHO	RO2R	ALD2
	MCO3	PAN	RCHO	PCO3	PPN	ACET	MGLY	MEK	GLYX	GCO3
	GPAN	ALK4	RO2N	R2O2	ALK7	ALKN	ETHE	PRPE	TBUT	TOLU
	CRES	DIAL	XYLE	TMBZ	RO2P	BZO	NPHE	PHEN	BZN2	NRHC
1.800E+03	2.396E-03	9.092E-05	1.531E-10	2.596E-01	2.495E-06	2.553E-06	3.549E-02	1.457E-15	1.718E-07	6.509E-06
1.000E+01	2.355E-01	3.793E-05	2.040E-05	9.247E-03	5.476E-05	3.006E-05	1.101E-02	8.892E-03	4.530E-05	4.212E-03
	2.316E-05	9.178E-03	9.202E-04	6.908E-06	2.724E-03	1.022E-02	1.268E-04	1.745E-02	1.045E-04	1.620E-07
	6.510E-05	9.340E-03	1.142E-06	8.319E-06	3.350E-03	2.432E-03	5.209E-04	2.213E-06	0.000E-01	1.973E-03
	6.632E-06	5.757E-05	5.691E-06	5.289E-09	7.974E-09	1.011E-08	1.228E-04	2.057E-07	3.223E-08	4.747E-02
NET RATES	5.426E-06	2.854E-07	-9.130E-07	7.795E-05	2.209E-08	2.131E-08	9.118E-06	-2.036E-07	8.796E-08	1.927E-08
	3.034E-05	-2.814E-07	-1.062E-07	6.673E-06	-3.768E-07	-1.822E-07	1.221E-05	-1.458E-06	-2.779E-07	-4.925E-08
	-1.446E-07	-1.344E-05	-7.454E-07	-4.026E-08	-3.358E-06	3.732E-06	-3.476E-07	3.605E-06	-2.899E-07	-1.425E-09
	-1.363E-07	-7.787E-06	-1.245E-08	-8.625E-08	-5.326E-06	-1.309E-07	-1.504E-06	-2.523E-08	0.000E-01	-3.042E-06
	-1.124E-07	-1.614E-07	-3.516E-08	-8.322E-11	-2.674E-10	8.023E-10	-1.169E-06	-2.043E-09	7.059E-10	0.000E-01

THE REACTION RATES ARE

8.15E-04 6.94E-03 5.03E-09 1.15E-09 6.83E-04 3.40E-05 6.15E-06 1.20E-12 1.01E-05 9.97E-06 7.66E-08 3.83E-09 2.53E-06 2.31E-05
6.04E-03 7.22E-05 9.47E-06 6.29E-05 1.45E-07 4.07E-07 2.80E-07 6.64E-06 1.10E-06 1.30E-05 4.70E-06 4.15E-05 1.76E-04 1.76E-04
2.07E-08 3.01E-05 6.15E-06 6.20E-06 4.04E-07 4.08E-07 1.75E-06 3.93E-06 5.62E-05 3.08E-05 5.40E-04 9.20E-06 5.05E-06 2.08E-06
4.44E-09 7.29E-06 3.33E-06 6.07E-06 1.26E-05 2.03E-05 2.19E-08 4.99E-06 1.68E-05 2.83E-07 4.20E-08 2.38E-05 4.16E-04 3.89E-06
5.62E-06 2.57E-06 4.29E-04 4.57E-06 1.93E-07 9.02E-09 7.09E-06 1.24E-04 1.16E-06 1.68E-06 7.66E-07 1.27E-04 2.00E-07 6.33E-07
4.87E-07 4.56E-06 3.35E-07 3.05E-07 2.60E-10 2.91E-06 1.66E-07 3.05E-06 2.72E-08 3.93E-08 1.80E-08 8.96E-07 5.47E-07 1.26E-09
7.79E-06 5.33E-06 1.30E-06 1.17E-06 1.92E-07 9.26E-11 1.52E-07 8.54E-06 1.40E-06 6.74E-10 1.11E-06 4.65E-05 7.61E-06 3.67E-09
6.03E-06 1.10E-06 4.02E-07 9.00E-11 2.48E-10 1.44E-08 1.08E-08 2.03E-12 6.88E-11 0.00E-01 0.00E-01 0.00E-01 0.00E-01 3.04E-06
4.38E-07 9.63E-07 3.52E-08 8.32E-11 6.73E-08 5.38E-07 8.18E-09 1.34E-09 6.46E-13 1.06E-09 5.38E-07 1.70E-09 6.06E-10 1.46E-09
2.88E-09 1.72E-06 1.71E-06 5.42E-09 1.93E-09 4.75E-12

THE PHOTOLYTIC RATE CONSTANTS ARE

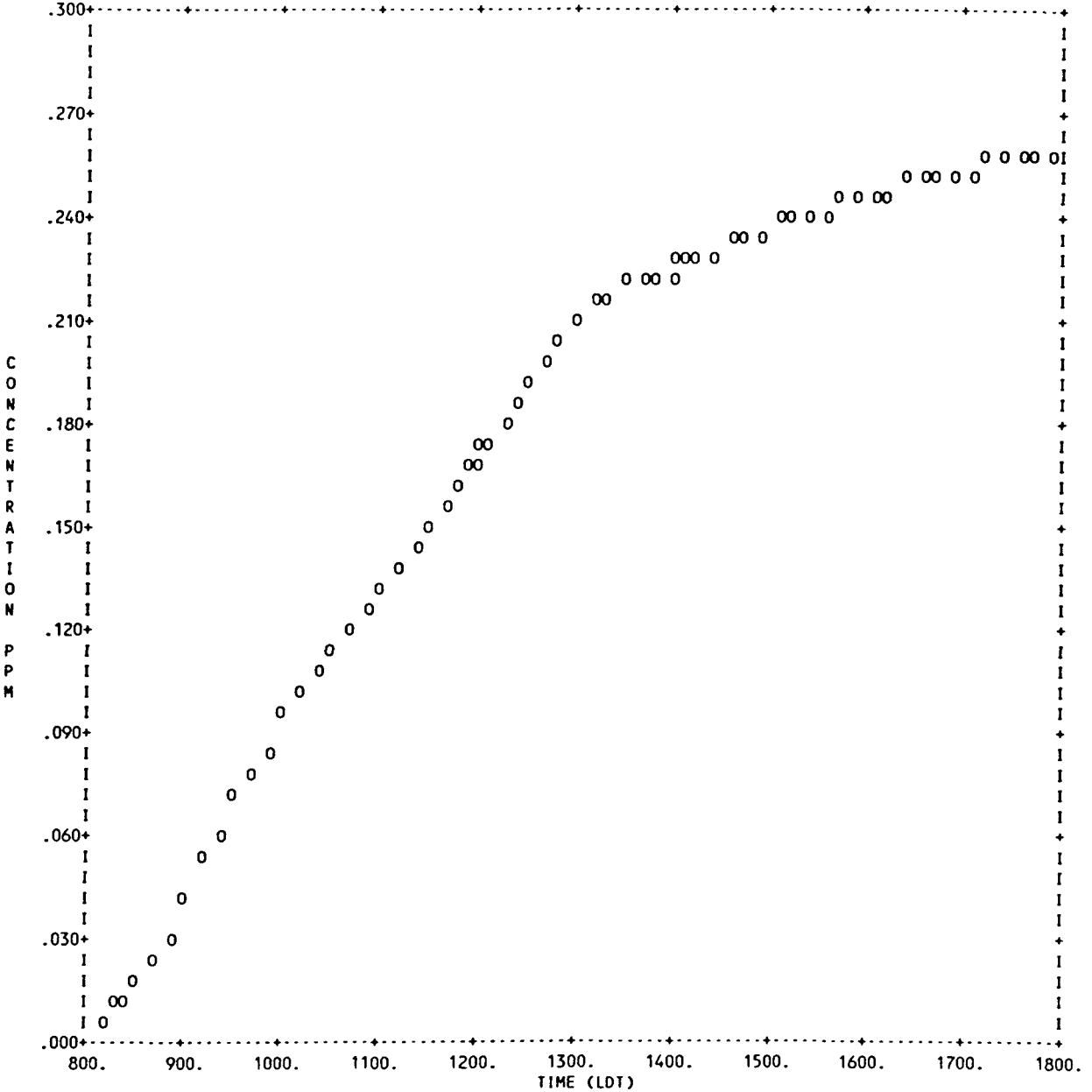
3.401E-01 1.016E+00 9.272E+00 2.327E-02 2.780E-04 6.245E-02 1.887E-04 1.887E-04 6.830E-04
1.422E-03 6.709E-05 2.102E-04 1.953E-05 2.793E-05 3.204E-03 7.062E-03 1.673E-02

THE CURRENT MIXING HEIGHT IS 1500.00
THE CURRENT TEMPERATURE IS 303.00
THE CURRENT ZENITH ANGLE IS 66.27

MAXIMUM O3 NOT REACHED, THE LAST ONE HOUR AVERAGE WAS .25701 PPM.

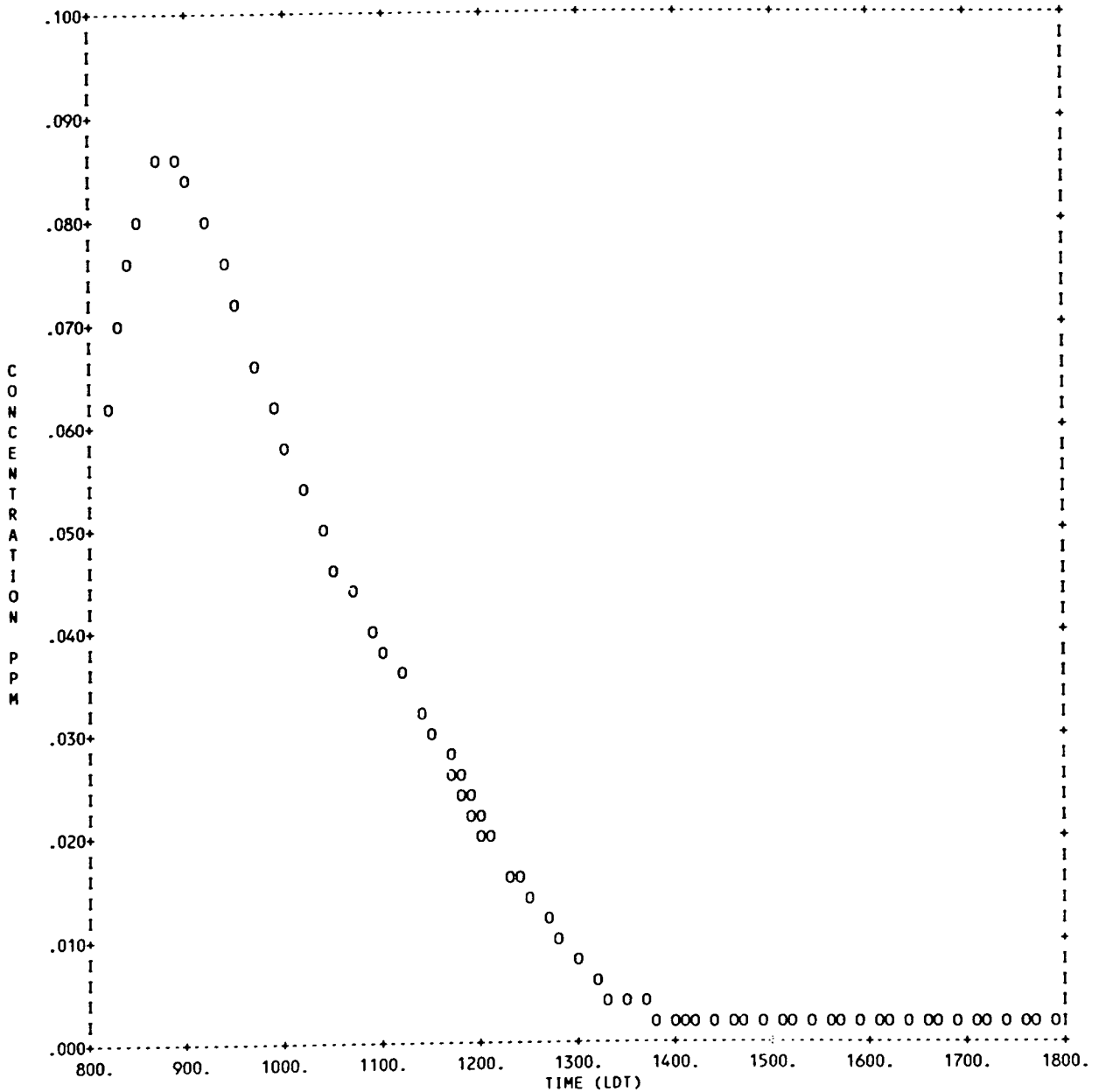
MAXIMUM ONE HOUR AVE NO2 = .08230 CENTERED AT 855. LDT

TABLE 2-19 (CONTINUED)



TEST PROBLEM #3 - OZIPM "CALC" RUN - 131 REACTION MECHANISM
O3 CONCENTRATION AS A FUNCTION OF TIME

TABLE 2-19 (CONTINUED)



TEST PROBLEM #3 - OZIPM "CALC" RUN - 131 REACTION MECHANISM
NO2 CONCENTRATION AS A FUNCTION OF TIME

TABLE 2-20. EXAMPLE #4

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****************************************
*                                      *
*   OZONE ISOPLETH PLOTTING PACKAGE    *
*     WITH OPTIONAL MECHANISMS         *
*                                      *
*             O Z I P M                *
*                                      *
*            VERSION 3.1               *
*                                      *
*          SEPTEMBER, 1985             *
*                                      *
****************************************
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THE INPUTS FOR THIS RUN ARE

