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MODELING OF SIMULATED PHOTOCHEMICAL SMOG WITH KINETIC MECHANISMS
Volume 2. CHEMK: A Computer Modeling Scheme for Chemical Kinetics

by

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ABSTRACT

Mechanisms that describe the formation of photochemical smog are developed using a computer modeling technique directed toward the simulation of data collected in two smog chambers: an indoor chamber and a dual outdoor chamber. The results of simulating 164 different experiemnts are presented in Vol. I. Individual compounds for which specific experiments were simulated and mechanisms developed include the following: formaldehyde, acetaldehyde, ethylene, propylene, butane, and toluene. Experiments in both chambers were simulated for all these compounds. The mechanisms reported describe the decay of the precursor organic compound, formation and decay of secondary organics, conversion of nitrogen oxides, formation of nitrates, and the appearance and decay of ozone. Special emphasis is given to the chemistry of toluene. Also included is a study of a generalized smog-based or carbon-bond mechanism developed in a previous study. Vol. II contains the user's manual and coding for a chemical kinetics computer program, CHEMK.

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SECTION 1

INTRODUCTION

Calculation of the time-dependent concentration profiles of a number of reacting species in a complex reaction mechanism is central to the science of chemical kinetics. Such calculations allow the validation of kinetic schemes and reaction rate constants through the comparison of predicted concentrations with experimental data. The need to rely on approximation methods such as steady-state assumptions, quantum yields, and a "rate-determining step" in making these calculations adds uncertainty to predicted concentrations and could possibly conceal inaccuracies in the kinetic mechanism if the experimental data were highly scattered. These approximation methods are also time-consuming in that the user must formulate them and evaluate their impact on the predictions.

Work by Whitten (1974) and Overton (1976) led to the development of fast and efficient computer programs that make complex calculations commonplace. These computer programs integrate the system of ordinary differential equations (ODEs) associated with a kinetic mechanism, given a set of initial conditions. The method used to integrate the system of ODEs was developed by Gear (1971) and modified by Hindmarsh (1974). Initial work by Whitten (1974) led to the development of a computer program that could handle 50 chemical species and 200 chemical reactions. That program, CHEMK, used the modified Gear routines documented by Hindmarsh (1974).

Since that time Spellmann and Hindmarsh (1975) have modified the Gear routines to handle sparse matrices. The Jacobian, or the matrix of partial differential equations, associated with a given chemical kinetic mechanism is usually sparse, meaning that it contains more zero elements than non-zero elements. Thus, the use of a routine designed specifically for sparse matrices would increase the efficiency of the computer program CHEMK in terms of central processing (CP) time. The work of Spellman and Hindmarsh and our experience with the limitations of the first versions of CHEMK led us to modify CHEMK.

In this report, we present a new version of CHEMK that can handle chemical kinetic mechanisms containing up to 89 species and up to 200 reactions. The new version can also handle photolysis rate constants and temperatures that vary with time, and reaction schemes with stoichiometric coefficients. The Gear routine used is that of Spellmann and Hindmarsh referred to above.

The version of CHEMK documented in this report requires approximately 44000 decimal words to load on a Control Data Corporation (CDC) 7600 computer. The efficiency of the new program has been increased about a factor of 3 from the original versions of CHEMK. Rather than present a detailed description of the program and its various routines, the emphasis in this report has been placed on providing a description of program inputs and options available to the user. A complete program listing is provided in Appendix A. Appendices B and C give the input data for an example run in the CHEMK and the EPA format, respectively. Appendix D gives the output of that example run in EPA format, and Appendix E provides an example of variable photolysis and print options.

SECTION 2

CHEMK INPUT

A brief description of each data input card and its argument list is given below. Both initial program specification and modified operation are treated in this presentation. The data input flow is illustrated schematically in Figure 1.

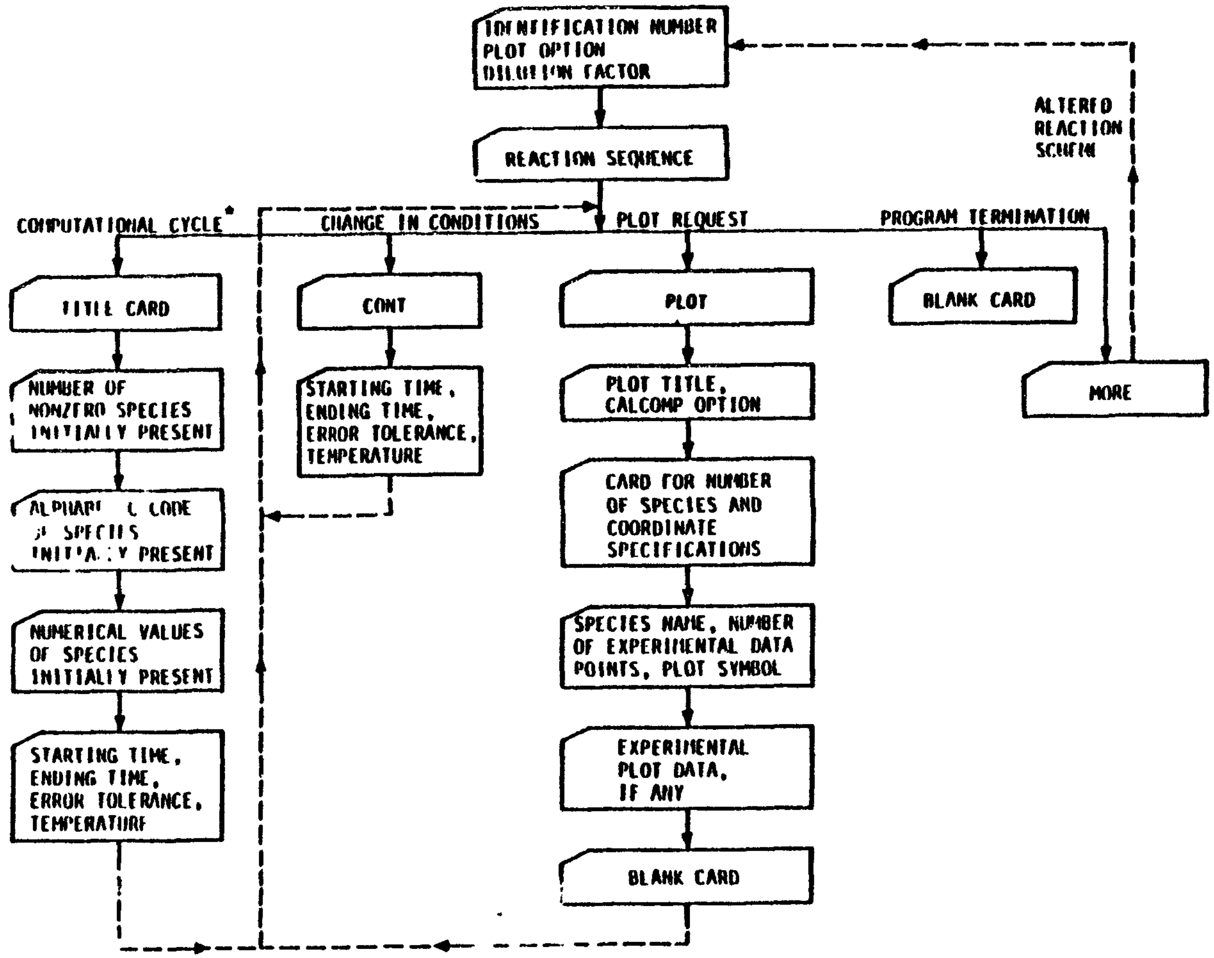
BASIC INPUT FOR A NEW PROBLEM

General Data Card

The arguments that can be entered on this card are:

> The last number of the reaction sequence.
> Choice of reaction format.
> Print option to print only instantaneous concentrations at specified intervals.
> Dilution factor.
> Number of time intervals in which the photolysis rate constants are changing.
> The time interval of each photolysis number.
> The number of photolysis reactions.
> The number of temperature values.
> The time interval of each temperature value.
> Option to plot the photolysis values as a function of time.

The last number of the reaction sequence should correspond to the number on the last card in the reaction scheme, even though it is not the highest reaction number. The next parameter (choice of reaction format) is to enable users of EPASIM (Overton, 1976) and users of the first versions of



* Must be executed for the first cycle

Figure 1. Data input flow chart

CHEMK to use the current version of CHEMK. A more detailed discussion of this option is presented in the section on kinetic mechanism cards.

An option has been added to the CHEMK program that will control the printing of the species' net rates of formation and the net rates of reaction. When this option is not used, only species concentrations are printed at specified time intervals.

To activate this option so that species net rates of formation and net rates of reaction will be printed at the same specified time intervals, the user enters any alphanumeric character anywhere in columns 11 through 14 of the General Data Card.

The dilution factor represents a constant dilution rate for every species such that:

$$\frac{dC_i}{dt} = -DC_i \qquad (1)$$

where

C_i = concentration of species i

D = dilution factor.

In many experiments all species are being diluted by a common first-order factor. If this factor is entered in the third field of the General Data Card (the one that identifies the last reaction and on all subsequent appearances of such a card), then this option will be activated. If one species (e.g., O_2) is part of the dilution gas, a first order "flow out" (e.g., O_2, the only reactant with no products) reaction with a negative rate constant equal to the dilution factor will cancel the dilution for such a species.

The next three parameters (number of time intervals in which the photolysis rate constants are changing, the time interval of each photolysis number, and number of photolysis reactions) are used to input the conditions of the time-varying photolysis rate constants. If a blank or zero is entered for the number of time intervals, then the time interval and number of photolysis reactions should not be entered. If the number of time intervals is nonzero then the first card after the General Data Card should contain the vector of reaction numbers that identify the reactions with varying photolysis rate constants. Up to seven numbers may be placed on each card.