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TITL
      TEST PROBLEM #4 - OZIPM "EKMA" RUN - 131 REACTION MECHANISM
MECH          132.      17.      13.       0.     303.
       1.     13.      14.      15.      16.      20.      35.
      42.     46.      47.      52.      61.      69.      71.
      73.     82.     114.
ALK4      ALK7      ETHE      PRPE      TBUT      TOLU      XYLE
TMBZ      HCHO      ALD2      RCHO      MEK       NRHC
 4.5       7.0       2.0       3.0       4.0       7.0       8.0
 9.0       1.0       2.0       3.0       4.0       1.0
NO2       HV     1  1.NO      1. O                       1.00E 00     0.
O                2  1.O3                                 4.87E+07 -1282.
O         NO2    3  1.NO                                 1.37E+04     0.
O         NO2    4  1.NO3                                3.29E+03  -894.
NO        O3     5  1.NO2                                2.68E+01  1370.
NO2       O3     6  1.NO3                                4.77E-02  2450.
NO        NO3    7  2.NO2                                2.75E+04  -252.
NO        NO     8  2.NO2                                1.50E-04  -529.
NO2       NO3    9  1.N2O5                               1.71E+03  -273.
N2O5            10  1.NO2     1. NO3                     2.08E+00 11379.
N2O5            11  2.HNO3                               3.00E-02     0.
NO2       NO3   12  1.NO      1. NO2                     5.98E-01  1229.
NO3       HV    13  1.NO                                 1.00E 00     0.
NO3       HV    14  1.NO2     1. O                       1.00E 00     0.
O3        HV    15  1.O                                  1.00E 00     0.
O3        HV    16  1.O*SD                               1.00E 00     0.
O*SD            17  2.OH                                 6.50E+09     0.
O*SD            18  1.O                                  4.32E+10     0.
NO        OH    19  1.HONO                               9.75E+03  -833.
HONO      HV    20  1.NO      1. OH                      1.00E 00     0.
NO2             21  1.HONO   -1. NO2       1. HNO3       1.17E-04     0.
NO2       OH    22  1.HNO3                               1.68E+04  -737.
HNO3      OH    23  1.NO3                                1.89E+02  -778.
CO        OH    24  1.HO2                                3.22E+02     0.
O3        OH    25  1.HO2                                1.00E+02   942.
NO        HO2   26  1.NO2     1. OH                      1.22E+04  -240.
NO2       HO2   27  1.HNO4                               2.02E+03  -773.
HNO4            28  1.NO2     1. HO2                     4.93E+00 10103.
HNO4      OH    29  1.NO2                                5.91E+03     0.
O3        HO2   30  1.OH                                 2.96E+00   579.
HO2       HO2   31  1.H2O2                               4.46E+03  -771.
HO2       HO2   32  1.H2O2                               5.08E+03 -2971.
NO3       HO2   33  1.HNO3                               4.46E+03  -771.
NO3       HO2   34  1.HNO3                               5.08E+03 -2971.
H2O2      HV    35  2.OH                                 1.00E 00     0.
H2O2      OH    36  1.HO2                                2.45E+03   187.
RO2       NO    37  1.NO                                 1.14E+04  -180.
RCO3      NO    38  1.NO                                 1.14E+04  -180.
RCO3      NO2   39  1.NO2                                7.57E+03  -180.
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TABLE 2-20 (CONTINUED)

THE INPUTS FOR THIS RUN ARE

RO2	HO2		40	1.HO2					4.43E+03	0.
RCO3	HO2		41	1.HO2					4.43E+03	0.
ROOH		HV	42	1.HO2	1. OH				1.00E 00	0.
RO2	RO2		43						1.48E+00	0.
RO2	RCO3		44						4.43E+03	0.
RCO3	RCO3		45						3.69E+03	0.
HCHO		HV	46	2.HO2	1. CO				1.00E 00	0.
HCHO		HV	47	1.CO					1.00E 00	0.
HCHO	OH		48	1.HO2	1. CO				1.33E+04	0.
HCHO	NO3		49	1.HNO3	1. HO2		1. CO		8.82E-01	2060.
HCHO	HO2		50	1.RO2R	1. RO2				1.48E+01	0.
ALD2	OH		51	1.MCO3	1. RCO3				2.36E+04	-250.
ALD2		HV	52	1.CO *	1. HCHO		1. HO2		1.00E 00	0.
1. RO2R			1. RO2							
ALD2	NO3		53	1.HNO3	1. MCO3		1. RCO3		3.69E+00	1427.
MCO3	NO		54	1.NO2 *	1. HCHO		1. RO2R		1.14E+04	-180.
1. RO2										
MCO3	NO2		55	1.PAN					7.57E+03	-180.
MCO3	HO2		56	1.ROOH	1. HCHO				4.43E+03	0.
MCO3	RO2		57	.5HO2	1. HCHO		1. RO2		4.43E+03	0.
MCO3	RCO3		58	1.HO2	1. HCHO		1. RCO3		3.69E+03	0.
PAN			59	1.MCO3	1. NO2		1. RCO3		2.21E-02	13542.
RCHO	OH		60	1.RCO3	1. PCO3				2.93E+04	-252.
RCHO		HV	61	1.ALD2*	1. HO2		1. CO		1.00E 00	0.
1. RO2R			1. RO2							
RCHO	NO3		62	1.HNO3	1. PCO3		1. RCO3		3.63E+00	1432.
PCO3	NO		63	1.NO2 *	1. ALD2		1. RO2R		1.14E+04	-180.
1. RO2										
PCO3	NO2		64	1.P N					7.57E+03	-180.
PCO3	HO2		65	1.ROOH	1. ALD2				4.43E+03	0.
PCO3	RO2		66	.5HO2	1. ALD2		1. RO2		4.43E+03	0.
PCO3	RCO3		67	1.HO2	1. ALD2		1. RCO3		3.69E+03	0.
PPN			68	1.PCO3	1. NO2		1. RCO3		2.21E-02	13542.
ACET		HV	69	1.MCO3*	1. HCHO		1. RCO3		1.00E 00	0.
1. RO2R			1. RO2							
ACET	OH		70	1.MGLY	1. RO2R		1. RO2		3.39E+02	1125.
MEK		HV	71	1.MCO3*	1. ALD2		1. RCO3		1.00E 00	0.
1. RO2R			1. RO2							
MEK	OH		72	1.5RO2R*	1.5 RO2		.5 MCO3		1.46E+03	745.
.5 ALD2		.5 HCHO		.5 PCO3	1. RCO3					
GLYX		HV	73	.13HCHO	1.87 CO				1.00E 00	0.
GLYX	OH		74	.63HO2 *	1.26 CO		.37 GCO3		1.70E+04	0.
.37 RCO3										
GLYX	NO3		75	1.HNO3*	.63 HO2		1.26 CO		8.88E-01	2058.
.37 GCO3		.37 RCO3								
GCO3	NO2		76	1.GPAN					7.57E+03	-180.
GCO3	NO		77	1.NO2	1. HO2		1. CO		1.14E+04	-180.
GPAN			78	1.GCO3	1. NO2		1. RCO3		2.21E-02	13542.
GCO3	HO2		79	1.ROOH	1. CO				4.43E+03	0.
GCO3	RO2		80	.5HO2	1. CO		1. RO2		4.43E+03	0.

THE INPUTS FOR THIS RUN ARE

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GCO3  RCO3      81   1.HO2      1. CO       1. RCO3    3.69E+03     0.
MGLY      HV    82   1.MCO3*    1. HO2      1. CO      1.00E 00     0.
   1. RCO3
MGLY  OH        83   1.MCO3     1. CO       1. RCO3    2.51E+04     0.
MGLY  NO3       84   1.HNO3*    1. MCO3     1. CO      3.69E+00  1427.
   1. RCO3
ALK4  OH        85  .19HCHO*   .31 ALD2    .17 RCHO    4.76E+03   353.
  .34 ACET    .44 MEK      .07 RO2N    .93 RO2R     .6 R2O2    1.6 RO2
ALK7  OH        86  .02HCHO*   .03 ALD2    .25 RCHO    9.11E+03   288.
  .36 ACET    .88 MEK      .18 RO2N    .82 RO2R    .84 R2O2   1.84 RO2
ALKN  OH        87   1.NO2 *   .15 MEK    1.05 RCHO    3.00E+03   709.
  .48 ALD2    .16 HCHO   1.39 R2O2   1.39 RO2
RO2N  NO        88   1.ALKN                           1.14E+04  -180.
RO2N  HO2       89   1.ROOH     1. MEK                4.43E+03     0.
RO2N  RO2       90   1.RO2      .5 HO2      1. MEK    1.48E+00     0.
RO2N  RCO3      91   1.RCO3     .5 HO2      1. MEK    4.43E+03     0.
R2O2  NO        92   1.NO2                            1.14E+04  -180.
R2O2  HO2       93   1.ROOH                           4.43E+03     0.
R2O2  RO2       94   1.RO2                            1.48E+00     0.
R2O2  RCO3      95   1.RCO3                           4.43E+03     0.
RO2R  NO        96   1.NO2      1. HO2                1.14E+04  -180.
RO2R  HO2       97   1.ROOH                           4.43E+03     0.
RO2R  RO2       98   .5HO2      1. RO2                1.48E+00     0.
RO2R  RCO3      99   .5HO2      1. RCO3               4.43E+03     0.
ETHE  OH       100   1.RO2R*    1. RO2    1.56 HCHO   1.26E+04  -411.
  .22 ALD2
ETHE  O3       101   1.HCHO    .12 HO2     .42 CO     2.57E-03  2634.
ETHE  O        102   1.HCHO*    1. HO2      1. CO     1.08E+03   792.
   1. RO2R     1. RO2
ETHE  NO3      103   1.NO2 *    2. HCHO     1. R2O2   1.62E-01  2923.
   1. RO2
PRPE  OH       104   1.RO2R*    1. HCHO     1. ALD2   3.89E+04  -504.
   1. RO2
PRPE  O3       105  .64HCHO*    .5 ALD2    .28 CO     1.67E-02  2105.
  .06 OH      .17 HO2      .13 RO2R    .13 RO2
PRPE  O        106   .6ACET*    .4 HCHO     .2 ALD2   5.88E+03   324.
   .2 HO2      .6 RO2R      .4 CO       .6 RO2
PRPE  NO3      107   1.NO2 *    1. HCHO     1. ALD2   1.12E+01  1935.
   1. R2O2     1. RO2
TBUT  OH       108   1.RO2R     2. ALD2     1. RO2    9.42E+04  -549.
TBUT  O3       109   1.ALD2*   .15 CO      .27 RO2R   2.96E-01  1137.
  .12 OH      .21 HO2      .27 RO2     .30 HCHO
TBUT  O        110   1.MEK      .4 HO2                3.45E+04   -10.
TBUT  NO3      111   1.NO2 *    2. ALD2     1. R2O2   5.61E+02   975.
   1. RO2
TOLU  OH       112  .16CRES*   .16 HO2     .84 RO2R   9.14E+03  -322.
   .4 DIAL    .84 RO2     .144 MGLY   .114 GLYX
DIAL  OH       113   1.PCO3     1. RCO3               4.43E+04     0.
DIAL      HV   114   1.HO2 *    1. CO       1. MCO3   1.00E 00     0.
   1. RCO3
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THE INPUTS FOR THIS RUN ARE

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XYLE  OH        115  .17CRES*   .17 HO2     .83 RO2R    3.62E+04  -116.
  .83 RO2     .65 DIAL   .316 MGLY   .095 GLYX
TMBZ  OH        116  .17CRES*   .17 HO2     .83 RO2R    9.16E+04     0.
  .83 RO2     .49 DIAL    .86 MGLY
CRES  OH        117   .2MGLY*   .15 RO2P    .85 RO2R    5.91E+04     0.
   1. RO2
CRES  NO3       118   1.HNO3     1. BZO                 3.25E+04     0.
RO2P  NO        119   1.NPHE                            1.14E+04  -180.
RO2P  HO2       120   1.ROOH                            4.43E+03     0.
RO2P  RO2       121   .5HO2      1. RO2                 1.48E+00     0.
RO2P  RCO3      122   .5HO2      1. RCO3                4.43E+03     0.
BZO   NO2       123   1.NPHE                            2.22E+04     0.
BZO   HO2       124   1.PHEN                            4.43E+03     0.
BZO             125   1.PHEN                            6.00E-02     0.
PHEN  OH        126   .2GLYX*   .15 RO2P    .85 RO2R    4.14E+04     0.
   1. RO2
PHEN  NO3       127   1.HNO3     1. BZO                 5.62E+03     0.
NPHE  NO3       128   1.HNO3     1. BZN2                5.62E+03     0.
BZN2  NO2       129                                     2.22E+04     0.
BZN2  HO2       130   1.NPHE                            4.43E+03     0.
BZN2            131   1.NPHE                            6.00E-02     0.
NRHC            132   1.NRHC                            1.00E-10     0.
ZENITH           17.
1.          1.0       1.0       1.0       1.0       1.0       1.0
   1.0      1.0       1.0       1.0
13.         2.3       2.3       2.3       2.3       2.4       2.6
   2.8      3.3       4.1       2.8
14.         20.       20.       21.       21.       22.       23.
   25.      30.       36.       26.
15.      5.52E-02  5.53E-02  5.56E-02  5.61E-02  5.71E-02  5.99E-02
  6.45E-02 7.43E-02  8.90E-02  6.60E-02
16.      4.56E-03  4.45E-03  4.12E-03  3.56E-03  2.86E-03  2.06E-03
  1.26E-03 5.98E-04  2.80E-04  1.54E-04
20.       .20       .20       .20       .20       .19       .19
   .19     .18       .18       .19
35.      9.08E-04  9.03E-04  8.82E-04  8.45E-04  7.91E-04  7.18E-04
  6.25E-04 5.12E-04  4.31E-04  3.83E-04
42.      9.08E-04  9.03E-04  8.82E-04  8.45E-04  7.91E-04  7.18E-04
  6.25E-04 5.12E-04  4.31E-04  3.83E-04
46.      3.65E-03  3.62E-03  3.53E-03  3.36E-03  3.11E-03  2.77E-03
  2.33E-03 1.81E-03  1.41E-03  1.10E-03
47.      5.59E-03  5.57E-03  5.50E-03  5.38E-03  5.19E-03  4.91E-03
  4.51E-03 3.97E-03  3.57E-03  3.43E-03
52.      5.87E-04  5.79E-04  5.51E-04  5.01E-04  4.36E-04  3.53E-04
  2.58E-04 1.63E-04  1.01E-04  5.98E-05
61.      1.19E-03  1.18E-03  1.14E-03  1.08E-03  9.94E-04  8.75E-04
  7.26E-04 5.53E-04  4.27E-04  3.31E-04
69.      1.34E-04  1.32E-04  1.27E-04  1.18E-04  1.06E-04  8.97E-05
  7.05E-05 4.98E-05  3.55E-05  2.49E-05
71.      1.91E-04  1.89E-04  1.82E-04  1.69E-04  1.51E-04  1.28E-04
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TABLE 2-20 (CONTINUED)

THE INPUTS FOR THIS RUN ARE

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  1.01E-04  7.11E-05  5.07E-05  3.56E-05
73.         7.79E-03  7.81E-03  7.87E-03  7.97E-03  8.17E 03  8.46E-03
  8.97E-03  9.88E-03  1.09E-02  9.73E-03
82.         1.72E-02  1.72E-02  1.74E-02  1.76E-02  1.80E-02  1.87E-02
  1.98E-02  2.17E-02  2.37E-02  2.14E-02
114.        6.38E-02  6.36E-02  6.29E-02  6.15E-02  5.95E-02  5.66E-02
  5.25E-02  4.70E-02  4.29E-02  4.27E-02
PLAC          39.000     77.00       5.0      1986.       8.0       21.
WASHINGTON, D.C.
DILU             250.      1000.      800.      1200.
REAC              13.       .25
      .260      .230      .020      .040      .020      .180      .080
      .030      .030      .020      .000      .000      .090
INIT              1.
CO
1.00
EMIS             -5.       .10       .10       .10       .05       .05
       .15       .15       .15       .075      .075
TRAN                       .060     -13.      -13.
      .001      .260      .230      .020      .040      .020      .180
      .080      .030      .030      .020      .000      .000      .090
      .030      .300      .200      .020      .010      .000      .100
      .020      .000      .040      .020      .000      .000      .290
EKMA              .210      8.0                1.0
      .000      .060      .001      .030
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TABLE 2-20 (CONTINUED)

THE REACTIONS											RATE CONSTANT	ACT. ENERGY(K)
1	NO2			=	NO	+	O				1.000E+00	0.000E-01
2	O			=	O3						4.870E+07	-1.282E+03
3	O	+	NO2	=	NO						1.370E+04	0.000E-01
4	O	+	NO2	=	NO3						3.290E+03	-8.940E+02
5	NO	+	O3	=	NO2						2.680E+01	1.370E+03
6	NO2	+	O3	=	NO3						4.770E-02	2.450E+03
7	NO	+	NO3	=	2 NO2						2.750E+04	-2.520E+02
8	NO	+	NO	=	2 NO2						1.500E-04	-5.290E+02
9	NO2	+	NO3	=	N2O5						1.710E+03	-2.730E+02
10	N2O5			=	NO2	+	NO3				2.080E+00	1.138E+04
11	N2O5			=	2 HNO3						3.000E-02	0.000E-01
12	NO2	+	NO3	=	NO	+	NO2				5.980E-01	1.229E+03
13	NO3			=	NO						1.000E+00	0.000E-01
14	NO3			=	NO2	+	O				1.000E+00	0.000E-01
15	O3			=	O						1.000E+00	0.000E-01
16	O3			=	O*SD						1.000E+00	0.000E-01
17	O*SD			=	2 OH						6.500E+09	0.000E-01
18	O*SD			=	O						4.320E+10	0.000E-01
19	NO	+	OH	=	HONO						9.750E+03	-8.330E+02
20	HONO			=	NO	+	OH				1.000E+00	0.000E-01
21	NO2			=	HONO	-	NO2	+	HNO3		1.170E-04	0.000E-01
22	NO2	+	OH	=	HNO3						1.680E+04	-7.370E+02
23	HNO3	+	OH	=	NO3						1.890E+02	-7.780E+02
24	CO	+	OH	=	HO2						3.220E+02	0.000E-01
25	O3	+	OH	=	HO2						1.000E+02	9.420E+02
26	NO	+	HO2	=	NO2	+	OH				1.220E+04	-2.400E+02
27	NO2	+	HO2	=	HNO4						2.020E+03	-7.730E+02
28	HNO4			=	NO2	+	HO2				4.930E+00	1.010E+04
29	HNO4	+	OH	=	NO2						5.910E+03	0.000E-01
30	O3	+	HO2	=	OH						2.960E+00	5.790E+02
31	HO2	+	HO2	=	H2O2						4.460E+03	-7.710E+02
32	HO2	+	HO2	=	H2O2						5.080E+03	-2.971E+03
33	NO3	+	HO2	=	HNO3						4.460E+03	-7.710E+02
34	NO3	+	HO2	=	HNO3						5.080E+03	-2.971E+03
35	H2O2			=	2 OH						1.000E+00	0.000E-01
36	H2O2	+	OH	=	HO2						2.450E+03	1.870E+02
37	RO2	+	NO	=	NO						1.140E+04	-1.800E+02
38	RCO3	+	NO	=	NO						1.140E+04	-1.800E+02
39	RCO3	+	NO2	=	NO2						7.570E+03	-1.800E+02
40	RO2	+	HO2	=	HO2						4.430E+03	0.000E-01
41	RCO3	+	HO2	=	HO2						4.430E+03	0.000E-01
42	ROOH			=	HO2	+	OH				1.000E+00	0.000E-01
43	RO2	+	RO2	=							1.480E+00	0.000E-01
44	RO2	+	RCO3	=							4.430E+03	0.000E-01
45	RCO3	+	RCO3	=							3.690E+03	0.000E-01
46	HCHO			=	2 HO2	+	CO				1.000E+00	0.000E-01
47	HCHO			=	CO						1.000E+00	0.000E-01
48	HCHO	+	OH	=	HO2	+	CO				1.330E+04	0.000E-01
49	HCHO	+	NO3	=	HNO3	+	HO2	+	CO		8.820E-01	2.060E+03
50	HCHO	+	HO2	=	RO2R	+	RO2				1.480E+01	0.000E-01

TABLE 2-20 (CONTINUED)

THE REACTIONS														RATE CONSTANT	ACT. ENERGY(K)
51	ALD2	+	OH	=		MCO3	+	RCO3						2.360E+04	-2.500E+02
52	ALD2			=		CO	+	HCHO	+	HO2	+	RO2R	+ RO2	1.000E+00	0.000E-01
53	ALD2	+	NO3	=		HNO3	+	MCO3	+	RCO3				3.690E+00	1.427E+03
54	MCO3	+	NO	=		NO2	+	HCHO	+	RO2R	+	RO2		1.140E+04	-1.800E+02
55	MCO3	+	NO2	=		PAN								7.570E+03	-1.800E+02
56	MCO3	+	HO2	=		ROOH	+	HCHO						4.430E+03	0.000E-01
57	MCO3	+	RO2	=	0.5	HO2	+	HCHO	+	RO2				4.430E+03	0.000E-01
58	MCO3	+	RCO3	=		HO2	+	HCHO	+	RCO3				3.690E+03	0.000E-01
59	PAN			=		MCO3	+	NO2	+	RCO3				2.210E-02	1.354E+04
60	RCHO	+	OH	=		RCO3	+	PCO3						2.930E+04	-2.520E+02
61	RCHO			=		ALD2	+	HO2	+	CO	+	RO2R	+ RO2	1.000E+00	0.000E-01
62	RCHO	+	NO3	=		HNO3	+	PCO3	+	RCO3				3.630E+00	1.432E+03
63	PCO3	+	NO	=		NO2	+	ALD2	+	RO2R	+	RO2		1.140E+04	-1.800E+02
64	PCO3	+	NO2	=		PPN								7.570E+03	-1.800E+02
65	PCO3	+	HO2	=		ROOH	+	ALD2						4.430E+03	0.000E-01
66	PCO3	+	RO2	=	0.5	HO2	+	ALD2	+	RO2				4.430E+03	0.000E-01
67	PCO3	+	RCO3	=		HO2	+	ALD2	+	RCO3				3.690E+03	0.000E-01
68	PPN			=		PCO3	+	NO2	+	RCO3				2.210E-02	1.354E+04
69	ACET			=		MCO3	+	HCHO	+	RCO3	+	RO2R	+ RO2	1.000E+00	0.000E-01
70	ACET	+	OH	=		MGLY	+	RO2R	+	RO2				3.390E+02	1.125E+03
71	MEK			=		MCO3	+	ALD2	+	RCO3	+	RO2R	+ RO2	1.000E+00	0.000E-01
72	MEK	+	OH	=	1.5	RO2R	+ 1.5	RO2	+ 0.5	MCO3	+ 0.5	ALD2	+ 0.5 HCHO + 0.5 PCO3 + RCO3	1.460E+03	7.450E+02
73	GLYX			=	0.13	HCHO	+ 1.87	CO						1.000E+00	0.000E-01
74	GLYX	+	OH	=	0.63	HO2	+ 1.26	CO	+ 0.37	GCO3	+ 0.37	RCO3		1.700E+04	0.000E-01
75	GLYX	+	NO3	=		HNO3	+ 0.63	HO2	+ 1.26	CO	+ 0.37	GCO3	+ 0.37 RCO3	8.880E-01	2.058E+03
76	GCO3	+	NO2	=		GPAN								7.570E+03	-1.800E+02
77	GCO3	+	NO	=		NO2	+	HO2	+	CO				1.140E+04	-1.800E+02
78	GPAN			=		GCO3	+	NO2	+	RCO3				2.210E-02	1.354E+04
79	GCO3	+	HO2	=		ROOH	+	CO						4.430E+03	0.000E-01
80	GCO3	+	RO2	=	0.5	HO2	+	CO	+	RO2				4.430E+03	0.000E-01
81	GCO3	+	RCO3	=		HO2	+	CO	+	RCO3				3.690E+03	0.000E-01
82	MGLY			=		MCO3	+	HO2	+	CO	+	RCO3		1.000E+00	0.000E-01
83	MGLY	+	OH	=		MCO3	+	CO	+	RCO3				2.510E+04	0.000E-01
84	MGLY	+	NO3	=		HNO3	+	MCO3	+	CO	+	RCO3		3.690E+00	1.427E+03
85	ALK4	+	OH	=	0.19	HCHO	+ 0.31	ALD2	+ 0.17	RCHO	+ 0.34	ACET	+ 0.44 MEK + 0.07 RO2N + 0.93 RO2R + 0.60 R2O2 + 1.6 RO2	4.760E+03	3.530E+02
86	ALK7	+	OH	=	.2	HCHO	+ .3	ALD2	+ 0.25	RCHO	+ 0.36	ACET	+ 0.88 MEK + 0.18 RO2N + 0.82 RO2R + 0.84 R2O2 + 1.84 RO2	9.110E+03	2.880E+02
87	ALKN	+	OH	=		NO2	+ 0.15	MEK	+ 1.5	RCHO	+ 0.48	ALD2	+ 0.16 HCHO + 1.39 R2O2 + 1.39 RO2	3.000E+03	7.090E+02
88	RO2N	+	NO	=		ALKN								1.140E+04	-1.800E+02
89	RO2N	+	HO2	=		ROOH	+	MEK						4.430E+03	0.000E-01

TABLE 2-20 (CONTINUED)