The next card(s) will contain the initial photolysis value and the values at the end of each time interval. If, for example, the user inputs 5 as the number of time intervals and 60 (minutes) as the time interval, then six photolysis values should be entered on the card (one for the initial value and one for every 60 minutes thereafter). Up to seven photolysis values may be entered on one card. The total time in which the photolysis rate constants are changing in the above example is 300 minutes. If the simulation is carried for a longer period of time (e.g., 600 minutes) then all photolysis rate constants are set to zero after 300 minutes. The maximum number of time intervals is 97 for each simulation. If more values are needed the MORE option may be used (see section on MORE option).

If the number of temperature values is nonzero, the next set of cards is the vector of temperature values (initial plus the end of each time interval specified on the General Data Card). The format for the temperature values is similar to that for the photolysis values. All temperature values must be in units of degrees Kelvin (K). All activation energies entered on each reaction card must also be in units of degrees Kelvin. The temperature at each specified printout time is printed with the rest of the species under the column TEMP.

If the user wishes to obtain a plot of the photolysis values as a function of time, then a nonzero value is declared in columns 56 to 60. A line printer plot is produced at the end of the species concentration versus time profiles. This option should be activated only when the plot option is declared.

2. Kinetic Mechanism Cards

Each chemical reaction in the mechanism must be entered individually. Entry requires (1) that the reaction be numbered, (2) that its components be specified in alphanumeric form, and (3) that the rate constant at 298K be specified. If the reaction is temperature-dependent, then the activation energy (in degrees Kelvin) can also be specified. A maximum of 200 reactions is allowed by the program.

The user has a choice of two different input formats for the reactions. To accommodate users of EPASIM (Overton, 1976) CHEMK allows nonunity stoichiometric coefficients for the products of the reactions. The reaction input format described in EPASIM and summarized in Table 1 is available for users of EPASIM and the current version of CHEMK. A maximum of three reactants and three products (with stoichiometric coefficients) are allowed under the EPASIM format. To use the EPASIM format, the user must enter a nonzero value in the second field of the General Data Card (see preceding subsection).

Reaction identification numbers are not used under the EPASIM format as described by Overton (1976). Therefore, we introduced this parameter in columns 17, 18, and 24 of the reaction card. The first field represents the reaction number from 1 through 99. If the user has more than 99 reactions, a modulus factor must be specified in column 24 to convert the reaction number to a number greater than 100. For example, a reaction identification number of 13 is given on the reaction card in columns 17 and 18 while column 24 is left blank. A reaction identification number of 123 is given on the reaction card first by input of 23 in columns 17 and 18 and 1 in column 24. For reaction 200, columns 17 and 18 are left blank (representing zero) and a 2 is entered in column 24.

For users of earlier versions of CHEMK and new users a different reaction input format is available. A maximum of three reactants and four products (without stoichiometric coefficients) is allowed under this format.

For the reacting species, any combinations of letters and numbers can be used to identify the individual entries with the exception that the letter M is exclusively reserved to designate the total pressure and TEMP is reserved for the temperature.

To specify a "flow in" reaction, that is, the continuous addition of a particular species, a reaction with only products can be used where the reaction rate k is equal to the flow rate. A reaction with a reactant but no products implies a first-order "flow out" process.

When preparing the data, one must ensure that the rate constant is in units consistent with the order of the reaction as specified in the reaction mechanism. Instead of input of a rate constant for each photolysis reaction, a photolysis ratio is entered when variable photolysis is used (see the section on the General Data Card). This ratio is the ratio of the actual photolysis rate constant to the photolysis values entered on the card(s) following the General Data Card. For example, if the user inputs photolysis values, then each of the photolysis reactions will have a photolysis constant determined at each instant in time from the product of the interpolated photolysis value and the ratio entered on the reaction card. All photolysis values must be declared on the card after the General Data Card, as discussed earlier. Therefore, for example, if the photolysis values represent NO_2 photolysis rate constants, then the NO_2 photolysis reaction identification number must be declared and a value of 1.0 entered for the rate constant. It is also wise to keep in mind the following points:

> HO2 and HOO will be treated as different species.
> 2NO will be treated as a new species and not as two NOs unless the EPASIM format is used.
> The maximum number of different species is 89.

Title Card

Each simulation is titled by entering the desired notation in columns 1 through 28 of this card. Anything may be entered in the first four columns of this card with the following exceptions:

> All blank: This card will terminate the program.
> CONT: This is an option indicating that concentrations and species from a previous run will be used as initial conditions for a new run.
> MORE: This choice indicates that new reactions or new photolysis and temperature values are to be added.
> PLOT: This entry activates the plotting routine.

Output Specification Card

The first two items on this card specify the number of reactants with nonzero initial concentrations and the number of integration steps between print cycles. Normally, the program suppresses the printing of the concentrations of all species as a function of the integration steps. However, the user may key the output to the frequency of the integration steps by entering a negative number of steps between print-outs in the appropriate slot on the data card. Thus, if the user enters a value of -5, the program will print the instantaneous concentrations every 5 iteration steps. If the user only wants concentrations printed at specified intervals, then this option should not be activated (i.e. leave this slot blank). To obtain output at specific times, the user enters the initial print time and then either a fixed time increment or a fixed multiple to be used between subsequent printings. For example, a user may specify an initial print time of 10 minutes and set the time increment at 10 minutes. In this case, output will be printed at 10 minutes, 20 minutes, 30 minutes, and so on. Or the user may specify an initial print time of 10 minutes and then set the print multiple at 2, in which case output is provided at 10 minutes, 20 minutes, 40 minutes, 80 minutes, and so on.

Initial Reactant Identification Card(s)

The vector containing the alphabetic designation of all reactants with a nonzero initial concentration is given on this card(s).

Initial Reactant Concentration Card(s)

The initial concentrations of all reactants, in appropriate units, are provided on this card in the same sequence as species are entered on the Initial Reactant Identification Card(s).

Time Specification Card

The simulation starting time and ending time are the first two arguments on this card. Their time unit should be identical to that used to specify rate constants. In addition, the absolute temperature and the error tolerance for the integration step may be entered on this card. Default values of these parameters are 298K and 10^{-2}, respectively.

After each simulation the user may choose the following options:

> Start a new simulation with the same mechanism by first inserting a new title card.
> Terminate the program by inserting a blank card.
> Provide a new or changed reaction sequence and start a new calculation using the MORE option.

- Continue the calculation using the current results but with some parameter changed using the CONT option.
- Plot the computed output using the PLOT option.

All of these possibilities are discussed in the following section.

PROGRAM OPTIONS

More Than One Computation

Rather than enter a terminating blank card, insert a new title card followed by a new set of initial condition data. The new data will provide computational results using the previously specified reaction scheme.

To Continue with Previously Calculated Species

If the new title card has CONT in its first four columns, the species from the previous calculation and their concentrations will be used as initial conditions for a problem in which either new reactions are entered or the temperature or error tolerance is changed. The next card must in this case be the time specification card, having the starting and ending times, error tolerance, and temperature.

New or Changed Reactions

To introduce either new or changed reactions into the kinetic mechanism, enter a card with the word MORE punched in columes 1 through 4 followed by the set of cards used for specifying the changes in the kinetic mechanism. This set includes a first card similar to the General Data Card. Any parameter controlled on the original General Data Card can be changed on this new version. The difference between this card and the original is that all blank fields will default to the parameters controlled on the original card or to the present values changed by previous uses of the MORE option. For example the dilution factor may be the only change desired. To accomplish this a MORE card followed by a card with only the new dilution factor in columns 21 through 30 would be used. The next card in this example might then be a CONT to continue the previous calculation or a new title to start an entirely new calculation with the same mechanism modified only by the new dilution factor.

The most frequent utilization of this option is typically for additions or alterations to the original mechanism. To alter any reaction a new reaction card is entered with the same identification number as the original. The new card must contain the complete reaction in its new form since it will replace the original. New reactions must have identification numbers not previously used in the original mechanism. In any case the identification number of the last reaction card to be read in at this time must appear on the new General Data Card in columns 1 to 3.

A new variable photolysis vector, a new variable temperature vector, or a new set of photolysis reactions controlled by the variable photolysis vector can also be introduced using this option. If a new photolysis reaction is to be added to the original set that varies with the time dependent photolysis vector, then the entire new set, including both the originals and the new additions, must be read in.

Plot Option Card

At the end of the computational cycle, a card with PLOT in its first four columns must be entered. This signals the program that the plot option is to be used and plot data are to follow.

Plot Title Card

If a plot has been selected by entering the word PLOT on the above card, then the user must supply a plot title card, which may have storage option entry and an option to print the species concentrations at certain time steps. The storage option entry determines whether the plotted output will be stored on a tape file for later access. If the output is to be stored, the user need only insert any nonzero number in the option argument space.

The data is stored on a file titled TAPE 7 in unformatted form. The following parameters are written to the file TAPE 7:

> NTIT--The plot title.
> NAME(L)--The Lth species being plotted.
> CLOW--The lowest concentration entered on the plot specification card.
> CHIGH--The highest concentration value entered on the plot specification card.
> TLOW--The lowest time value entered on the plot specification card.
> THIGH--The highest time value entered on the plot specification card.
> NDAT--Number of observed data points.
> NPNT--Number of calculated data points.
> (TIME(J),J=1,NDAT)--The vector of time values of the observed data.
> (DATA(J),J=1,NDAT)--The vector of observed concentration values.
> (SAVTIM(J),J=1,NPNT)--The vector of time values of the calculated data.
> (SAVCON(L,J),J=1,NPNT)--The vector of calculated concentrations.

The twelve parameters are written with a single WRITE statement and should be read in the same manner.

If the user is interested in the actual concentrations of the species being plotted, then a nonzero value entered for this option will activate the printing of the actual concentrations at the times closest to every one-eightieth of the total simulation time. Thus, if the total simulation time is 400 minutes then calculated concentrations at 5-minute intervals are printed.

Plot Specification Card

The plotting routine can handle up to three species on one plot. This is done by specifying the number of species to be plotted on the plot specification card. The information entered on this card is: The number of species to be plotted, the concentration labels for the vertical axis (five labels must be entered), the lowest and highest values of the concentrations, and the lowest and highest values of the integration time.