THE REACTIONS														RATE CONSTANT	ACT. ENERGY(K)
90	RO2N	+	RO2	=		RO2	+	0.5	HO2	+		MEK		1.480E+00	0.000E-01
91	RO2N	+	RCO3	=		RCO3	+	0.5	HO2	+		MEK		4.430E+03	0.000E-01
92	R2O2	+	NO	=		NO2								1.140E+04	-1.800E+02
93	R2O2	+	HO2	=		ROOH								4.430E+03	0.000E-01
94	R2O2	+	RO2	=		RO2								1.480E+00	0.000E-01
95	R2O2	+	RCO3	=		RCO3								4.430E+03	0.000E-01
96	RO2R	+	NO	=		NO2	+		HO2					1.140E+04	-1.800E+02
97	RO2R	+	HO2	=		ROOH								4.430E+03	0.000E-01
98	RO2R	+	RO2	=	0.5	HO2	+		RO2					1.480E+00	0.000E-01
99	RO2R	+	RCO3	=	0.5	HO2	+		RCO3					4.430E+03	0.000E-01
100	ETHE	+	OH	=		RO2R	+		RO2	+	1.56	HCHO	+ 0.22 ALD2	1.260E+04	-4.110E+02
101	ETHE	+	O3	=		HCHO	+	0.12	HO2	+	0.42	CO		2.570E-03	2.634E+03
102	ETHE	+	O	=		HCHO	+		HO2	+		CO	+ RO2R	1.080E+03	7.920E+02
				+		RO2									
103	ETHE	+	NO3	=		NO2	+	2	HCHO	+		R2O2	+ RO2	1.620E-01	2.923E+03
104	PRPE	+	OH	=		RO2R	+		HCHO	+		ALD2	+ RO2	3.890E+04	-5.040E+02
105	PRPE	+	O3	=	0.64	HCHO	+	0.5	ALD2	+	0.28	CO	+ . 6 OH	1.670E-02	2.105E+03
				+	0.17	HO2	+	0.13	RO2R	+	0.13	RO2			
106	PRPE	+	O	=	0.6	ACET	+	0.4	HCHO	+	0.2	ALD2	+ 0.2 HO2	5.880E+03	3.240E+02
				+	0.6	RO2R	+	0.4	CO	+	0.6	RO2			
107	PRPE	+	NO3	=		NO2	+		HCHO	+		ALD2	+ R2O2	1.120E+01	1.935E+03
				+		RO2									
108	TBUT	+	OH	=		RO2R	+	2	ALD2	+		RO2		9.420E+04	-5.490E+02
109	TBUT	+	O3	=		ALD2	+	0.15	CO	+	0.27	RO2R	+ 0.12 OH	2.960E-01	1.137E+03
				+	0.21	HO2	+	0.27	RO2	+	0.3	HCHO			
110	TBUT	+	O	=		MEK	+	0.4	HO2					3.450E+04	-1.000E+01
111	TBUT	+	NO3	=		NO2	+	2	ALD2	+		R2O2	+ RO2	5.610E+02	9.750E+02
112	TOLU	+	OH	=	0.16	CRES	+	0.16	HO2	+	0.84	RO2R	+ 0.4 DIAL	9.140E+03	-3.220E+02
				+	0.84	RO2	+	0.144	MGLY	+	0.114	GLYX			
113	DIAL	+	OH	=		PCO3	+		RCO3					4.430E+04	0.000E-01
114	DIAL			=		HO2	+		CO	+		MCO3	+ RCO3	1.000E+00	0.000E-01
115	XYLE	+	OH	=	0.17	CRES	+	0.17	HO2	+	0.83	RO2R	+ 0.83 RO2	3.620E+04	-1.160E+02
				+	0.65	DIAL	+	0.316	MGLY	+	. 95	GLYX			
116	TMBZ	+	OH	=	0.17	CRES	+	0.17	HO2	+	0.83	RO2R	+ 0.83 RO2	9.160E+04	0.000E-01
				+	0.49	DIAL	+	0.86	MGLY						
117	CRES	+	OH	=	0.2	MGLY	+	0.15	RO2P	+	0.85	RO2R	+ RO2	5.910E+04	0.000E-01
118	CRES	+	NO3	=		HNO3	+		BZO					3.250E+04	0.000E-01
119	RO2P	+	NO	=		NPHE								1.140E+04	-1.800E+02
120	RO2P	+	HO2	=		ROOH								4.430E+03	0.000E-01
121	RO2P	+	RO2	=	0.5	HO2	+		RO2					1.480E+00	0.000E-01
122	RO2P	+	RCO3	=	0.5	HO2	+		RCO3					4.430E+03	0.000E-01
123	BZO	+	NO2	=		NPHE								2.220E+04	0.000E-01
124	BZO	+	HO2	=		PHEN								4.430E+03	0.000E-01
125	BZO			=		PHEN								6.000E-02	0.000E-01
126	PHEN	+	OH	=	0.2	GLYX	+	0.15	RO2P	+	0.85	RO2R	+ RO2	4.140E+04	0.000E-01
127	PHEN	+	NO3	=		HNO3	+		BZO					5.620E+03	0.000E-01
128	NPHE	+	NO3	=		HNO3	+		BZN2					5.620E+03	0.000E-01
129	BZN2	+	NO2	=										2.220E+04	0.000E-01
130	BZN2	+	HO2	=		NPHE								4.430E+03	0.000E-01
131	BZN2			=		NPHE								6.000E-02	0.000E-01
132	NRHC			=		NRHC								1.000E-10	0.000E-01

TABLE 2-20 (CONTINUED)

THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION NO.	SPECIES	ZENITH ANGLE (DEG) 0	10	20	30	40	50	60	70	78	86
1	NO2	6.00E-01	5.95E-01	5.86E-01	5.64E-01	5.32E-01	4.85E-01	4.09E-01	2.88E-01	1.55E-01	3.49E-02
13	NO3	1.38E+00	1.37E+00	1.35E+00	1.30E+00	1.28E+00	1.26E+00	1.14E+00	9.51E-01	6.36E-01	9.77E-02
14	NO3	1.20E+01	1.19E+01	1.23E+01	1.18E+01	1.17E+01	1.12E+01	1.02E+01	8.65E+00	5.59E+00	9.07E-01
15	O3	3.31E-02	3.29E-02	3.26E-02	3.16E-02	3.04E-02	2.91E-02	2.64E-02	2.14E-02	1.38E-02	2.30E-03
16	O3	2.74E-03	2.65E-03	2.41E-03	2.01E-03	1.52E-03	9.99E-04	5.15E-04	1.72E-04	4.35E-05	5.37E-06
20	HONO	1.20E-01	1.19E-01	1.17E-01	1.13E-01	1.01E-01	9.22E-02	7.77E-02	5.19E-02	2.79E-02	6.63E-03
35	H2O2	5.45E-04	5.37E-04	5.16E-04	4.77E-04	4.21E-04	3.48E-04	2.55E-04	1.48E-04	6.69E-05	1.34E-05
42	ROOH	5.45E-04	5.37E-04	5.16E-04	4.77E-04	4.21E-04	3.48E-04	2.55E-04	1.48E-04	6.69E-05	1.34E-05
46	HCHO	2.19E-03	2.15E-03	2.07E-03	1.90E-03	1.65E-03	1.34E-03	9.52E-04	5.22E-04	2.19E-04	3.84E-05
47	HCHO	3.35E-03	3.32E-03	3.22E-03	3.04E-03	2.76E-03	2.38E-03	1.84E-03	1.14E-03	5.54E-04	1.20E-04
52	ALD2	3.52E-04	3.45E-04	3.23E-04	2.83E-04	2.32E-04	1.71E-04	1.05E-04	4.70E-05	1.57E-05	2.09E-06
61	RCHO	7.14E-04	7.02E-04	6.68E-04	6.09E-04	5.29E-04	4.24E-04	2.97E-04	1.59E-04	6.63E-05	1.16E-05
69	ACET	8.04E-05	7.86E-05	7.44E-05	6.66E-05	5.64E-05	4.35E-05	2.88E-05	1.44E-05	5.51E-06	8.69E-07
71	MEK	1.15E-04	1.12E-04	1.07E-04	9.53E-05	8.03E-05	6.21E-05	4.13E-05	2.05E-05	7.87E-06	1.24E-06
73	GLYX	4.67E-03	4.65E-03	4.61E-03	4.50E-03	4.34E-03	4.10E-03	3.67E-03	2.85E-03	1.69E-03	3.40E-04
82	MGLY	1.03E-02	1.02E-02	1.02E-02	9.93E-03	9.57E-03	9.07E-03	8.09E-03	6.25E-03	3.68E-03	7.47E-04
114	DIAL	3.83E-02	3.79E-02	3.68E-02	3.47E-02	3.16E-02	2.75E-02	2.15E-02	1.35E-02	6.66E-03	1.49E-03

TABLE 2-20 (CONTINUED)

TEST PROBLEM #4 - OZIPM "EKMA" RUN - 131 REACTION MECHANISM

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

WASHINGTON, D.C.

LATITUDE	39.000			
LONGITUDE	77.000			
TIME ZONE	5.0			
DATE	8	21	1986	
TIME	800	TO	1800	LOCAL DAYLIGHT TIME

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS	INITIAL	250.	FINAL	1000.
TIMING	START	800.	STOP	1200.

MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME	800	900	1000	1100	1200
HEIGHT	250.0	449.5	679.6	869.6	1000.0

REACTIVITY

EMISSIONS	ALK4 FRACTION	.260	ALK7 FRACTION	.230	ETHE FRACTION	.020	
EMISSIONS	PRPE FRACTION	.040	TBUT FRACTION	.020	TOLU FRACTION	.180	
EMISSIONS	XYLE FRACTION	.080	TMBZ FRACTION	.030	HCHO FRACTION	.030	
EMISSIONS	ALD2 FRACTION	.020	RCHO FRACTION	.000	MEK FRACTION	.000	
EMISSIONS	NRHC FRACTION	.090					

TABLE 2-20 (CONTINUED)

SURFACE LAYER	ALK4 FRACTION	.260	ALK7 FRACTION	.230	ETHE FRACTION	.020	
SURFACE LAYER	PRPE FRACTION	.040	TBUT FRACTION	.020	TOLU FRACTION	.180	
SURFACE LAYER	XYLE FRACTION	.080	TMBZ FRACTION	.030	HCHO FRACTION	.030	
SURFACE LAYER	ALD2 FRACTION	.020	RCHO FRACTION	.000	MEK FRACTION	.000	
SURFACE LAYER	NRHC FRACTION	.090					
ALOFT	ALK4 FRACTION	.300	ALK7 FRACTION	.200	ETHE FRACTION	.020	
ALOFT	PRPE FRACTION	.010	TBUT FRACTION	.000	TOLU FRACTION	.100	
ALOFT	XYLE FRACTION	.020	TMBZ FRACTION	.000	HCHO FRACTION	.040	
ALOFT	ALD2 FRACTION	.020	RCHO FRACTION	.000	MEK FRACTION	.000	
ALOFT	NRHC FRACTION	.290					
NO2/NOX	.250						

TRANSPORTED CONCENTRATIONS

SURFACE LAYER	OZONE	.000	HYDROCARBON	.001	NOX	.000 PPM
SURFACE LAYER	CO	1.000				
ALOFT	OZONE	.060	HYDROCARBON	.030	NOX	.000 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES	HOUR	1	2	3	4	5
VOC	FRACTION	.100	.100	.100	.050	.050
NOX	FRACTION	.150	.150	.150	.075	.075

TABLE 2-20 (CONTINUED)

EKMA CALCULATIONS ARE PERFORMED TO ESTIMATE

SITE-SPECIFIC VOC CONTROL REQUIREMENTS

BASE YEAR OZONE	.210 PPM
BASE YEAR NMOC/NOX	8.000
ANTICIPATED CHANGE IN NOX	.000 PERCENT
FUTURE OZONE TRANSPORTED ALOFT	.060 PPM
FUTURE NMOC TRANSPORTED ALOFT	.030 PPMC
FUTURE NOX TRANSPORTED ALOFT	.000 PPM
FUTURE OZONE IN THE SURFACE LAYER	.000 PPM
FUTURE NMOC IN THE SURFACE LAYER	.001 PPMC
FUTURE NOX IN THE SURFACE LAYER	.000 PPM

THE FOLLOWING SIMULATIONS WERE DONE.

NMOC	NOX	RATIO	O3	TIME
1.00000	.12500	8.00000	.19632	NOT MAX
1.06969	.13371	8.00000	.20346	NOT MAX
1.13349	.14169	8.00000	.20980	NOT MAX
.11335	.14169	.80000	.02505	1218.
.54299	.14169	3.83234	.07154	NOT MAX
.99075	.14169	6.99258	.18472	NOT MAX
.73470	.14169	5.18538	.11399	NOT MAX
.76186	.14169	5.37711	.12116	NOT MAX
.75745	.14169	5.34600	.11996	NOT MAX

VOC CONTROL REQUIREMENT IS 33.2 PERCENT

3. SPECIATION OF NONMETHANE ORGANIC COMPOUNDS

Knowledge of NMOC speciation is essential for modeling urban ozone air quality with up-to-date chemical mechanisms. Most photochemical air quality simulation models require NMOC speciation information for emissions, initial concentrations, and boundary concentrations. The speciation data needs to be compiled using the NMOC classification scheme that is used by the specific mechanism incorporated into the simulation model. The NMOC classes in the SAPRC/ERT OZIPM mechanism are shown in Table 3-1. Also shown in the table are the molecular weights and number of carbons per molecule of the surrogate species used to represent each class of compounds. Photochemical models require this information to convert concentrations and emissions from mass and molar carbon units to molar units.

The classification scheme shown in Table 3-1 is also recommended for the initial compilation of data for use with the condensed mechanism since proper use of that mechanism requires knowledge of the splits between the two alkane classes, the two higher alkene classes, and the two higher aromatic classes. Final inputs for the condensed mechanism should be classified into the classes shown in Table 3-2.

3.1 Assignment of Individual Species to Classes

The assignment of individual organic species to the organic classes in the OZIPM mechanism is shown in Table 3-3. Given detailed chemical speciation for either emissions or ambient concentrations, the individual species should be classified according to the assignments shown in the table. Unlike the Carbon Bond approach, where almost all species are divided into two or more classes, all of the carbon in individual species is assigned to one compound class in this classification scheme. The only exceptions to this are propane, methanol, and benzene, which are split between the C4-C5 alkanes and nonreactive classes. Also included in the table are estimates of the uncertainty in the assignments. The uncertainty is expressed on a scale of 0 to 4, where 0 indicates that the species is treated explicitly in the mechanism, and 4 indicates that reactivity is totally unknown.

TABLE 3-1

NMOC CLASSES FOR THE OZIPM MECHANISM

Compound Class	Symbol	Molecular Weight	No. of Carbons Per Molecule
Ethene	ETHE	28.	2
Terminal Alkenes	PRPE	42.	3
Internal Alkenes	TBUT	56.	4
C4-C5 Alkanes	ALK4	65.	4.5
C6+ Alkanes	ALK7	100.	7
Mono-Alkylbenzenes	TOLU	92.	7
Di-Alkylbenzenes	XYLE	106.	8
Tri-Alkylbenzenes	TMBZ	120.	9
Formaldehyde	HCHO	30.	1
Acetaldehyde	ALD2	46.	2
Higher Aldehydes	RCHO	58.	3
Ketones	MEK	72.	4
Nonreactive	NROG	15.	1

TABLE 3-2

NMOC CLASSES FOR THE CONDENSED MECHANISM

Compound Class	Symbol	Molecular Weight	No. of Carbons Per Molecule
Ethene	ETHE	28.	2
Higher Alkenes	ALKE	47.6*	3.4*
C4+ Alkanes	ALKA	84.9*	5.92*
Mono-Alkylbenzenes	TOLU	92.	7
Higher Aromatics	AROM	111.6*	8.4*
Formaldehyde	HCHO	30.	1
Higher Aldehydes	ALD2	46.	2
Ketones	MEK	72.	4
Nonreactive	NROG	15.	1

*Default values. Speciated emissions inventory data should be used, if available, to determine more accurate values.

TABLE 3-3

ORGANIC SPECIES CLASSIFICATION FOR THE OZIPM CHEMICAL MECHANISM

ID No.	Compound Name	Classification	Uncertainty Classification
43814	1,1,1-TRICHLOROETHANE	NONREACTIVE	1
43820	1,1,2-TRICHLOROETHANE	NONREACTIVE	1
43813	1,1-DICHLOROETHANE	NONREACTIVE	1
45225	1,2,3-TRIMETHYLBENZENE	TRI-ALKYL BENZENE	1
45208	1,2,4-TRIMETHYLBENZENE	TRI-ALKYL BENZENE	1
99016	1,2-DICHLOROPROPANE	NONREACTIVE	1
45207	1,3,5-TRIMETHYLBENZENE	TRI-ALKYL BENZENE	0
43218	1,3-BUTADIENE	INTERNAL ALKENES	2
46201	1,4-DIOXANE	C6+ ALKANES	2
43213	1-BUTENE	TERMINAL ALKENES	1
98104	1-CHLOROBUTANE	C4-C5 ALKANES	2
43268	1-DECENE	TERMINAL ALKENES	3
98111	1-ETHOXY-2-PROPANOL	C6+ ALKANES	2
98113	1-HEPTANOL	C6+ ALKANES	1
98005	1-HEPTENE	TERMINAL ALKENES	3
43245	1-HEXENE	TERMINAL ALKENES	3
98037	1-METHYLCYCLOHEXANE	C6+ ALKANES	1
43267	1-NONENE	TERMINAL ALKENES	3
99901	1-OCTENE	TERMINAL ALKENES	3
43224	1-PENTENE	TERMINAL ALKENES	2
43312	1-T-2-O-4-TM-CYCLOPENTANE	C6+ ALKANES	1
43269	1-UNDECENE	TERMINAL ALKENES	3
43296	2,2,3-TRIMETHYLPENTANE	C6+ ALKANES	1
43276	2,2,4-TRIMETHYLPENTANE	C6+ ALKANES	1
43299	2,2,5-TRIMETHYLPENTANE	C6+ ALKANES	1
98033	2,2,5-TRIMETHYLHEXANE	C6+ ALKANES	1
43291	2,2-DIMETHYBUTANE	C6+ ALKANES	1
43280	2,3,3-TRIMETHYLPENTANE	C6+ ALKANES	1
43279	2,3,4-TRIMETHYLPENTANE	C6+ ALKANES	1
43234	2,3-DIMETHYL-1-BUTENE	TERMINAL ALKENES	2
98001	2,3-DIMETHYLBUTANE	C6+ ALKANES	1
43274	2,3-DIMETHYLPENTANE	C6+ ALKANES	1
98054	2,4,4-TRIMETHYL-1-PENTENE	TERMINAL ALKENES	3
98055	2,4,4-TRIMETHYL-2-PENTENE	INTERNAL ALKENES	3
43277	2,4-DIMETHYLHEXANE	C6+ ALKANES	1
43271	2,4-DIMETHYLPENTANE	C6+ ALKANES	1
43278	2,5-DIMETHYLHEXANE	C6+ ALKANES	1
98110	2-(-BUTOXYETHOXY)-ETHANOL	C6+ ALKANES	2
43308	2-BUTYLETHANOL	C6+ ALKANES	1
98108	2-BUTYLTETRAHYDROFURAN	C6+ ALKANES	2
98051	2-CHLOROTOLUENE	MONO-ALKYL BENZENE	2
43452	2-ETHOXYETHYL ACETATE	C6+ ALKANES	3
43311	2-ETHOXYETHANOL	C6+ ALKANES	2
98002	2-ETHYL-1-BUTENE	TERMINAL ALKENES	2
98112	2-ETHYL-1-HEXANOL	C6+ ALKANES	1
43310	2-METHOXYETHANOL	C6+ ALKANES	2

TABLE 3-3 (continued)

ID No.	Compound Name	Classification	Uncertainty Classification
43229	2-METHYL PENTANE	C6+ ALKANES	1
98076	2-METHYL-3-HEXANONE	KETONES	1
98004	2-METHYL-2-PENTENE	INTERNAL ALKENES	2
43228	2-METHYL-2-BUTENE	INTERNAL ALKENES	1
98040	2-METHYL-1-PENTENE	TERMINAL ALKENES	3
43225	2-METHYL-1-BUTENE	TERMINAL ALKENES	2
43275	2-METHYLHEXANE	C6+ ALKANES	1
98032	3,5,5-TRIMETHYLHEXANE	C6+ ALKANES	1
98105	3-(CHLOROMETHYL)-HEPTANE	C6+ ALKANES	2
99021	3-CARENE*	INTERNAL ALKENES	3
98041	3-HEPTENE	INTERNAL ALKENES	3
43230	3-METHYL PENTANE	C6+ ALKANES	1
43223	3-METHYL-1-BUTENE	TERMINAL ALKENES	1
43270	3-METHYL-T-2-PENTENE	INTERNAL ALKENES	2
43211	3-METHYL-1-PENTENE	TERMINAL ALKENES	2
43298	3-METHYLHEPTANE	C6+ ALKANES	1
43295	3-METHYLHEXANE	C6+ ALKANES	1
43293	4-METHYL-T-2-PENTENE	INTERNAL ALKENES	2
43297	4-METHYLHEPTANE	C6+ ALKANES	1
98042	4-NONENE	INTERNAL ALKENES	3
45221	A-METHYLSTYRENE	TERMINAL ALKENES	3
98025	A-PINENE*	INTERNAL ALKENES	3
98097	A-TERPINEOL*	INTERNAL ALKENES	3
43503	ACETALEHYDE	ACETALDEHYDE	0
43404	ACETIC ACID	NONREACTIVE	2
43551	ACETONE**	KETONES	1
43702	ACETONITRILE	NONREACTIVE	1
43206	ACETYLENE	NONREACTIVE	2
43505	ACROLEIN (ACRYLIC ALDHYDE)	ACETALDEHYDE	3
43704	ACRYLONITRILE	ETHENE	3
98085	ALKYL SUBSTITUTED CYCLOHEXANE	C6+ ALKANES	2
99001	ALLYL CHLORIDE	ETHENE	3
98015	ANTHRACENE	TRI-ALKYL BENZENE	3
98020	B-METHYLSTYRENE	INTERNAL ALKENES	3
98026	B-PINENE*	TERMINAL ALKENES	3
45201	BENZENE	NONREACTIVE 70% C6+ ALKANES 30%	3
45402	BENZOIC ACID	NONREACTIVE	3
98024	BENZYL CHLORIDE	MONO-ALKYL BENZENE	3
99017	BROMODICHLOROMETHANE	NONREACTIVE	1
99019	BROMOFORM	NONREACTIVE	1
98080	BUTANDIOL	C6+ ALKANES	2
98074	BUTYL CELLOSOLVE	C6+ ALKANES	2
43510	BUTYRALDEHYDE	HIGHER ALDEHYDES	1
98086	C2 ALKYL DECALIN	C6+ ALKANES	2
98084	C2 ALKYL INDAN	DI-ALKYL BENZENE	3
43512	C5 ALDEHYDE	HIGHER ALDEHYDES	2
98075	C5 ESTER	C4-C5 ALKANES	3
98095	C6 ALDEHYDE	HIGHER ALDEHYDES	2

TABLE 3-3 (continued)

ID No.	Compound Name	Classification	Uncertainty Classification
98093	C6 ESTER	C6+ ALKANES	3
98096	CARBITOL	C6+ ALKANES	2
98030	CARBON SULFIDE	NONREACTIVE	4
43807	CARBON TETRABROMIDE	NONREACTIVE	0
43804	CARBON TETRACHLORIDE	NONREACTIVE	0
98031	CARBONYL SULFIDE	NONREACTIVE	1
98087	CARVOMENTHENE*	INTERNAL ALKENE	3
98088	CARVONE*	INTERNAL ALKENE	3
43443	CELLOSOLVE ACETATE	C6+ ALKANES	3
99020	CHLORODIBROMOMETHANE	NONREACTIVE	1
43825	CHLORODIFLUOROMETHANE (F-22)	NONREACTIVE	1
43830	CHLOROFLUOROHYDROCARBONS	NONREACTIVE	3
43803	CHLOROFORM	NONREACTIVE	1
43827	CHLOROPENTAFLUOROETHANE (F-115)	NONREACTIVE	0
43826	CHLOROTRIFLUOROMETHANE (F-13)	NONREACTIVE	0
43217	CIS-2-BUTENE	INTERNAL ALKENES	1
43227	CIS-2-PENTENE	INTERNAL ALKENES	1
43227	CIS-3-PENTENE	INTERNAL ALKENES	1
98019	CRYOFLOURANE (F 114)	NONREACTIVE	1
43264	CYCLOHEXANONE	KETONES	2
43248	CYCLOHEXANE	C6+ ALKANES	1
43273	CYCLOHEXENE	INTERNAL ALKENES	2
43292	CYCLOPENTENE	INTERNAL ALKENES	2
43242	CYCLOPENTANE	C4-C5 ALKANES	1
43207	CYCLOPROPANE	NONREACTIVE	1
98027	D-LIMONENE*	INTERNAL ALKENES	3
43320	DIACETONE ALCOHOL	HIGHER KETONE	3
99015	DIBENZOFURAN	DI-ALKYL BENZENE	3
98107	DIBUTYL ETHER	C6+ ALKANES	1
43823	DICHLORODIFLUOROMETHANE (F-12)	NONREACTIVE	0
43802	DICHLOROMETHANE	NONREACTIVE	1
43828	DICHLOROTETRAFLUOROETHANE	NONREACTIVE	0
98062	DIETHYLCYCLOHEXANE	C6+ ALKANES	1
43450	DIMETHYL FORMAMIDE	DI-ALKYL BENZENE	4
98018	DIMETHYL ETHER	C4-C5 ALKANES	1
98059	DIMETHYLCYCLOHEXANE	C6+ ALKANES	1
45103	DIMETHYLETHYLBENZENE	TRI-ALKYL BENZENE	1
98091	DIMETHYLHEPTANE	C6+ ALKANES	1
98012	DIMETHYLNAPHTHALENE	TRI-ALKYL BENZENE	3
98017	DM-2,3,DH-1H-INDENE	TRI-ALKYL BENZENE	3
99006	EPICHLOROHYDRIN	NONREACTIVE	2
43202	ETHANE	NONREACTIVE	2
43433	ETHYL ACETATE	C4-C5 ALKANES	3
43438	ETHYL ACRYLATE	TERMINAL ALKENE	3
43302	ETHYL ALCOHOL	C4-C5 ALKANES	1
43812	ETHYL CHLORIDE	NONREACTIVE	1
43351	ETHYL ETHER	C4-C5 ALKANES	1
98106	ETHYL ISOPROPYL ETHER	C6+ ALKANES	1
43219	ETHYLACETYLENE	ETHENE	3

TABLE 3-3 (continued)