Species Information Card

This card contains the name of the species to be plotted (the species identification code), the number of data points to be plotted from experimental data, and the plot output symbol. If the number of experimental data points is zero, the next card is not entered. A species identification card must be entered for each species to be plotted.

Experimental Plot Data Cards

A unique feature of the PLOT program is its ability to overlay experimental data over a computer concentration profile. To do this, pairs of time and concentration values must be entered for each species. Four pairs of these values appear on each card, and the number of entries corresponds to the value specified on the previous data card.

End of Plot Data Card

A blank card must be entered to signal the end of the plot data. The next card can start a new simulation.

End of Program Card

A blank card entered instead of a new title or option card ends the program.

Table 1 provides an individual description of each data card, its argument list, format code, and column entries.

Calculation of the Round-Off Error

The variable UROUND in block data ALPHA1 should be set to the round-off error associated with each computer system. Currently, UROUND is set to the round-off error of 7.5×10^{-15} associated with a CDC 7600 computer system. To reset UROUND, the card (W.16) in block data ALPHA1 should be changed:

```
DATA     UROUND/user's round-off error/     (card W.16)
```

UROUND is calculated from the number of significant digits (N) used for the mantissa of a floating point constant:

$$UROUND = 2^{-N}$$

For example, on the UNIVAC 1110 computer, each word contains 36-BITs of which 27 are used for the mantissa. Thus, 2^{-27} is equal to approximately 7.5×10^{-9}. This is the value required for UROUND in CHEMK.

TABLE 1. INPUT CARD DESCRIPTION

Card	Column	Format	Description
General Data Card	1-3	I3	Last number of reaction sequence
	6-10	I5	Choice of reaction input format: Nonzero=EPASIM, default=CHEMK format
	11-14	A4	Print option for net rates of reaction and species rate of formation: default=printing is suppressed
	15-20	--	Not read
	21-30	F10.0	Dilution factor
	31-35	I5	Number of photolysis time units
	36-40	I5	Time interval of each photolysis time unit
	41-45	I5	Number of photolysis reactions
	46-50	I5	Number of temperature time units
	51-55	I5	Time interval of each temperature time unit
	56-60	--	Option to plot photolysis values as a function of time
	61-80	--	Not read
Next card(s)	1-10 11-20 21-30 • • • 61-70	7I10	If there are variable photolysis rate constants, the reaction identification vector identifying number of each photolysis reaction is read here
	71-80	--	Not read
Next card(s)	1-10 11-20 21-30 31-40 • • • 61-70	7F10.0	The initial photolysis and the value at the end of each time unit. If photolysis occurs for N units of time, then there should be N+1 photolysis values
	71-80	--	Not read

Table 1 (Continued)

Card	Column	Format	Description
Next card(s)	1-10 11-20 21-30 31-40 . . . 61-70	7F10.0	If variable temperature is used then the temperature values are read here. If there are N units of time in which the temperature changes, then there should N+1 temperature values
	71-80	--	Not read
Kinetic Mechanism Card (EPASIM format)	1-4, 7-11, 13-16,	A4 A4 A4	The names of the reactants (up to three are allowed)
	17-18	I2	The identification number of the reaction (number may be between 0 and 99; 0 only if next field is nonzero)
	19-23	F5.0	The stoichiometric coefficient of the first product; a blank implies a default value of 1
	24	I1	Modulus factor for reaction identification numbers greater than 100 (values are 0 or blank, 1, and 2); if a value of 1 is entered, the reaction identification number will be between 100 and 199 depending on the value in columns 17 and 18
	25-28	A4	The name of the first product
	32-36	F5.0	The stoichiometric coefficient of the second product
	37-40	A4	The name of the second product
	41-45	F5.0	The stoichiometric coefficient of the third product

Table 1 (Continued)

Card	Column	Format	Description
	49-52	A4	The name of the third product
	55-64	F10.0	The rate constant at 298K or, for photolysis reactions, the ratio of the photolysis value to reaction number 1
	66-72	F7.0	The activation energy in degrees Kelvin (K)
Kinetic Mechanism Card (CHEMK format)*	1- 3	I3	The reaction identification number
	6- 9 11-14 16-19	A4	The names of the reactants (up to three allowed)
	21-24 26-29 31-34 36-39	A4	The names of the products (up to four allowed)
	41-50	F10.0	The rate constant at 298K or the photolysis ratio for photolysis reactions
	51-60	F10.0	The activation energy in degrees Kelvin (K)
Title Card	1-72	18A4	The first four columns must not all be blank or contain one of the following: MORE, CONT, PLOT
Output Specification Card	1- 3	I3	Number of reactants with initial nonzero concentrations (maximum is 89)
	21-30	I10	Number of integration steps between print cycles; default is 10^4 to suppress printing keyed to step size.
	31-40	F10.0	Specific time of initial print (independent of step size)

TABLE 1 (Continued)

Card	Column	Format	Description
	41-50	F10.0	Time interval
	51-60	F10.0	Time multiple (note that at least one of the above two fields must be blank)
Initial Reactant Card(s)	1- 4, 11-14 21-24 • • • 61-64	A4	Alphanumeric identification of the reactants with initial nonzero concentrations seven species per card
	65-80	--	Not read
Initial Reactant Concentration Card(s)	1-10 11-20 21-30 • • 61-70	F10.0	Initial concentrations of reactants. Concentrations must be given in the same sequence as the species are given on Initial Reactant Card(s)
	71-80	--	Not read
Time Specification Card	1-10	F10.0	Simulation starting time. Time must be in the same units as the rate constants
	11-20	F10.0	Simulation ending time. Time must be in the same units as the rate constants
	21-30	F10.0	Temperature (constant throughout the simulation if variable temperature profile is not used; default=298K)
	31-40	F10.0	Error tolerance; default=10^{-2}
	41-80	--	Not read

TABLE 1 (Continued)

Card	Column	Format	Description
Options Card	1- 4	A4	Plot initiated if PLOT is entered. Additional kinetic steps are processed if MORE is entered. A new starting time is used if CONT is entered. Program terminates if blank card is inserted.
	5-80	--	Not read
Plot Option Cards:			
Plot Title	1-12	3A4	Title of simulation
	13-54	--	Not read
	55-60		Option to print actual concentrations of all plotted species
	61-65	I5	Data storage option. If nonzero, plot data is saved on a file named TAPE7
	66-80	--	Not read
Plot Specification Card	1- 5	--	Not read
	6- 7	I2	Number of species to be plotted; up to three species may be placed on one plot
	8-15	--	Not read
	16-19 21-24 26-29 31-34 36-39	A4	Concentration labels: Five arguments must be entered
	41-50	F10.0	Lowest concentration value
	51-60	F10.0	Highest concentration value
	61-70	F10.0	Lowest time value
	71-80	F10.0	Highest time value

TABLE 1 (Concluded)

Card	Column	Format	Description
Species Identification Card (one card for each species)	1 - 4	A4	Name of species to be plotted
	6- 7	I2	Number of data points to be plotted from experimental data. Value must be between 1 and 80. If set at zero, no experimental data are read
	8	--	Not read
	9	A1	Symbol for plotted output
	10-80	--	Not read
Experimental Plot Data	1-10	F10.0	Time
	11-20	F10.0	Concentration
	21-30 31-40 . . . 61-70, 71-80	F10.0	(A total of four sets of time and concentration are placed on each card)
End of Plot Data	1- 4	A4	Blank card
	5-80	--	Not read
End of Program	1- 4	A4	Blank card
	5-80	--	Not read