ID No.	Compound Name	Classification	Uncertainty Classification
43721	ETHYLAMINE	DI-ALKYL BENZENE	4
45203	ETHYLBENZENE	MONO-ALKYL BENZENE	1
43288	ETHYLCYCLOHEXANE	C6+ ALKANES	1
98057	ETHYLCYCLOPENTANE	C6+ ALKANES	1
99014	ETHYLENE DIBROMIDE	NONREACTIVE	2
43601	ETHYLENE OXIDE	NONREACTIVE	2
43815	ETHYLENE DICHLORIDE	NONREACTIVE	2
43370	ETHYLENE GLYCOL	C4-C5 ALKANES	3
43203	ETHYLENE	ETHENE	0
98011	ETHYLNAPHTHALENE	TRI-ALKYL BENZENE	3
43502	FORMALDEHYDE	FORMALDEHYDE	0
99902	FURAN	DI-ALKYL BENZENE	3
43368	GLYCOL	C4-C5 ALKANES	3
43367	GLYCOL ETHER	C6+ ALKANES	2
99903	GLYOXAL**	FORMALDEHYDE	2
43232	HEPTANE	C6+ ALKANES	1
98077	HEPTANONE	KETONES	1
99007	HEXACHLOROCYCLOPENTADIENE	NONREACTIVE	2
43231	HEXANE	C6+ ALKANES	1
43371	HEXYLENE GLYCOL	C6+ ALKANES	2
98044	INDAN	DI-ALKYL BENZENE	3
98048	INDENE	TRI-ALKYL BENZENE	3
98115	ISOAMYL ISOBUTYRATE	C6+ ALKANES	3
43214	ISOBUTANE	C4-C5 ALKANES	1
43451	ISOBUTYL ISOBUTYRATE	C6+ ALKANES	3
43446	ISOBUTYL ACETATE	C4-C5 ALKANES	3
43306	ISOBUTYL ALCOHOL	C4-C5 ALKANES	1
98047	ISOBUTYLBENZENE	MONO-ALKYL BENZENE	1
43215	ISOBUTYLENE	TERMINAL ALKENES	2
98036	ISOBUTYRALDEHYDE	HIGHER ALDEHYDES	1
99904	ISOMERS OF HEPTENE	INTERNAL ALKENES	3
43105	ISOMERS OF HEXANE	C6+ ALKANES	1
43106	ISOMERS OF HEPTANE	C6+ ALKANES	1
99905	ISOMERS OF HEXENE	INTERNAL ALKENES	3
45102	ISOMERS OF XYLENE	DI-ALKYL BENZENE	3
45105	ISOMERS OF BUTYLBENZENE	MONO-ALKYL BENZENE	3
43108	ISOMERS OF NONANE	C6+ ALKANES	1
45106	ISOMERS OF DIETHYLBENZENE	DI-ALKYL BENZENE	3
43110	ISOMERS OF UNDECANE	C6+ ALKANES	2
43122	ISOMERS OF PENTANE	C4-C5 ALKANES	1
45104	ISOMERS OF ETHYLTOLUENE	DI-ALKYL BENZENE	3
43112	ISOMERS OF DODECANE	C6+ ALKANES	2
43107	ISOMERS OF OCTANE	C6+ ALKANES	1
43109	ISOMERS OF DECANE	C6+ ALKANES	2
99906	ISOMERS OF OCTENE	INTERNAL ALKENES	3
43243	ISOPRENE*	INTERNAL ALKENES	2
98043	ISOPROPYLBENZENE (CUMENE)	MONO-ALKYL BENZENE	1
43444	ISOPROPYL ACETATE	C4-C5 ALKANES	3
43304	ISOPROPYL ALCOHOL	C4-C5 ALKANES	1

TABLE 3-3 (continued)

ID No.	Compound Name	Classification	Uncertainty Classification
98089	ISOPULEGONE*	TERMINAL ALKENES	3
98056	ISOVALERALDEHYDE	HIGHER ALDEHYDES	2
43119	LACTOL SPIRITS	C6+ ALKANES	4
98022	M-CRESOL (3-M-BENZENOL)**	MONO-ALKYL BENZENE	2
98045	M-DIETHYLBENZENE	DI-ALKYL BENZENE	1
45212	M-ETHYLTOLUENE	DI-ALKYL BENZENE	1
45205	M-XYLENE	DI-ALKYL BENZENE	0
99008	MALEIC ANHYDRIDE	NONREACTIVE	2
43201	METHANE	NONREACTIVE	1
43432	METHYL ACETATE	NONREACTIVE	2
43301	METHYL ALCOHOL	NONREACTIVE 50% C4-C5 ALKANES 50%	3
43445	METHYL AMYL ACETATE	C6+ ALKANES	3
43561	METHYL AMYL KETONE	KETONES	1
43819	METHYL BROMIDE	NONREACTIVE	1
43801	METHYL CHLORIDE	NONREACTIVE	1
43552	METHYL ETHYL KETONE	KETONES	0
98114	METHYL ISOBUTYRATE	C4-C5 ALKANES	3
43560	METHYL ISOBUTYL KETONE	KETONES	1
43559	METHYL N-BUTYL KETONE	KETONES	1
43209	METHYLACETYLENE	ETHENE	3
98016	METHYLANTHRACENE	TRI-ALKYL BENZENE	3
43262	METHYLCYCLOPENTANE	C6+ ALKANES	1
43261	METHYLCYCLOHEXANE	C6+ ALKANES	1
43272	METHYLCYCLOPENTENE	INTERNAL ALKENES	3
43805	METHYLENE BROMIDE	NONREACTIVE	0
98010	METHYLNAPHTHALENE	TRI-ALKYL BENZENE	3
45234	METHYLPROPYLBENZENE	DI-ALKYL BENZENE	1
43118	MINERAL SPIRITS	MONO-ALKYL BENZENE	4
45801	MONOCHLOROBENZENE	NONREACTIVE	3
43212	N-BUTANE	C4-C5 ALKANES	1
43305	N-BUTYL ALCOHOL	C4-C5 ALKANES	1
43435	N-BUTYL ACETATE	C4-C5 ALKANES	3
43238	N-DECANE	C6+ ALKANES	2
43255	N-DODECANE	C6+ ALKANES	2
43220	N-PENTANE	C6+ ALKANES	1
98063	N-PENTYLCYCLOHEXANE	C6+ ALKANES	2
43303	N-PROPYL ALCOHOL	C4-C5 ALKANES	1
45209	N-PROPYLBENZENE	MONO-ALKYL BENZENE	1
45101	NAPHTHA	MONO-ALKYL BENZENE	4
98046	NAPHTHALENE	TRI-ALKYL BENZENE	3
99009	NITROBENZENE	NONREACTIVE	3
43235	NONANE	C6+ ALKANES	1
98021	O-CRESOL (2-M-BENZENOL)**	MONO-ALKYL BENZENE	2
45211	O-ETHYLTOLUENE	DI-ALKYL BENZENE	1
45204	O-XYLENE	DI-ALKYL BENZENE	1
43233	OCTANE	C6+ ALKANES	1
98023	P-CRESOL (4-M-BENZENOL)**	MONO-ALKYL BENZENE	2

TABLE 3-3 (continued)

ID No.	Compound Name	Classification	Uncertainty Classification
45807	P-DICHLOROBENZENE	NONREACTIVE	3
45206	P-XYLENE	DI-ALKYL BENZENE	1
98094	PENTYL ALCOHOL	C4-C5 ALKANES	1
43817	PERCHLOROETHYLENE	NONREACTIVE	1
45300	PHENOLS**	MONO-ALKYL BENZENE	3
98028	PHTHALIC ANHYDRIDE	DI-ALKYL BENZENE	3
43208	PROPADIENE	TERMINAL ALKENES	3
43204	PROPANE	NONREACTIVE 50% C4-C5 ALKANES 50%	3
43504	PROPIONALDEHYDE	HIGHER ALDEHYDES	1
43434	PROPYL ACETATE	C4-C5 ALKANES	3
45108	PROPYLBENZENE	MONO-ALKYL BENZENE	1
98109	PROPYLCYCLOHEXANONE	KETONES	2
43602	PROPYLENE OXIDE	C4-C5 ALKANES	3
43369	PROPYLENE GLYCOL	C4-C5 ALKANES	2
43205	PROPYLENE	TERMINAL ALKENES	0
98013	PROPYLNAPHTHALENE	TRI-ALKYL BENZENE	3
45216	SEC-BUTYLBENZENE	MONO-ALKYL BENZENE	1
45220	STYRENE	TERMINAL ALKENES	3
98116	SUBSTITUTED C7 ESTER (C12)	C6+ ALKANES	3
98117	SUBSTITUTED C9 ESTER (C12)	C6+ ALKANES	3
43123	TERPENES*	INTERNAL ALKENES	3
98079	TERPINENE*	INTERNAL ALKENES	3
45215	TERT-BUTYLBENZENE	MONO-ALKYL BENZENE	1
43309	TERT-BUTYL-ALCOHOL	C4-C5 ALKANES	1
43390	TETRAHYDROFURAN	C6+ ALKANES	1
45232	TETRAMETHYLBENZENE	TRI-ALKYL BENZENE	1
45202	TOLUENE	MONO-ALKYL BENZENE	0
99018	TRANS-1,2-DICHLOROETHENE	ETHENE	3
43216	TRANS-2-BUTENE	INTERNAL ALKENES	0
43227	TRANS-2-PENTENE	INTERNAL ALKENES	1
43226	TRANS-2-PENTENE	INTERNAL ALKENES	1
43227	TRANS-3-PENTENE	INTERNAL ALKENES	1
45233	TRI/TETRAALKYL BENZENE	TRI-ALKYL BENZENE	1
43821	TRICHLOROTRIFLUOROETHANE	NONREACTIVE	0
43811	TRICHLOROFLUOROMETHANE	NONREACTIVE	0
43824	TRICHLOROETHYLENE	ETHENE	3
45107	TRIMETHYLBENZENE	TRI-ALKYL BENZENE	1
43740	TRIMETHYL AMINE	TRI-ALKYL BENZENE	4
98060	TRIMETHYLCYCLOHEXANE	C6+ ALKANES	1
98058	TRIMETHYLCYCLOPENTANE	C6+ ALKANES	1
98014	TRIMETHYLNAPHTHALENE	TRI-ALKYL BENZENE	3
43822	TRIMETHYLFLUOROSILANE	NONREACTIVE	1
43241	UNDECANE	C6+ ALKANES	2
43860	VINYL CHLORIDE	ETHENE	3
45401	XYLENE BASE ACIDS	DI-ALKYL BENZENE	4

*Biogenic compound.

**These species can either be represented by the assigned class or explicitly.

TABLE 3-3 (continued)

Uncertainty Classifications:

0 = Explicitly represented in mechanism (for reactive compounds), or known not to react in the troposphere (for nonreactive compounds)

1 = Representation shown is probably a good approximation

2 = Representation shown may not be a good approximation, but the mechanism does not contain more appropriate species.

3 = Representation shown is probably a poor approximation, but the mechanism does not contain more appropriate species.

4 = Appropriate representation is unknown.

Chemical structure is largely the basis for the assignment of the individual species to classes. Alkanes are assigned to one of the alkane classes on the basis of carbon number. Alkenes are assigned based on the position of the double bond within the molecule (i.e., on whether the double bond is located in the terminal position or in an internal position). The aromatics are assigned based on the number of alkyl groups attached to the benzene ring. Aldehydes are assigned on the basis of carbon number. However, about 20% of the compounds on the list are not kinetically or structurally similar to any of the surrogate species. These are the species that have been assigned a high uncertainty rating (3 or 4) in Table 3-3. The assignments for these species are primarily based on similarity between their OH rate constants (when available) and the OH rate constants of the surrogate species in the mechanism and, secondarily, on similarity of structure and reactivity of products (when known). The OH rate constants were obtained from Atkinson (1986). Although these compounds represent 20% of the species on the list, it is unlikely that they represent a significant (i.e., more than 5%) fraction of NMOC in urban areas.

VOC emission inventories can be speciated using published data. Emission speciation profiles are available for a moderate number of stationary and some mobile sources in the "Volatile Organic Compound Species Data Manual" (EPA 1980) and "Improvements of the Emission Inventory for ROG and NO_x in the SoCAB" (Oliver and Peoples 1985). Additional speciation data for mobile sources are available from EPA's "Forty-Six Car Study" (EPA 1985). Profiles for stationary sources are generally assigned on the basis of Source Classification Code (SCC). The detailed profiles can be transformed to NMOC class profiles using the assignments shown in Table 3-3.

Speciated ambient NMOC data are needed for photochemical modeling. Region-specific data should be employed in the modeling whenever possible. Recognizing that speciated NMOC ambient data are often not available default speciation profiles have been developed for NMOC in the surface layer and aloft. These profiles are shown in Table 3-4. They are based on analysis of surface data from 25 urban areas and aircraft data from 4 urban areas (Lurmann et al. 1987). Plausible ranges of the speciation fractions are shown in Table 3-5. The ranges generally

TABLE 3-4

RECOMMENDED DEFAULT NMOC COMPOSITION PROFILES

	Carbon Fractions of NMOC	
Compound Class	Surface Layer	Aloft
C4-C5 Alkanes	.21	.21
C6+ Alkanes	.28	.18
Ethene	.03	.015
Terminal Alkenes	.06	.03
Internal Alkenes	.04	.005
Mono-alkylbenzenes	.16	.07
Di-alylbenzenes	.06	.04
Tri-alkylbenzenes	.04	.02
Formaldehyde	.03	.05
Acetaldehyde	.02	.03
Unreactive	.07	.35

TABLE 3-5

RANGE OF NMOC COMPOSITION FRACTIONS

	Carbon Fractions of NMOC	
Compound Class	Surface Layer	Aloft
C4-C5 Alkanes	.11 - .31	.11 - .31
C6+ Alkanes	.14 - .42	.09 - .27
Ethene	.015 - .045	.0 - .03
Terminal Alkenes	.03 - .09	.0 - .045
Internal Alkenes	.02 - .06	.0 - .01
Mono-alkylbenzenes	.08 - .24	.04 - .11
Di-alylbenzenes	.03 - .09	.0 - .06
Tri-alkylbenzenes	.02 - .06	.0 - .04
Formaldehyde	.015 - .06	.01 - .08
Acetaldehyde	.01 - .04	.01 - .08
Unreactive	.04 - .11	.15 - .75

reflected ±50% variations about the mean fractions. If ambient samples shown variations beyond these ranges (particularly the upper values), then the sample may reflect strong influence by local point sources and may not be representative of the entire urban area.