* Default reaction format

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Appendix A
Program Listing

```
C***********************************************************************
C
C     CHEMK IS A FORTRAN PROGRAM WHICH, WHEN GIVEN A PREDETERMINED
C     KINETIC MECHANISM, COMPUTES THE CONCENTRATIONS OF THE VARIOUS
C     REACTANTS IN TIME. IT WAS WRITTEN BY GARY Z. WHITTEN OF SYSTEMS
C     APPLICATIONS INCORPORATED IN SAN RAFAEL, CA AND INCORPORATES
C     THE GEAR INTEGRATION PACKAGE OF A. HINDMARSH OF LAWRENCE LIVERMORE
C     LABORATORIES IN LIVERMORE, CA.  THE PRINTER-PLOT ROUTINE WAS
C     PROVIDED BY DAVID C. WHITNEY OF SAI AND THE PROGRAM WAS CONVERTED
C     ANSI FORTRAN BY JIM MEYER OF SAI. THE  COMPUTER CODE THAT FOLLOWS
C     IS EXECUTABLE ON ANY IBM OR CDC MACHINE WITH A FORTRAN IV COMPILER
C
C     TWO SEPARATE SETS OF DATA ARE NEEDED TO EXECUTE THE PROGRAM. ONE
C     SET CONTROLS THE COMPUTATIONAL PART OF THE PROGRAM AND IS
C     NECESSARY TO ESTABLISH THE INTEGRATION ROUTINE.  THE SECOND SET OF
C     CONTROLS THE PLOTTER OUTPUT AND PROVIDES THE PARAMETERS NECESSARY
C     SPECIFY THE  OUTPUT FORMAT.  THE READER IS REFERED TO THE PROGRAM
C     FOR FURTHER INFORMATION.
C
C                                GARY Z. WHITTEN
C                                SYSTEMS APPLICATIONS INCORPORATED
C                                950 NORTHGATE DRIVE
C                                SAN RAFAEL, CALIFORNIA  94903
C                                (415) 472-4011
C
C***********************************************************************
C
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT
      COMMON /NAMES/ SPECIS(91),REACT(91),NS
      COMMON /FRPLOT/ NIT(3),SAVCON(90,80),SAVTIM(80),JGRID(89,40),NT
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER
      COMMON /APLOT/ JVERT(52,2),JBLANK,JSTAR,JPLUS,JBAR
      COMMON /GEAR1/ T,GUESS,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART
      COMMON /GEAR2/ YMAX(100)
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP
      COMMON /SPARSE/ IA(91),JA(1000)
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST,
     1IPH(30),QM(100),PM(100),PSTOP
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10
      DIMENSION C(91), IRS(200,7), KRS(7), SC1(7)
      INTEGER SPECIS,REACT,PHI,TMI,AST
C
C     ALPHAMERIC DATA ARE PREASSIGNED IN BLOCK DATA ALPHA1
C
      DATA NPLOT/4HSAVE/,IBLK/1H /
      DATA IN2,IN3,IN5,IN6,IN7,IN8,IN9/7*1/
      DATA XN4,XN6,XN9/3*1.0/
```

```
C
C     INITIAL PARAMETERS
C
      IN=5
      IOUT=6
      ITAPE=7
C
C     CLEAR PATTERN MATRIX AND SET THE FIRST ELEMENTS
C     ALSO SET STOICHIOMETRIC COEFFICIENTS EQUAL TO 1
C
      DO 5 J=1,200
      DO 5 K=1,7
      IRS(J,K)=IBLANK
      SC(J,K)=1.
    5 KR(J,K)=0
      DO 10 J=1,200
      A(J)=0.
      R(J)=0.
   10 S(J)=0.
      NR=0
      NS=0
C
C     NX = LAST NUMBER OF THE REACTION SEQUENCE
C     NPLOT = PLOT OPTION
C     DILUT= DILUTION FACTOR
C
      READ (IN,185) NX,NEPA,NPLIT,DILUT,NPHOT,PHI,IL,NTEMP,TMI,IPP
      GO TO 20
   15 NS=NS-1
      READ (IN,185) NX,IN2,IN3,XN4,IN5,IN6,IN7,IN8,IN9,IN10
      IF (IABS(IN2).NE.0) NEPA=IN2
      NPLIT=IN3
      IF (ABS(XN4).NE.0) DILUT=XN4
      IF (IABS(IN5).NE.0) NPHOT=IN5
      IF (IABS(IN6).NE.0) PHI=IN6
      IF (IABS(IN7).NE.0) IL=IN7
      IF (IABS(IN8).NE.0) NTEMP=IN8
      IF (IABS(IN9).NE.0) TMI=IN9
      IF (IABS(IN10).NE.0) IPP=IN10
   20 IF (IL.LE.0.OR.IN7.LE.0) GO TO 25
      READ (IN,200) (IPH(I),I=1,IL)
   25 IF (NPHOT.LE.0.OR.IN5.LE.0) GO TO 30
      NPHOT=NPHOT+1
      READ (IN,190) (PM(I),I=1,NPHOT)
      PM(NPHOT+1)=2.0*PM(NPHOT)-PM(NPHOT-1)
      PM(NPHOT+2)=3.0*PM(NPHOT)-2.0*PM(NPHOT-1)
      PSTOP=FLOAT((NPHOT-1)*PHI)
   30 IF (NTEMP.LE.0.OR.IN8.LE.0) GO TO 35
      NTEMP=NTEMP+1
      READ (IN,190) (QM(I),I=1,NTEMP)
```

```
      QM(NTEMP+1)=2.*QM(NTEMP)-QM(NTEMP-1)
      QM(NTEMP+2)=3.0*QM(NTEMP)-2.0*QM(NTEMP-1)
      TEMEND=FLOAT((NTEMP-1)*TMI)
   35 IF (NX.GT.0) WRITE (IOUT,130)
      IF (NX.LE.0) NS=NS+1
      IF (NX.LE.0) GO TO 80
C
C     REACTION INPUT DATA
C
   40 IF (NEPA.LE.0) READ (IN,135) J,(IRS(J,I),I=1,7),A(J),S(J)
      IF (NEPA.LE.0) GO TO 55
      READ (IN,220) (KRS(I),I=1,3),J,SC1(1),JJ,KRS(4),(SC1(LL-3),KRS(LL)
     1,LL=5,6),RTE,ENERGY
      IF (JJ.GT.0) J=JJ*100+J
      DO 45 II=1,6
   45 IRS(J,II)=KRS(II)
      A(J)=RTE
      S(J)=ENERGY
      DO 50 II=4,6
   50 SC(J,II)=SC1(II-3)
   55 DO 60 I=1,7
   60 IF (SC(J,I).LE.0.) SC(J,I)=1.
      DO 75 K=1,7
      NL=K*5
      NF=NL-4
      DO 65 LK=NF,NL
   65 AST(LK)=IBLK
      IPL(K)=IBLK
      IF (K.EQ.1.OR.K.EQ.4) GO TO 70
      IF (IRS(J,K).NE.IBLANK) IPL(K-1)=JPLUS
   70 IF (IRS(J,K).NE.IBLANK) CALL VALU (SC(J,K),K,NF,NL)
   75 CONTINUE
      WRITE (IOUT,140) J,(AST(I),I=1,5),IRS(J,1),IPL(1),(AST(I),I=6,10),
     1IRS(J,2),IPL(2),(AST(I),I=11,15),IRS(J,3),IPL(3),(AST(I),I=16,20),
     2IRS(J,4),IPL(4),(AST(I),I=21,25),IRS(J,5),IPL(5),(AST(I),I=26,30),
     3IRS(J,6),IPL(6),(AST(I),I=31,35),IRS(J,7),IPL(7),A(J),S(J)
      KR(J,1)=100
      IF (J.GT.NR) NR=J
      IF (J.NE.NX) GO TO 40
C
C     ESTABLISH REACTION MATRIX AND SET UP SPARSE JACOBIAN VECTORS
C
      CALL MATRX (C,IRS)
      CALL SPARS (IA,JA,NS-2)
      INX=1
C
C     TITLE CARD AND OPTIONS
C
   80 READ (IN,195) (ITITLE(I),I=1,7)
      NFL=0
```

```
      IF (ITITLE(1).EQ.IGO(1)) GO TO 15
      IF (ITITLE(1).EQ.IGO(2)) GO TO 115
      IF (ITITLE(1).EQ.IGO(3)) GO TO 85
      IF (ITITLE(1).EQ.IBLANK) STOP
      GO TO 90
C
C     CALL PLOT
C
   85 READ (IN,180) (NIT(I),I=1,3),IDT,KALCMP
      NT=NT-2
      CALL PLOT (NIT,NT,NS,SPECIS,SAVTIM,SAVCON,IDT,KALCMP,JGRID)
      GO TO 80
C
C     OPTIONS CARD
C
   90 READ (IN,155) N,NPRNT,TPRNT,TSTEP,TFACT
C
C     TIME STEP SKIP OPTION
C
      IF (NPRNT*NPRNT.EQ.0) NPRNT=100000
C
C     TIME STEP LENGTH OPTION
C
      IF (TPRNT*TPRNT.EQ.0.) TPRNT=1.E10
C
C     CONCENTRATION OF SPECIES INITIALLY PRESENT
C
      READ (IN,125) (REACT(I),I=1,N)
      READ (IN,190) (C(I),I=1,N)
C
C     STARTING AND ENDING INTEGRATION TIMES
C
      READ (IN,175) START,STOPP,TEMP,ERR
      IF (START*START.EQ.0.) START=0.
C
C     SPECIFICATION OF THE TEMPERATURE IF UNSPECIFIED IN INPUT
C
      IF (TEMP.LE.0.) TEMP=298.
C
C     SPECIFICATION OF THE ERROR BOUND IF UNSPECIFIED IN INPUT
C
      IF (ERR*ERR.EQ.0.) ERR=1.E-2
C
C     OUTPUT OF THE INITIAL CONDITIONS