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APPENDIX A

PHOTOLYTIC REACTION RATE DATA

TABLE A-1

SOLAR ACTINIC FLUXES FOR ZERO ELEVATION AND BEST ESTIMATE ALBEDO*

WAVELENGTH BAND (um)	EXP	PHOTONS/CM**2-SEC SOLAR ZENITH ANGLE 0	10	20	30	40	50	60	70	78	86
.295-.300	14	0.041	0.038	0.030	0.019	0.009	0.003	0.000	0.000	0.000	0.000
.300-.305	14	0.39E	0.381	0.331	0.255	0.167	0.084	0.027	0.004	0.001	0.000
.305-.310	14	1.41	1.37	1.25	1.05	0.80	0.513	0.244	0.064	0.011	0.002
.310-.315	14	3.14	3.10	2.91	2.58	2.13	1.56	0.922	0.357	0.090	0.009
.315-.320	14	4.35	4.31	4.10	3.74	3.21	2.52	1.67	0.793	0.264	0.030
.320-.325	14	5.48	5.41	5.19	4.80	4.23	3.43	2.43	1.29	0.502	0.073
.325-.330	14	7.89	7.79	7.51	7.01	6.27	5.21	3.83	2.17	0.928	0.167
.330-.335	14	8.35	8.25	7.98	7.50	6.76	5.72	4.30	2.54	1.15	0.241
.335-.340	14	8.24	8.16	7.91	7.46	6.78	5.79	4.43	2.69	1.25	0.282
.340-.345	14	8.89	8.80	8.54	8.09	7.38	6.36	4.93	3.04	1.44	0.333
.345-.350	14	8.87	8.79	8.54	8.11	7.43	6.44	5.04	3.15	1.51	0.352
.350-.355	14	10.05	9.96	9.70	9.22	8.48	7.39	5.83	3.69	1.77	0.414
.355-.360	14	9.26	9.18	8.94	8.52	7.86	6.88	5.47	3.50	1.69	0.391
.360-.365	14	10.25	10.16	9.91	9.46	8.76	7.71	6.17	3.99	1.94	0.444
.365-.370	15	1.26	1.25	1.22	1.17	1.08	0.958	0.772	0.505	0.247	0.055
.370-.375	15	1.14	1.13	1.10	1.06	0.983	0.873	0.708	0.467	0.230	0.051
.375-.380	15	1.27	1.26	1.23	1.18	1.10	0.983	0.802	0.535	0.265	0.058
.380-.385	15	1.05	1.04	1.02	0.980	0.917	0.820	0.673	0.453	0.226	0.049
.385-.390	15	1.15	1.15	1.12	1.08	1.01	0.909	0.750	0.510	0.257	0.054
.390-.395	15	1.19	1.18	1.16	1.11	1.05	0.943	0.783	0.537	0.273	0.057
.395-.400	15	1.44	1.43	1.40	1.35	1.28	1.15	0.962	0.666	0.341	0.070
.400-.405	15	1.73	1.72	1.69	1.63	1.53	1.39	1.16	0.809	0.418	0.085
.405-.410	15	1.94	1.93	1.90	1.83	1.73	1.57	1.32	0.926	0.482	0.097
.410-.415	15	2.05	2.04	2.00	1.93	1.83	1.66	1.41	0.993	0.522	0.104
.415-.420	15	2.08	2.07	2.03	1.96	1.86	1.70	1.44	1.03	0.543	0.107
.420-.430	15	4.08	4.06	3.99	3.87	3.67	3.36	2.87	2.07	1.11	0.216
.430-.440	15	4.20	4.18	4.11	3.99	3.80	3.49	3.01	2.19	1.20	0.229
.440-.450	15	4.87	4.85	4.77	4.64	4.43	4.09	3.54	2.61	1.45	0.272
.450-.460	15	5.55	5.51	5.43	5.27	5.03	4.64	4.02	2.99	1.67	0.312
.460-.470	15	5.68	5.65	5.57	5.42	5.17	4.79	4.17	3.12	1.77	0.325
.470-.480	15	5.82	5.79	5.70	5.55	5.31	4.91	4.32	3.26	1.87	0.341
.480-.490	15	5.78	5.75	5.67	5.53	5.29	4.93	4.33	3.29	1.90	0.339
.490-.500	15	5.79	5.76	5.68	5.54	5.31	4.96	4.37	3.34	1.95	0.344
.500-.510	15	5.99	5.96	5.87	5.71	5.47	5.09	4.47	3.41	1.99	0.340
.510-.520	15	5.88	5.86	5.77	5.62	5.38	5.02	4.43	3.40	2.00	0.340
.520-.530	15	5.98	5.95	5.87	5.72	5.48	5.11	4.52	3.47	2.04	0.336
.530-.540	15	5.98	5.95	5.87	5.72	5.48	5.12	4.52	3.48	2.05	0.326
.540-.550	15	5.88	5.85	5.77	5.62	5.40	5.04	4.46	3.44	2.03	0.317
.550-.560	15	5.94	5.91	5.83	5.68	5.44	5.08	4.49	3.46	2.04	0.312
.560-.570	15	5.99	5.96	5.88	5.73	5.49	5.13	4.54	3.50	2.06	0.306
.570-.580	15	6.12	6.09	6.00	5.85	5.61	5.24	4.63	3.57	2.10	0.301
.580-.600	16	1.25	1.24	1.22	1.19	1.14	1.07	0.951	0.737	0.439	0.064
.600-.620	16	1.26	1.26	1.24	1.21	1.16	1.08	0.963	0.748	0.448	0.065
.620-.640	16	1.27	1.26	1.24	1.17	1.10	1.10	0.980	0.771	0.473	0.074
.640-.660	16	1.30	1.30	1.28	1.25	1.20	1.13	1.01	0.803	0.502	0.086
.660-.680	16	1.33	1.33	1.31	1.28	1.23	1.16	1.04	0.828	0.527	0.096
.680-.700	16	1.33	1.32	1.30	1.27	1.23	1.16	1.04	0.839	0.541	0.104

* THE SECOND COLUMN (EXP) LISTS THE POWER OF TEN BY WHICH ALL ENTRIES SHOULD BE MULTIPLIED. DATA FROM PETERSON (1976).

Table A-2

Photolytic Data for $NO_2 + h\nu \rightarrow NO + O$

Wavelength (um)	Absorption Cross-section*	Quantum Yield
.295	9.67E-20	.984
.300	1.17E-19	.980
.305	1.66E-19	.976
.310	1.76E-19	.972
.315	2.25E-19	.968
.320	2.54E-19	.964
.325	2.79E-19	.960
.330	2.99E-19	.956
.335	3.45E-19	.952
.340	3.88E-19	.948
.345	4.07E-19	.944
.350	4.10E-19	.940
.355	5.13E-19	.936
.360	4.51E-19	.932
.365	5.78E-19	.928
.370	5.42E-19	.850
.375	5.35E-19	.770
.376	5.48E-19	.780
.377	5.61E-19	.920
.378	5.73E-19	.820
.379	5.86E-19	.870
.380	5.99E-19	.900
.381	5.98E-19	.810
.382	5.97E-19	.700
.383	5.96E-19	.680
.384	5.95E-19	.700
.385	5.94E-19	.770
.386	5.95E-19	.840
.387	5.96E-19	.750
.388	5.98E-19	.810
.389	5.99E-19	.780
.390	6.00E-19	.800
.391	5.98E-19	.880
.392	5.96E-19	.840
.393	5.93E-19	.900
.394	5.91E-19	.900
.395	5.89E-19	.840
.396	6.06E-19	.830
.397	6.24E-19	.820
.398	6.41E-19	.770
.399	6.59E-19	.780
.400	6.76E-19	.680
.401	6.67E-19	.650
.402	6.58E-19	.620
.403	6.50E-19	.570
.404	6.41E-19	.420
.405	6.32E-19	.320
.406	6.21E-19	.330
.407	6.10E-19	.250
.408	5.99E-19	.200
.409	5.88E-19	.190
.410	5.77E-19	.150
.411	5.88E-19	.100
.415	6.30E-19	.067
.420	6.23E-19	.023
.425	6.00E-19	.000

* in cm^2 per molecule

Table A-3

Photolytic Data for NO3 + hv --> NO + O2

Wavelength (um)	Absorption Cross-section	Quantum Yield
.585	2.77E-18	.000
.590	5.14E-18	.250
.595	4.08E-18	.400
.600	2.83E-18	.250
.605	3.45E-18	.200
.610	1.48E-18	.200
.615	1.96E-18	.100
.620	3.58E-18	.100
.625	9.25E-18	.050
.630	5.66E-18	.050
.635	1.45E-18	.030
.640	1.11E-18	.000

Table A-4

Photolytic Data for NO3 + hv --> NO2 + O

Wavelength (um)	Absorption Cross-section	Quantum Yield
.400	0.00E-01	1.000
.405	3.00E-20	1.000
.410	4.00E-20	1.000
.415	5.00E-20	1.000
.420	8.00E-20	1.000
.425	1.00E-19	1.000
.430	1.30E-19	1.000
.435	1.80E-19	1.000
.440	1.90E-19	1.000
.445	2.20E-19	1.000
.450	2.80E-19	1.000
.455	3.30E-19	1.000
.460	3.70E-19	1.000
.465	4.30E-19	1.000
.470	5.10E-19	1.000
.475	6.00E-19	1.000
.480	6.40E-19	1.000
.485	6.90E-19	1.000
.490	8.80E-19	1.000
.495	9.50E-19	1.000
.500	1.01E-18	1.000
.505	1.10E-18	1.000
.510	1.32E-18	1.000
.515	1.40E-18	1.000
.520	1.45E-18	1.000
.525	1.48E-18	1.000
.530	1.94E-18	1.000
.535	2.04E-18	1.000
.540	1.81E-18	1.000
.545	1.81E-18	1.000
.550	2.36E-18	1.000
.555	2.68E-18	1.000
.560	3.07E-18	1.000
.565	2.53E-18	1.000
.570	2.54E-18	1.000
.575	2.74E-18	1.000
.580	3.05E-18	1.000
.585	2.77E-18	1.000
.590	5.14E-18	.750
.595	4.08E-18	.600
.600	2.83E-18	.550
.605	3.45E-18	.400
.610	1.45E-18	.300
.615	1.96E-18	.250
.620	3.58E-18	.200
.625	9.25E-18	.150
.630	5.66E-18	.050
.635	1.45E-18	.000

Table A-5

Photolytic Data for O3 + hv --> O(1D) + O2 at 270 K

Wavelength (um)	Absorption Cross-section	Quantum Yield
.260	1.07E-17	.900
.270	7.74E-18	.900
.280	3.79E-18	.900
.290	1.34E-18	.900
.300	3.80E-19	.900
.305	1.88E-19	.860
.310	9.80E-20	.460
.313	7.50E-20	.160
.315	5.20E-20	.070
.317	4.16E-20	.030
.320	2.60E-20	.000

Table A-6

Photolytic Data for O3 + hv --> O(1D) + O2 at 300 K

Wavelength (um)	Absorption Cross-section	Quantum Yield
.260	1.07E-17	.900
.270	7.74E-18	.900
.280	3.79E-18	.900
.290	1.34E-18	.900
.300	3.80E-19	.900
.305	1.88E-19	.890
.310	9.80E-20	.560
.313	7.50E-20	.260
.315	5.20E-20	.130
.317	4.16E-20	.050
.320	2.60E-20	.000

Table A-7

Photolytic Data for O3 + hv --> O(1D) + O2 at 330 K

Wavelength (um)	Absorption Cross-section	Quantum Yield
.260	1.07E-17	.900
.270	7.74E-18	.900
.280	3.79E-18	.900
.290	1.34E-18	.900
.300	3.80E-19	.900
.305	1.88E-19	.900
.310	9.80E-20	.630
.313	7.50E-20	.360
.315	5.20E-20	.220
.317	4.16E-20	.120
.320	2.60E-20	.030
.322	2.30E-20	.000

Table A-8

Photolytic Data for O3 + hv --> O(3P) + O2

Wavelength (um)	Absorption Cross-section	Quantum Yield
.260	1.07E-07	.100
.270	7.74E-18	.100
.280	3.79E-18	.100
.290	1.34E-18	.100
.300	3.16E-19	.100
.310	9.80E-20	.443
.320	2.60E-20	1.000
.330	6.70E-21	1.000
.340	1.70E-21	1.000
.350	4.00E-22	1.000
.355	0.00E-01	1.000
.400	0.00E-01	1.000
.450	1.60E-22	1.000
.500	1.34E-21	1.000
.550	3.32E-21	1.000
.600	5.06E-21	1.000
.650	2.45E-21	1.000
.660	2.13E-21	1.000
.670	1.82E-21	1.000
.680	1.50E-21	1.000
.690	1.19E-21	1.000
.700	8.70E-22	1.000

Table A-9

Photolytic Data for H2O2 + hv --> 2 OH

Wavelength (um)	Absorption Cross-section	Quantum Yield
.250	8.30E-20	1.000
.255	6.70E-20	1.000
.260	5.20E-20	1.000
.265	4.20E-20	1.000
.270	3.20E-20	1.000
.275	2.50E-20	1.000
.280	2.00E-20	1.000
.285	1.50E-20	1.000
.290	1.13E-20	1.000
.295	8.70E-21	1.000
.300	6.60E-21	1.000
.305	4.90E-21	1.000
.310	3.70E-21	1.000
.315	2.80E-21	1.000
.320	2.00E-21	1.000
.325	1.50E-21	1.000
.330	1.20E-21	1.000
.335	9.00E-22	1.000
.340	7.00E-22	1.000
.345	5.00E-22	1.000
.350	3.00E-22	1.000
.355	3.00E-22	.000