C
      WRITE (IOUT,145) (ITITLE(I),I=1,7),(REACT(I),I=1,N)
   95 WRITE (IOUT,150) (C(I),I=1,N)
C
C     COMPUTE THE NET RATES OF REACTION
C
```

```
      IF (NTEMP.GT.0) TEMP=QM(1)
      IF (ITITLE(1).EQ.IGO(2).AND.NTEMP.GT.0) TEMP=TEMOLD
      CALL RATES (C,N)
C
C     OUTPUT OF THE TEMPERATURE AND ERROR BOUND
C
      WRITE (IOUT,160) TEMP,ERR
C
C     OUTPUT OF THE DILUTION FACTOR
C
      IF (DILUT*DILUT.EQ.0.) DILUT=0.
      IF (DILUT.NE.0.) WRITE (IOUT,170) DILUT
C
C     SET LIMITS FOR TIMED OUTPUTS
C
      IF (TSTEP.NE.0.) YMAX(1)=TSTEP
      IF (TSTEP.NE.0.) PC=TSTEP
      IF (TSTEP*TSTEP.EQ.0.) YMAX(1)=1.E10
      IF (TSTEP*TSTEP.EQ.0.) PC=1.E10
      IF (TFACT.NE.0.) YMAX(2)=TFACT
      IF (TFACT*TFACT.EQ.0.) YMAX(2)=1.
C
C     RATE CONSTANTS
C
      WRITE (IOUT,165) (R(I),I=1,NR)
C
C     WRITE INITIAL CONDITIONS OF THE CELL
C
      IF (NPHOT.LE.0) GO TO 105
      WRITE (IOUT,215) (IPH(I),I=1,IL)
      DO 100 I=1,IL
      J=IPH(I)
      YMAX(10+I)=R(J)
  100 CONTINUE
      WRITE (IOUT,225) (YMAX(10+I),I=1,IL)
      NPT=NPHOT
      WRITE (IOUT,205) PHI,(PM(I),I=1,NPT)
  105 IF (NTEMP.LE.0) GO TO 110
      NPT=NTEMP
      WRITE (IOUT,210) TMI,(QM(I),I=1,NPT)
  110 GUESS=1.E-10
      T=START
      IF (NPLOT.EQ.IBLANK) YMAX(3)=0.
      IF (NPLOT.NE.IBLANK) YMAX(3)=1.
      IF (NPLIT.NE.IBLANK) YMAX(4)=1.
      IF (NPLIT.EQ.IBLANK) YMAX(4)=0.
C
C     INITIALIZE PARAMETERS
C
      CALL YFIX (NS,TPRNT,C,NPRNT,INX)
```

```
      INX=4
      TEMOLD=TEMP
      GO TO 80
C
C     CONTINUATION OF DATA
C
  115 READ (IN,175) START,STOPP,TEMP,ERR
      IF (TEMP.LE.0.) TEMP=298.
      IF (TEMOLD.NE.298..AND.TEMOLD.NE.0.) TEMP=TEMOLD
      IF (ERR*ERR.EQ.0.) ERR=1.E-2
      DO 120 I=1,NS
  120 REACT(I)=SPECIS(I)
C
C     INITIAL CONDITIONS
C
      WRITE (IOUT,145) (ITITLE(I),I=1,7),(REACT(I),I=1,NS)
      N=NS
      GO TO 95
C
C
  125 FORMAT (7(A4,6X))
  130 FORMAT (1H1,14H THE REACTIONS,86X,13HRATE CONSTANT,2X,15HACT. ENER
     1GY (K))
  135 FORMAT (I3,2X,7(A4,1X),2F10.0)
  140 FORMAT (/,2X,I3,2X,3(5A1,1X,A4,2X,A1),1H=,2X,4(5A1,1X,A4,2X,A1),1P
     1E11.3,2X,E13.3)
  145 FORMAT (1H1,30X,7A4,//,23H INITIAL CONCENTRATION ,//(10X,10(4X,A4,
     14X)))
  150 FORMAT (/(8X,1P10E12.3))
  155 FORMAT (I3,17X,I6,4X,3F10.0)
  160 FORMAT (/,34H THE TEMPERATURE OF THE CELL WAS =,1PE9.2,26H AND THE
     1 ERROR TOLERANCE =,E9.2)
  165 FORMAT (/,29H THE RATE CONSTANTS USED WERE,/,(/,8X,1P10E12.3))
  170 FORMAT (/,30H THE OVERALL DILUTION RATE WAS,1PE9.2)
  175 FORMAT (8F10.0)
  180 FORMAT (3A4,43X,2I5)
  185 FORMAT (I3,2X,I5,A4,6X,F10.2,6I5)
  190 FORMAT (7F10.3)
  195 FORMAT (7A4)
  200 FORMAT (7I10)
  205 FORMAT (/44H0THE NO2 PHOTOLYSIS NUMBERS IN INTERVALS OF ,I3,15H TI
     1ME UNITS ARE,/,(1H0,1P10E13.3))
  210 FORMAT (/34H0THE TEMPERATURES IN INTERVALS OF ,I3,15H TIME UNITS A
     1RE/(1H0,1P10E13.3))
  215 FORMAT (/29H0THE PHOTOLYSIS REACTIONS ARE,/(1H0,9I13))
  220 FORMAT (2(A4,2X),A4,I2,F5.1,I1,A4,2X,2(F5.0,1X,A4,2X),F10.2,1X,F7.
     12)
  225 FORMAT (57H0THE PHOTOLYSIS RATIOS OF EACH OF THE REACTIONS ABOVE A
     1RE/(1H0,4X,1P9E13.3))
      END
```

```
      SUBROUTINE YFIX (NO,TLAST,C,NQ,INDEX)
C
C***********************************************************************
C
C     THIS IS THE NORMAL OUTPUT ROUTINE
C
C***********************************************************************
C
      COMMON /SPARSE/ IA(91),JA(1000)
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT
      COMMON /NAMES/ SPECIS(91),REACT(91),NS
      COMMON /FRPLOT/ NIT(3),SAVCON(90,80),SAVTIM(80),JGRID(89,40),NT
      COMMON /GEAR1/ D,H,DUM(4),IDUM(4)
      COMMON /GEAR2/ YMAX(100)
      COMMON /INOUT/ INPP,IOUT,ITAPE
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST,
     1IPH(30),QM(100),PM(100),PSTOP
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10
      DIMENSION C(91), RT(200)
      INTEGER SPECIS,REACT,TMI,PHI,AST
      DATA IGO/4HCONT/
      DATA NT1/1/
      DATA START1/0.0/
      N=NS-1
      NS2=NS-2
      NFRST=1
C
C     TIME INTERVALS
C
      IF (ITITLE(1).NE.IGO) GO TO 30
      IF (NT1.EQ.0) GO TO 30
      TDC=(STOPP-START1)/80.
      TD=START1+TDC
      J=0
      NTSV=NT
      DO 25 I=1,80
    5 J=J+1
      IF (J.GT.NTSV) GO TO 20
      IF (SAVTIM(J).GE.TD) GO TO 10
      GO TO 5
   10 SAVTIM(I)=SAVTIM(J)
      DO 15 K=1,NS
   15 SAVCON(K,I)=SAVCON(K,J)
      NT=I
      GO TO 25
   20 IF (I.EQ.1) NT=1
      SAVTIM(I)=TD
   25 TD=TD+TDC
```

```
      GO TO 40
   30 TDC=(STOPP-START)/80.
      TD=START
      DO 35 I=1,80
      TD=TD+TDC
   35 SAVTIM(I)=TD
      START1=START
      NT=1
   40 NC=0
C
C     INITIALIZE PARAMETERS
C
      NHS=0
      MS=IABS(NQ)
      TPRNT=TLAST+START
      TSTEP=PC
      TFACT=YMAX(2)
      IF (TFACT.GT.1.) TSTEP=0.
      MT=50-((NS-1)/10)*3-(NR-1)/10
      NN=NS+1-MIN0(NS/10,1)
      IF (YMAX(3).EQ.0.) NPLOT=0
      IF (YMAX(3).NE.0.) NPLOT=1
      IF (YMAX(4).EQ.0.) NOPT=0
      IF (YMAX(4).NE.0.) NOPT=1
      IF (NOPT.EQ.0) MT=50-((NS-1)/10)*2
      NTP=0
      NT1=NPLOT
      IF (NPLOT.EQ.0) NT=-1
      IN=INDEX
      T=START
      TNEXT=START+1.
      CALL DIFFUN (NS2,TNEXT,C,RT)
      CALL SAVLIN (T,C,NS2)
      NFRST=2
      IF (T-START) 60,60,50
   45 TNEXT=AMIN1(TPRNT,STOPP)
      IF (T.EQ.START) GO TO 55
   50 IF (NQ.LT.0.AND.IABS(NQ).NE.0) IN=3
   55 CALL DRIVES (NS2,T,H,C,TNEXT,ERR,21,IN,IA,JA)
      T=TNEXT
      IF (T.GE.STOPP) TPRNT=STOPP
   60 IF (T.EQ.START) TIMNW=START
      IF (T.NE.START) TIMNW=TPRNT
      IF (T.EQ.START) GO TO 65
      IF (NQ.LT.0.AND.IABS(NQ).NE.0) TIMNW=T
      NHS=NHS+1
      IF (NHS.GE.MS.OR.T.GE.TPRNT) GO TO 65
      GO TO 45
   65 NHS=0
      CALL DIFFUN (NS2,TIMNW,C,RT)
```

```
      IF (NOPT.LE.0) NTP=NTP+(N/10)+4
      IF (NOPT.GT.0) NTP=NTP+(N/10)*3+(NR-1)/10+12
      IF (NTP.GT.MT.OR.T.EQ.START) WRITE (IOUT,120)
      IF (T.EQ.START) GO TO 70
      IF (NOPT.LE.0.AND.NTP.LE.MT) GO TO 75
   70 CONTINUE
      IF (NTP.GT.MT) NTP=0
      IF (NN.GE.11) WRITE (IOUT,115) (SPECIS(I),I=1,NN)
      IF (NN.LE.10) WRITE (IOUT,125) (SPECIS(I),I=1,NN)
   75 CONTINUE
      IF (NS.GE.11) WRITE (IOUT,130) TIMNW,(C(I),I=1,10),H,(C(I),I=11,NS
     12),TEMP,SG
      IF (NS.LE.10) WRITE (IOUT,130) TIMNW,(C(I),I=1,NS2),TEMP,SG,H
      IF (NOPT.EQ.0) WRITE (IOUT,135)
      IF (NOPT.EQ.0) GO TO 95
      RT(NS)=0.
      RT(N)=0.
      DO 80 I=1,NS2
   80 RT(NS)=RT(NS)+RT(I)
      WRITE (IOUT,105) (RT(I),I=1,NS)
      DO 90 I=1,NR
      J=KR(I,1)
      IF (J.EQ.0) RT(I)=0.
      IF (J.EQ.0) GO TO 90
      JT=ITYPE(I)
      XT=1.
      DO 85 L=1,JT
      J=KR(I,L)
      XJ=1.
      IF (J.GT.0.AND.J.LE.NS2) XJ=C(J)**ISC(I,L)
      IF (ISC(I,L).EQ.-1) XJ=C(J)**SC(I,L)
      IF (J.EQ.NS) XJ=SG
      XT=XT*XJ
   85 CONTINUE
      RT(I)=XT*R(I)
   90 CONTINUE
      WRITE (IOUT,110) (RT(I),I=1,NR)
   95 IF (TIMNW.EQ.START) GO TO 55
      IF (T.GE.STOPP) RETURN
      IF (IN.EQ.3.AND.T.LT.TPRNT) GO TO 45
      TPRNT=TPRNT*TFACT+TSTEP
      GO TO 45
C
C
  105 FORMAT (/,10H NET RATES,2X,1P10E12.3,/,(12X,1P10E12.3))
  110 FORMAT (//,2X,22HTHE REACTION RATES ARE,/,(1H ,1P10E13.2))
  115 FORMAT (/,4X,5HTIME ,4X,10(4X,A4,4X),/,2X,8HINTERVAL,3X,10(4X,A4,4
     1X),/,(13X,10(4X,A4,4X)))
  120 FORMAT (1H1)
  125 FORMAT (/,4X,5HTIME ,4X,10(4X,A4,4X),/)
```

```
130 FORMAT (/,1P11E12.3/,11E12.3/,(12X,10E12.3))
135 FORMAT (1H )
    END
```

```
      SUBROUTINE RATES (C,N)
C
C***********************************************************************
C
C     THIS SUBROUTINE SETS THE INITIAL CONCENTRATIONS AND CALCULATES THE
C     RATE CONSTANTS
C
C***********************************************************************
C
      INTEGER SPECIS,REACT
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT
      COMMON /NAMES/ SPECIS(91),REACT(91),NS
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER
      DIMENSION C(91)
      FCT=1./298.-1./TEMP
      SIGG=0.
      DO 5 I=1,91
    5 SIG(I)=0.
      DO 15 I=1,N
      DO 10 J=1,NS
      IF (SPECIS(J).EQ.REACT(I)) SIG(J)=C(I)
      IF (SPECIS(J).EQ.REACT(I)) GO TO 15
   10 CONTINUE
      SIGG=SIGG+C(I)
   15 CONTINUE
      N=NS
      M=N-1
      C(N)=0.
      DO 20 I=1,M
      C(N)=C(N)+SIG(I)
   20 C(I)=SIG(I)
      BK=0.
C
C     IF SIG(N) DOES NOT EQUAL ZERO, IT IMPLIES THAT THAT THE CONCENTRAT
C     SPECIES N HAS BEEN READ. OTHERWISE M IS THE SUM OF THE INITIAL
C     CONCENTRATIONS.
C
      C(N)=C(N)+SIGG
      IF (SIG(N).NE.0.) BK=SIG(N)-C(N)
      IF (SIG(N).NE.0.) C(N)=SIG(N)
      NP=0
      DO 25 I=1,NR
      IF (KR(I,1).EQ.0) GO TO 25
C
C     CALCULATE THE RATE CONSTANTS
C
      IF (ABS(S(I)).EQ.0.) R(I)=A(I)
      IF (ABS(S(I)).NE.0.) R(I)=A(I)*EXP(S(I)*FCT)
```

```
25 CONTINUE
   IF (NS.LE.9) SPECIS(NS+1)=JINTER
   RETURN
   END
```

```
      SUBROUTINE DIFFUN (N,T,X,XT)
C
C***********************************************************************
C
C     THIS SUBROUTINE CALCULATES THE DERIVATIVE VECTOR OF THE ODE!S
C
C***********************************************************************
C
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT
      COMMON /NAMES/ SPECIS(91),REACT(91),NS
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST,
     1IPH(30),QM(100),PM(100),PSTOP
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),R1,IN10
      DIMENSION XT(N), X(N)
      INTEGER PHI,TMI
      INTEGER SPECIS
      P=BK
      DO 5 I=1,N
      XT(I)=-DILUT*X(I)
    5 P=P+X(I)
      SG=P
      IF (NFRST.EQ.1) FCT=((3355.7046E-6)*TEMP-1.)/TEMP
      IF (NFRST.EQ.1) GO TO 10
      IF (T.EQ.TOLD) GO TO 30
      IF (T.LE.1.) GO TO 30
   10 IF (NPHOT.LE.0) GO TO 30
      IF (NFRST.NE.1) GO TO 15
      PINT=FLOAT(PHI)
      PINV=1./PINT
   15 CONTINUE
      IF (T.GT.PSTOP) GO TO 20
      IZ=IFIX(T*PINV)+1
      Z=T*PINV-FLOAT(IZ-1)
      IF (T.LE.PINT) R1=PM(1)+(0.5*PM(3)*(Z-1.)+0.5*PM(1)*(Z-3.)-PM(2)*(
     1Z-2.))*Z
      IF (T.LE.PINT) GO TO 20
      R1=PM(IZ)+0.25*Z*(5.*PM(IZ+1)-3.0*PM(IZ)-PM(IZ-1)-PM(IZ+2)+(PM(IZ-
     11)-PM(IZ)-PM(IZ+1)+PM(IZ+2))*Z)
   20 IF (R1.LT.0.) R1=0.
      DO 25 IK=1,IL
      IR=IPH(IK)
      R(IR)=R1*A(IR)
   25 IF (R(IR).LT.0.) R(IR)=0.
   30 TNOW=TEMP
      IF (NFRST.EQ.1) GO TO 35
      IF (T.EQ.TOLD) GO TO 50
      IF (T.LE.1.) GO TO 50
   35 CONTINUE
```

```
      IF (T.GT.TEMEND) GO TO 50
      IF (NFRST.NE.1) GO TO 40
      TINT=FLOAT(TMI)
      TINV=1./TINT
   40 CONTINUE
      IZ=IFIX(T*TINV)+1
      Z=T*TINV-FLOAT(IZ-1)
      IF (T.LE.TINT) TNOW=QM(1)+(0.5*QM(3)*(Z-1.)+0.5*QM(1)*(Z-3.)-QM(2)
     1*(Z-2.))*Z
      IF (T.LE.TINT) GO TO 45
      TNOW=QM(IZ)+0.25*Z*((5.*QM(IZ+1)-3.0*QM(IZ)-QM(IZ-1)-QM(IZ+2))+(QM
     1(IZ-1)-QM(IZ)-QM(IZ+1)+QM(IZ+2))*Z)
   45 CONTINUE
      IF (TNOW.NE.TEMP.AND.TNOW.GT.0.) FCT=((3355.7046E-6)*TNOW-1.)/TNOW
   50 DO 70 IR=1,NR
      I=KR(IR,1)
      IF (I.EQ.0.OR.R(IR).EQ.0.) GO TO 70
C
C     CHECK FOR A ZEROTH ORDER REACTION
C
      RT=1.
      JT=ITYPE(IR)
      DO 55 L=1,JT
      I=KR(IR,L)
      IF (I.EQ.99.OR.I.EQ.0) GO TO 55
      IF (I.NE.NS) RT=RT*X(I)
      IF (I.EQ.NS) RT=RT*P
   55 CONTINUE
      IF (ABS(S(IR)).NE.0..AND.T.GT.1.) R(IR)=A(IR)*EXP(S(IR)*FCT)
      RT=RT*R(IR)
      DO 60 L=1,JT
      I=KR(IR,L)
      IF (I.EQ.0.OR.I.GT.N) GO TO 60
      XT(I)=XT(I)-RT
   60 CONTINUE
      DO 65 K=4,7
      I=KR(IR,K)
      IF (I.EQ.0) GO TO 70
C
C     I WILL BE NEGATIVE IF CLEAN HAS BEEN CALLED
C
      IF (I.LT.0) GO TO 65
      XT(I)=XT(I)+SC(IR,K)*RT
   65 CONTINUE
   70 CONTINUE
      TEMP=TNOW
      TOLD=T
      RETURN
      END
```

```
      SUBROUTINE MATRX (C,KR)
C
C***********************************************************************
C
C     MATRX CREATES A NR X 7 MATRIX OF THE REACTION SCHEME WHERE EACH
C     ROW REPRESENTS A  REACTION.  THE FIRST THREE COLUMNS ARE REACTANTS
C     AND THE LAST FOUR ARE THE PRODUCTS.  THE ELEMENTS CORRESPOND
C     TO THE INDIVIDUAL SPECIES AND WILL BE USED AS SUBSCRIPTS.
C
C***********************************************************************
C
      INTEGER SPECIS,REACT
      COMMON /DATA/ NR,IR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT
      COMMON /NAMES/ SPECIS(91),REACT(91),NS
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP
      DIMENSION C(91), KR(200,7)
      NOLD=NS+1
      DO 90 I=1,NR
C
C     SKIP REACTIONS ALREADY PROCESSED
C
      IF (IR(I,2).EQ.NOLD.OR.IR(I,3).EQ.NOLD) IR(I,3)=99
      IF (IR(I,2).EQ.NOLD) IR(I,2)=0
      IF (IR(I,1).EQ.NOLD) IR(I,1)=99
      IF (IR(I,1).EQ.NOLD) IR(I,3)=99
      IF (IABS(IR(I,1)).NE.100) GO TO 90
C
C     IF LESS THAN THREE REACTANTS, FILL FIRST SLOTS.
C
      IF (KR(I,1).NE.IBLANK) GO TO 5
      IF (KR(I,3).NE.IBLANK) KR(I,1)=KR(I,3)
      IF (KR(I,3).NE.IBLANK) SC(I,1)=SC(I,3)
      SC(I,3)=1.