Table A-10

Photolytic Data for HONO + hv --> NO + OH

Wavelength (um)	Absorption Cross-section	Quantum Yield	Wavelength (um)	Absorption Cross-section	Quantum Yield
.311	0.00E-01	1.000	.352	1.14E-19	1.000
.312	2.00E-21	1.000	.353	3.71E-19	1.000
.313	4.20E-21	1.000	.354	4.96E-19	1.000
.314	4.60E-21	1.000	.355	2.46E-19	1.000
.315	4.20E-21	1.000	.356	1.19E-19	1.000
.316	3.00E-21	1.000	.357	9.35E-20	1.000
.317	4.60E-21	1.000	.358	7.78E-20	1.000
.318	3.60E-20	1.000	.359	7.29E-20	1.000
.319	6.10E-20	1.000	.360	6.83E-20	1.000
.320	2.10E-20	1.000	.361	6.90E-20	1.000
.321	4.27E-20	1.000	.362	7.32E-20	1.000
.322	4.01E-20	1.000	.363	9.00E-20	1.000
.323	3.93E-20	1.000	.364	1.21E-19	1.000
.324	4.01E-20	1.000	.365	1.33E-19	1.000
.325	4.04E-20	1.000	.366	2.13E-19	1.000
.326	3.13E-20	1.000	.367	3.52E-19	1.000
.327	4.12E-20	1.000	.368	4.50E-19	1.000
.328	7.55E-20	1.000	.369	2.93E-19	1.000
.329	6.64E-20	1.000	.370	1.19E-19	1.000
.330	7.29E-20	1.000	.371	9.46E-20	1.000
.331	8.70E-20	1.000	.372	8.85E-20	1.000
.332	1.38E-19	1.000	.373	7.44E-20	1.000
.333	5.91E-20	1.000	.374	4.77E-20	1.000
.334	5.91E-20	1.000	.375	2.70E-20	1.000
.335	6.45E-20	1.000	.376	1.90E-20	1.000
.336	5.91E-20	1.000	.377	1.50E-20	1.000
.337	4.58E-20	1.000	.378	1.90E-20	1.000
.338	1.91E-19	1.000	.379	5.80E-20	1.000
.339	1.63E-19	1.000	.380	7.78E-20	1.000
.340	1.05E-19	1.000	.381	1.14E-19	1.000
.341	8.70E-20	1.000	.382	1.40E-19	1.000
.342	3.35E-19	1.000	.383	1.72E-19	1.000
.343	2.01E-19	1.000	.384	1.99E-19	1.000
.344	1.02E-19	1.000	.385	1.90E-19	1.000
.345	8.54E-20	1.000	.386	1.19E-19	1.000
.346	8.32E-20	1.000	.387	5.65E-20	1.000
.347	8.20E-20	1.000	.388	3.20E-20	1.000
.348	7.49E-20	1.000	.389	1.90E-20	1.000
.349	7.13E-20	1.000	.390	1.20E-20	1.000
.350	6.83E-20	1.000	.391	5.00E-21	1.000
.351	1.74E-19	1.000	.392	0.00E-01	1.000

Table A-11

Photolytic Data for HCHO + hv --> 2 HO2 + CO

Wavelength (um)	Absorption Cross-section	Quantum Yield
.240	3.00E-22	.210
.250	1.30E-21	.240
.260	4.70E-21	.300
.270	8.60E-21	.400
.280	1.86E-20	.590
.290	2.51E-20	.710
.300	2.62E-20	.780
.310	2.45E-20	.770
.320	1.85E-20	.620
.330	1.76E-20	.310
.340	1.18E-20	.000

Table A-12

Photolytic Data for HCHO + hv --> H2 + CO

Wavelength (um)	Absorption Cross-section	Quantum Yield
.240	3.00E-22	.420
.250	1.30E-21	.460
.260	4.70E-21	.480
.270	8.60E-21	.460
.280	1.86E-20	.350
.290	2.51E-20	.260
.300	2.62E-20	.220
.310	2.45E-20	.230
.320	1.85E-20	.380
.330	1.76E-20	.690
.340	1.18E-20	.690
.350	4.20E-21	.400
.360	6.00E-22	.120
.370	0.00E-01	.000

Table A-13

Photolytic Data for ALD2 + hv --> HCHO + HO2 + RO2R + CO

Wavelength (um)	Absorption Cross-section	Quantum Yield
.260	2.16E-20	.310
.270	3.46E-20	.380
.280	4.32E-20	.590
.290	4.76E-20	.550
.295	4.45E-20	.490
.300	4.03E-20	.415
.305	3.42E-20	.325
.310	2.72E-20	.235
.315	2.09E-20	.150
.320	1.60E-20	.075
.325	1.13E-20	.030
.330	6.80E-21	.000

Table A-14

Photolytic Data for RCHO + hv --> ALD2 + HO2 + RO2R + CO

Wavelength (um)	Absorption Cross-section	Quantum Yield
.280	5.26E-20	.200
.290	5.77E-20	.200
.300	5.05E-20	.200
.310	3.68E-20	.200
.320	1.66E-20	.200
.330	6.49E-21	.200
.340	1.44E-21	.200
.345	0.00E-01	.200

Table A-15

Photolytic Data for ACET + hv --> HCHO + RO2R + MCO3

Wavelength (um)	Absorption Cross-section	Quantum Yield
.210	1.10E-21	.070
.220	1.20E-21	.070
.230	4.60E-21	.070
.240	1.30E-20	.070
.250	2.68E-20	.070
.260	4.21E-20	.070
.270	5.54E-20	.070
.280	5.92E-20	.070
.290	5.16E-20	.070
.300	3.44E-20	.070
.310	1.53E-20	.070
.320	4.60E-21	.070
.330	1.10E-21	.070
.340	0.00E-01	.070

Table A-16

Photolytic Data for MEK + hv --> ALD2 + RO2R + MCO3

Wavelength (um)	Absorption Cross-section	Quantum Yield
.210	1.10E-21	.100
.220	1.20E-21	.100
.230	4.60E-21	.100
.240	1.30E-20	.100
.250	2.68E-20	.100
.260	4.21E-20	.100
.270	5.54E-20	.100
.280	5.92E-20	.100
.290	5.16E-20	.100
.300	3.44E-20	.100
.310	1.53E-20	.100
.320	4.60E-21	.100
.330	1.10E-21	.100
.340	0.00E-01	.100

Table A-17

Photolytic Data for DIAL + hv --> HO2 + CO + MCO3

Wavelength (um)	Absorption Cross-section	Quantum Yield
.200	7.90E-20	1.000
.350	7.90E-20	1.000
.360	7.90E-20	0.000

Table A-18

Photolytic Data for GLYX+ hv --> .13 HCHO + .87 H2 + 1.87 CO

Wavelength (um)	Absorption Cross-section	Quantum Yield	Wavelength (um)	Absorption Cross-section	Quantum Yield
.230	2.87E-21	.029	.414	7.50E-20	.029
.235	2.87E-21	.029	.414	8.11E-20	.029
.240	4.30E-21	.029	.415	8.11E-20	.029
.245	5.73E-21	.029	.415	6.89E-20	.029
.250	8.60E-21	.029	.416	4.26E-20	.029
.255	1.15E-20	.029	.417	4.86E-20	.029
.260	1.43E-20	.029	.418	5.88E-20	.029
.265	1.86E-20	.029	.419	6.69E-20	.029
.270	2.29E-20	.029	.420	3.85E-20	.029
.275	2.58E-20	.029	.421	5.67E-20	.029
.280	2.87E-20	.029	.421	4.46E-20	.029
.285	3.30E-20	.029	.422	5.27E-20	.029
.290	3.15E-20	.029	.422	1.05E-19	.029
.295	3.30E-20	.029	.423	8.51E-20	.029
.300	3.58E-20	.029	.424	6.08E-20	.029
.305	2.72E-20	.029	.425	7.29E-20	.029
.310	2.72E-20	.029	.426	1.18E-19	.029
.312	2.87E-20	.029	.426	1.30E-19	.029
.315	2.29E-20	.029	.427	1.07E-19	.029
.320	1.43E-20	.029	.428	1.66E-19	.029
.325	1.15E-20	.029	.429	4.05E-20	.029
.327	1.43E-20	.029	.430	5.07E-20	.029
.330	1.15E-20	.029	.431	4.86E-20	.029
.335	2.87E-21	.029	.432	4.05E-20	.029
.340	0.00E-01	.029	.433	3.65E-20	.029
.355	0.00E-01	.029	.434	4.05E-20	.029
.360	2.29E-21	.029	.434	6.08E-20	.029
.365	2.87E-21	.029	.435	5.07E-20	.029
.370	8.03E-21	.029	.436	8.11E-20	.029
.375	1.00E-20	.029	.436	1.13E-19	.029
.380	1.72E-20	.029	.437	5.27E-20	.029
.382	1.58E-20	.029	.438	1.01E-19	.029
.384	1.49E-20	.029	.438	1.38E-19	.029
.386	1.49E-20	.029	.439	7.70E-20	.029
.388	2.87E-20	.029	.440	2.47E-19	.029
.390	3.15E-20	.029	.441	8.11E-20	.029
.391	3.24E-20	.029	.442	6.08E-20	.029
.392	3.04E-20	.029	.443	7.50E-20	.029
.393	2.23E-20	.029	.444	9.32E-20	.029
.394	2.63E-20	.029	.445	1.13E-19	.029
.395	3.04E-20	.029	.446	5.27E-20	.029
.396	2.63E-20	.029	.447	2.43E-20	.029
.397	2.43E-20	.029	.448	2.84E-20	.029
.398	3.24E-20	.029	.449	3.85E-20	.029
.399	3.04E-20	.029	.450	6.08E-20	.029
.400	2.84E-20	.029	.451	1.09E-19	.029
.401	3.24E-20	.029	.451	9.32E-20	.029
.402	4.46E-20	.029	.452	1.22E-19	.029
.403	5.27E-20	.029	.453	2.39E-19	.029
.404	4.26E-20	.029	.454	1.70E-19	.029
.405	3.04E-20	.029	.455	3.40E-19	.029
.406	3.04E-20	.029	.455	4.05E-19	.029
.407	2.84E-20	.029	.456	1.01E-19	.029
.408	2.43E-20	.029	.457	1.62E-20	.029
.409	2.84E-20	.029	.458	1.22E-20	.029
.410	6.08E-20	.029	.458	1.42E-20	.029
.411	5.07E-20	.029	.459	4.05E-21	.029
.411	6.08E-20	.029	.460	4.05E-21	.029
.412	4.86E-20	.029	.460	6.08E-21	.029
.413	8.31E-20	.029	.461	2.03E-21	.029
.413	6.48E-20	.029	.462	0.00E-01	.029

Table A-19

Photolytic Data for MGLY + hv --> HO2 + CO + MCO3

Wavelength (um)	Absorption Cross-section	Quantum Yield	Wavelength (um)	Absorption Cross-section	Quantum Yield
.220	2.10E-21	.107	.394	2.31E-20	.107
.225	2.10E-21	.107	.396	2.48E-20	.107
.230	4.21E-21	.107	.398	2.61E-20	.107
.235	7.57E-21	.107	.400	2.78E-20	.107
.240	9.25E-21	.107	.402	2.99E-20	.107
.245	8.41E-21	.107	.404	3.20E-20	.107
.250	9.25E-21	.107	.406	3.79E-20	.107
.255	9.25E-21	.107	.408	3.95E-20	.107
.260	9.67E-21	.107	.410	4.33E-20	.107
.265	1.05E-20	.107	.412	4.71E-20	.107
.270	1.26E-20	.107	.414	4.79E-20	.107
.275	1.43E-20	.107	.416	4.88E-20	.107
.280	1.51E-20	.107	.418	5.05E-20	.107
.285	1.43E-20	.107	.420	5.22E-20	.107
.290	1.47E-20	.107	.422	5.30E-20	.107
.295	1.18E-20	.107	.424	5.17E-20	.107
.300	1.14E-20	.107	.426	5.30E-20	.107
.305	9.25E-21	.107	.428	5.22E-20	.107
.310	6.31E-21	.107	.430	5.55E-20	.107
.315	5.47E-21	.107	.432	5.13E-20	.107
.320	3.36E-21	.107	.434	5.68E-20	.107
.325	1.68E-21	.107	.436	6.22E-20	.107
.330	8.41E-22	.107	.438	6.06E-20	.107
.335	0.00E-01	.107	.440	5.47E-20	.107
.350	0.00E-01	.107	.441	6.14E-20	.107
.354	4.21E-22	.107	.442	5.47E-20	.107
.358	1.26E-21	.107	.443	5.55E-20	.107
.360	2.10E-21	.107	.433	6.81E-20	.107
.362	2.10E-21	.107	.444	5.97E-20	.107
.364	2.94E-21	.107	.445	5.13E-20	.107
.366	3.36E-21	.107	.446	4.88E-20	.107
.368	4.21E-21	.107	.447	5.72E-20	.107
.370	5.47E-21	.107	.448	5.47E-20	.107
.372	5.89E-21	.107	.449	6.56E-20	.107
.374	7.57E-21	.107	.450	5.05E-20	.107
.376	7.99E-21	.107	.451	3.03E-20	.107
.378	8.83E-21	.107	.452	4.29E-20	.107
.380	1.01E-20	.107	.453	2.78E-20	.107
.382	1.09E-20	.107	.454	2.27E-20	.107
.384	1.35E-20	.107	.456	1.77E-20	.107
.386	1.51E-20	.107	.458	8.41E-21	.107
.388	1.72E-20	.107	.460	4.21E-21	.107
.390	2.06E-20	.107	.464	1.68E-21	.107
.392	2.10E-20	.107	.468	0.00E-01	.107