      KR(I,3)=IBLANK
      IF (KR(I,1).NE.IBLANK) GO TO 5
      KR(I,1)=KR(I,2)
      KR(I,2)=IBLANK
      SC(I,1)=SC(I,2)
      SC(I,2)=1.
    5 IF (KR(I,2).NE.IBLANK) GO TO 10
      IF (KR(I,3).NE.IBLANK) SC(I,2)=SC(I,3)
      SC(I,3)=1.
      IF (KR(I,3).NE.IBLANK) KR(I,2)=KR(I,3)
      KR(I,3)=IBLANK
   10 DO 15 K=4,7
C
C     GET RID OF M AS A PRODUCT
```

```
C
      IF (KR(I,K).EQ.MBLANK) KR(I,K)=IBLANK
   15 CONTINUE
C
C     IF LESS THAN FOUR PRODUCTS, FILL FIRST SLOTS.
C
      IF (KR(I,4).NE.IBLANK) GO TO 30
      DO 20 K=1,3
      INDEX=8-K
      IF (KR(I,INDEX).NE.IBLANK) GO TO 25
   20 CONTINUE
      INDEX=5
   25 KR(I,4)=KR(I,INDEX)
      KR(I,INDEX)=IBLANK
      SC(I,4)=SC(I,INDEX)
      SC(I,INDEX)=1.
      IF (KR(I,1).NE.IBLANK.OR.KR(I,4).NE.IBLANK) GO TO 30
      IR(I,1)=0
      GO TO 90
   30 CONTINUE
      IF (KR(I,5).NE.IBLANK) GO TO 35
      IF (KR(I,7).NE.IBLANK) KR(I,5)=KR(I,7)
      IF (KR(I,7).NE.IBLANK) SC(I,5)=SC(I,7)
      SC(I,7)=1.
      KR(I,7)=IBLANK
      IF (KR(I,5).NE.IBLANK) GO TO 35
      KR(I,5)=KR(I,6)
      KR(I,6)=IBLANK
      SC(I,5)=SC(I,6)
      SC(I,6)=1.
   35 K=KR(I,6)
      IF (K.NE.IBLANK) GO TO 40
      KR(I,6)=KR(I,7)
      KR(I,7)=K
      SC(I,6)=SC(I,7)
      SC(I,7)=1.
   40 DO 85 J=1,7
      K=KR(I,J)
C
C     PROCESS REACTANTS HERE
C
      IF (J.GT.3) GO TO 65
C
C     ALL M DEPENDENT REACTIONS ARE TO HAVE A 99 IN THE THIRD SLOT
C
      IF (K.NE.MBLANK) GO TO 60
      GO TO (45,50,55),J
   45 KR(I,1)=KR(I,2)
      SC(I,1)=SC(I,2)
   50 KR(I,2)=KR(I,3)
```

```
      SC(I,2)=SC(I,3)
      SC(I,3)=1.
      KR(I,3)=MBLANK
   55 IR(I,3)=99
   60 K=KR(I,J)
C
C     ZERO ORDER REACTIONS HAVE 99 IN FIRST SLOT
C
      IF (KR(I,1).EQ.IBLANK) IR(I,1)=99
      IF (KR(I,1).EQ.IBLANK) K=99
C
C     ALL BLANKS ARE SET EQUAL TO ZERO
C
      IF (J.EQ.3.AND.K.EQ.MBLANK) K=99
   65 IF (K.EQ.MBLANK.OR.K.EQ.IBLANK) IR(I,J)=0
      IF (K.EQ.IBLANK.OR.K.EQ.99) GO TO 85
      IF (NS.NE.0) GO TO 70
      NS=1
      GO TO 80
   70 DO 75 L=1,NS
      IF (K.NE.SPECIS(L)) GO TO 75
C
C     SLOT SET TO SPECIES NUMBER
C
      IR(I,J)=L
      GO TO 85
   75 CONTINUE
C
C     IF NO SPECIES ARE FOUND, ADD ONE TO THE LIST
C
      IF (SPECIS(NS).NE.ITEMP) NS=NS+1
   80 SPECIS(NS)=K
      C(NS+2)=C(NS+1)
      C(NS+1)=C(NS)
      C(NS)=0.
      IR(I,J)=NS
   85 CONTINUE
   90 CONTINUE
      IF (SPECIS(NS).NE.ITEMP) NS=NS+1
      SPECIS(NS)=ITEMP
      SPECIS(NS+1)=MBLANK
      NS=NS+1
      DO 95 IK=1,NR
      DO 95 MT=1,3
      J=IFIX(SC(IK,MT)+UROUND)
      ISC(IK,MT)=J
   95 IF (SC(IK,MT)-FLOAT(J).GT.4.*UROUND) ISC(IK,MT)=-1
      DO 100 I=1,NR
      IF (IR(I,1).EQ.0) GO TO 100
      ITYPE(I)=2
```

```
C
C     CHECK FOR 99 CODE AND SUBSTITUTE M WHICH IS THE LAST SPECIES
C
      IF (IR(I,1).EQ.99.AND.IR(I,3).EQ.99) IR(I,1)=NS
      IF (IR(I,1).EQ.NS.AND.IR(I,3).EQ.99) IR(I,3)=0
      IF (IR(I,2).EQ.0.AND.IR(I,3).EQ.99) IR(I,2)=NS
      IF (IR(I,2).EQ.NS.AND.IR(I,3).EQ.99) IR(I,3)=0
      IF (IR(I,2).EQ.0) ITYPE(I)=1
      IF (IR(I,3).NE.0) ITYPE(I)=3
      IF (IR(I,3).EQ.99) IR(I,3)=NS
  100 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE PLOT (NTIT,NPNT,NTOT,NAME,SAVTIM,SAVCON,IDT,KCP,JGRID)
C SUBROUTINE ****** P L O T ******
C
C THIS SUBROUTINE READS THE PLOT CARDS AND PLOTS THE RESULTS AS PART
C OF THE PRINTED OUTPUT -- IT DOES NOT DRIVE A PLOTTER.
C
C SYMBOL DESCRIPTIONS --
C
C CGRID     THE LENGTH OF THE VERTICAL AXIS, PPM
C CHIGH     HIGHEST CONCENTRATION VALUE, PPM
C CLOW      LOWEST CONCENTRATION VALUE, PPM
C CSPAN     CONCENTRATION NORMALIZATION FACTOR
C DATA      CONCENTRATION DATA POINTS, PPM, UP TO 80
C IDT       IF NOT ZERO THEN PRINT RAW DATA USED FOR PLOTS
C J         DO-LOOP INDICES OR LOCAL POINTERS
C JBLANK    A HOLLERITH WORD OF FOUR BLANK CHARACTERS
C JCONC     CONCENTRATION LABELS
C JGRID     THE PLOTTING GRID
C JN        HOLLERITH SYMBOL FOR NO DATA POINTS
C JPLUS     THE CHARACTER >+>
C JSTAR     THE CHARACTER >*>
C JSYMB     SYMBOL TO BE USED FOR PLOTTING SAVED POINTS
C JVERT     VERTICAL LEGEND
C JX        THE CHARACTER >X>
C K         DO-LOOP INDICES OR LOCAL POINTERS
C KCP       IF NOT EQUAL TO ZERO SAVE DATA FOR OFFLINE PLOTTING
C KCON      CONCENTRATION COORDINATE ON GRID
C KTIM      TIME COORDINATE ON GRID
C L         DO-LOOP INDICES OR LOCAL POINTERS
C M         DO-LOOP INDICES OR LOCAL POINTERS
C MAXCON    LIMIT ON NUMBER OF VERTICAL POINTS
C MAXPNT    MAXIMUM NUMBER OF SAVED TIME AND CONCENTRATION POINTS
C MAXTIM    LIMIT ON NUMBER OF HORIZONTAL POINTS
C N         DO-LOOP INDICES OR LOCAL POINTERS
C NAME      SPECIES NAMES, ONE PER SPECIES
C NDAT      NUMBER OF CONCENTRATION DATA POINTS
C NIN       THE FORTRAN INPUT UNIT (NORMALLY 5)
C NOUT      THE FORTRAN OUTPUT UNIT NUMBER (NORMALLY 6)
C NPLT      THE NUMBER OF SPECIES TO BE PLOTTED
C NPNT      NUMBER OF SAVED TIMES AND CONCENTRATIONS
C NTEST     SPECIES NAME FOR TESTING
C NTIT      USER-INPUT TITLE FOR PRINTOUT, 3 FOUR-CHARACTER WORDS
C NTOT      TOTAL NUMBER OF SPECIES
C NX        FLAG FOR CORRECT SPECIES TEST
C SAVCON    SPECIES CONCENTRATIONS, PPM, ONE PER SPECIES AT 80 TIMES
C SAVTIM    TIMES THAT CONCENTRATIONS ARE SAVED, MIN, UP TO 80 VALUES
C TGRID     THE LENGTH OF THE HORIZONTAL AXIS, MIN
C THIGH     HIGHEST TIME VALUE, MIN
C TIME      TIMES AT WHICH CONCENTRATIONS ARE INPUT, MIN, UP TO 80
C TLOW      LOWEST TIME VALUE, MIN
```

```
C TPRINT   TIMES FOR PRINTOUT ON HORIZONTAL AXIS, MIN
C TSPAN    TIME NORMALIZATION FACTOR
C
C BEGINNING OF PROGRAM.
C
C ENTRY POINT
C
C SET DIMENSIONS OF INCOMING ARRAYS
C
      DIMENSION SAVCON(90,80), SAVTIM(80), NTIT(3), NAME(91)
C
C SET DIMENSIONS OF LOCAL ARRAYS
C
      DIMENSION JCONC(5), TIME(80), DATA(80), JN(3)
      DIMENSION JGRID(89,40), TPRINT(9), KVERT(52)
C
C DEFINE THE VERTICAL LABEL AND ESTABLISH ALPHAMERIC DATA
C
      COMMON /APLOT/ JVERT(52,2),JBLANK,JSTAR,JPLUS,JBAR
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10
C
C DEFINE MISCELLANEOUS DATA VALUES
C
      COMMON /INOUT/ NIN,NOUT,ITAPE
      DATA MAXTIM/89/,MAXCON/40/,MAXPNT/80/
      DATA TGRID/88./,CGRID/40./,JX/1HX/,JNO/1H /
      DATA KVERT/11*4H    ,4H P  ,4H H  ,4H O  ,4H T  ,4H O  ,4H L  ,4H
     1Y  ,4H S  ,4H I  ,4H S  ,4H    ,4H C  ,4H O  ,4H N  ,4H S  ,4H T
     2,4H A  ,4H N  ,4H T  ,22*4H    /
C
C DEFINE VERTICAL AXIS VIA ASSIGNMENT STATEMENTS
C
      IF (IDT*IDT.EQ.0) GO TO 10
      WRITE (NOUT,150)
      WRITE (NOUT,145) (NAME(I),I=1,NTOT)
      DO 5 J=1,NPNT
    5 WRITE (NOUT,155) SAVTIM(J),(SAVCON(I,J),I=1,NTOT)
   10 DO 15 J=1,40
      JGRID(1,J)=JBAR
   15 CONTINUE
      JGRID(1,1)=JPLUS
      JGRID(1,11)=JPLUS
      JGRID(1,21)=JPLUS
      JGRID(1,31)=JPLUS
      JN(1)=JSTAR
      JN(2)=JPLUS
      JN(3)=JX
      TSPAN=-10.
C
C READ PLOT CONTROL CARD
```

```
C
   20 READ (NIN,130) NPLT,JCONC,CLOW,CHIGH,TLOW,THIGH
C
C TEST FOR END PLOTTING
C
      IF (NPLT.EQ.0) GO TO 105
      WRITE (NOUT,160) NTIT
C
C SET NORMALIZATION FACTORS AND VERTICAL LABELS
C
      CSPAN=CGRID/(CHIGH-CLOW)
      TSPAN=TGRID/(THIGH-TLOW)
      JVERT(1,2)=JCONC(5)
      JVERT(11,2)=JCONC(4)
      JVERT(21,2)=JCONC(3)
      JVERT(31,2)=JCONC(2)
C
C SET HORIZONTAL TIME LABELS
C
      DO 25 J=1,9
      TPRINT(J)=FLOAT(J-1)/8.*(THIGH-TLOW)+TLOW
   25 CONTINUE
C
C CLEAR GRID
C
      DO 35 K=1,MAXCON
      DO 30 J=2,MAXTIM
      JGRID(J,K)=JBLANK
   30 CONTINUE
   35 CONTINUE
      NX=0
      DO 95 LK=1,NPLT
      READ (NIN,135) NTEST,NDAT,JSYMB
C
C TEST NUMBER OF DATA POINTS AND READ DATA
C
      IF (NDAT.LE.0) GO TO 45
      IF (NDAT.LE.MAXPNT) GO TO 40
      WRITE (NOUT,185) MAXPNT
      GO TO 125
C
C READ DATA POINTS
C
   40 READ (NIN,140) (TIME(J),DATA(J),J=1,NDAT)
C
C TEST FOR CORRECT SPECIES NAME
C
   45 DO 50 L=1,NTOT
      IF (NTEST.EQ.NAME(L)) GO TO 55
   50 CONTINUE
```

```
      WRITE (NOUT,190) NTEST
      NX=NX+1
      IF (NPLT.EQ.1.OR.NX.EQ.3) GO TO 20
      IF (NPLT.EQ.2.AND.NX.EQ.2) GO TO 20
      GO TO 95
C
C IF THERE ARE CALCULATED POINTS, GET THEIR COORDINATES
C
   55 IF (NPNT.LE.0) GO TO 65
      DO 60 J=1,NPNT
      KTIM=IFIX((SAVTIM(J)-TLOW)*TSPAN+1.5)
      Y=(SAVCON(L,J)-CLOW)*CSPAN-0.5
      IF (Y.LT.0.0) GO TO 60
      KCON=IFIX(Y)
      KCON=MAXCON-KCON
C
C CHECK FOR BEING WITHIN GRID, THEN PLACE ON GRID
C
      IF (KTIM.LT.2) GO TO 60
      IF (KCON.LT.1) GO TO 60
      IF (KTIM.GT.MAXTIM) GO TO 60
      IF (KCON.GT.MAXCON) GO TO 60
      JGRID(KTIM,KCON)=JSYMB
   60 CONTINUE
C
C IF THERE ARE DATA POINTS, GET THEIR COORDINATES
C
   65 IF (NDAT.LE.0) GO TO 75
      DO 70 J=1,NDAT
      KTIM=IFIX((TIME(J)-TLOW)*TSPAN+1.5)
      Y=(DATA(J)-CLOW)*CSPAN-0.5
      IF (Y.LT.0.0) GO TO 70
      KCON=IFIX(Y)
      KCON=MAXCON-KCON
C
C CHECK FOR BEING WITHIN GRID, THEN PLACE ON GRID
C
      IF (KTIM.LT.2) GO TO 70
      IF (KCON.LT.1) GO TO 70
      IF (KTIM.GT.MAXTIM) GO TO 70
      IF (KCON.GT.MAXCON) GO TO 70
      IF (LK.EQ.1) JGRID(KTIM,KCON)=JSTAR
      IF (LK.EQ.2) JGRID(KTIM,KCON)=JPLUS
      IF (LK.EQ.3) JGRID(KTIM,KCON)=JX
   70 CONTINUE
   75 IF (NDAT.GT.0) GO TO 85
      WRITE (NOUT,195) NTEST,JNO,JSYMB
      GO TO 90
   85 WRITE (NOUT,195) NTEST,JN(LK),JSYMB
C
```

```
C SAVE DATA FOR OFFLINE PLOTS IF DESIRED
C
   90 IF (KCP*KCP.EQ.0) GO TO 95
      WRITE (ITAPE) NTIT,NAME(L),CLOW,CHIGH,TLOW,THIGH,NDAT,NPNT,(TIME(J
     1),J=1,NDAT),(DATA(J),J=1,NDAT),(SAVTIM(J),J=1,NPNT),(SAVCON(L,J),J
     2=1,NPNT)
   95 CONTINUE
      DO 100 K=1,MAXCON
      WRITE (NOUT,165) JVERT(K,1),JVERT(K,2),(JGRID(J,K),J=1,MAXTIM)
  100 CONTINUE
C
C PRINT THE HORIZONTAL AXIS AND LABELS
C
      WRITE (NOUT,170) JCONC(1)
      IF (THIGH.GT.80.) WRITE (NOUT,175) TPRINT
      IF (THIGH.LE.80.) WRITE (NOUT,180) TPRINT
      GO TO 20
C
C END OF SUBROUTINE -- RETURN TO CALLER
C
  105 IF (IPP.LE.0) RETURN
      IF (IN10.LE.0) RETURN
      IF (TSPAN.LE.0.) RETURN
      JVERT(1,2)=4H0.80
      JVERT(11,2)=4H0.60
      JVERT(21,2)=4H0.40
      JVERT(31,2)=4H0.20
      JCONC(1)=4H0.00
      CSPAN=CGRID/0.8
      WRITE (NOUT,200) NTIT
      DO 110 I=1,MAXCON
      DO 110 J=2,MAXTIM
  110 JGRID(J,I)=JBLANK
      DO 115 I=1,NPNT
      KTIM=IFIX((RTIM(I)-TLOW)*TSPAN+1.5)
      Y=(RDAT(I)-CLOW)*CSPAN-0.5
      IF (Y.LT.0.0) GO TO 115
      KCON=IFIX(Y)
      KCON=MAXCON-KCON
      IF (KCON.LT.1) GO TO 115
      IF (KTIM.LT.2) GO TO 115
      IF (KTIM.GT.MAXTIM) GO TO 115
      IF (KCON.GT.MAXCON) GO TO 115
      JGRID(KTIM,KCON)=JSTAR
  115 CONTINUE
      DO 120 K=1,MAXCON
      WRITE (NOUT,165) KVERT(K),JVERT(K,2),(JGRID(J,K),J=1,MAXTIM)
  120 CONTINUE
      WRITE (NOUT,170) JCONC(1)
      IF (TPRINT(9).GT.80.) WRITE (NOUT,175) TPRINT
```

```
      IF (TPRINT(9).LE.80.) WRITE (NOUT,180) TPRINT
      RETURN
  125 CONTINUE
      STOP
C
C LIST OF FORMAT STATEMENTS
C
C
C
  130 FORMAT (5X,I2,8X,5(A4,1X),4F10.0)
  135 FORMAT (A4,1X,I2,1X,A1)
  140 FORMAT (8F10.0)
  145 FORMAT (/,4X,5HTIME ,4X,10(4X,A4,4X),/,(13X,10(4X,A4,4X)))
  150 FORMAT (1H1)
  155 FORMAT (1P11E12.4,/,(12X,10E12.4))
  160 FORMAT (1H1,//////////,62X,3A4,/,32X,7HSPECIES,2X,5HEXPT.,2X,4HSIM
     1.)
  165 FORMAT (16X,2A4,89A1)
  170 FORMAT (20X,A4,1H+,8(11H----------+))
  175 FORMAT (I25,2X,8F11.0,/,62X,14HTIME (MINUTES),/)
  180 FORMAT (I25,2X,8F11.3,/,62X,14HTIME (MINUTES),/)
  185 FORMAT (33H PROGRAM CANNOT HANDLE MORE THAN ,I4,28H PLOT POINTS --
     1 JOB ABORTED.)
  190 FORMAT (33X,13HSPECIES NAME ,A4,26H NOT FOUND IN SPECIES LIST)
  195 FORMAT (33X,A4,6X,A1,5X,A1)
  200 FORMAT (1H1,//////////,62X,3A4,//)
      END
```

```
      SUBROUTINE VALU (VAL,N,NF,NL)
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST,
     1IPH(30),QM(100),PM(100),PSTOP
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART
      DIMENSION AC(5), AD(5), BC(5)
      INTEGER AC,AD,BC,AST
      DATA IBLK/1H /,IPER/1H./,IZRO/1H0/
      AVAL=ALOG10(VAL)
      IF (AVAL.EQ.0.) RETURN
      DO 5 I=1,5
      AC(I)=IBLK
      AD(I)=IZRO
    5 BC(I)=IZRO
      IAD=IFIX(AVAL+UROUND)
      IF (IAD) 30,10,10
   10 IREM=3-IAD
      IAD=IAD+1
      JREM=IFIX(VAL+UROUND)
      REM=VAL-FLOAT(JREM)
      IF (REM.GT.UROUND.AND.IREM.GT.0) GO TO 15
      CALL CONVT (JREM,AC,5)
      GO TO 50
   15 CALL CONVT (JREM,AD,IAD)
      JREM=IFIX(REM*(10.**IREM)+0.1)
      CALL CONVT (JREM,BC,IREM)
      DO 20 J=1,IAD
   20 AC(J)=AD(J)
      AC(IAD+1)=IPER
      DO 25 K=1,IREM
   25 AC(K+IAD+1)=BC(K)
      GO TO 40
   30 IAD=IABS(IFIX(AVAL-0.1))-1
      IVAL=IFIX(VAL*10000.+0.1)
      CALL CONVT (IVAL,AC,5)
      AC(1)=IPER
      DO 35 I=1,IAD
   35 AC(I+1)=IZRO
   40 IF (AC(5).NE.IZRO) GO TO 50
      DO 45 K=1,4
      L=6-K
   45 AC(L)=AC(L-1)
      AC(1)=IBLK
      GO TO 40
   50 DO 55 I=NF,NL
      K=I-NF+1
   55 AST(I)=AC(K)
      RETURN
      END
```

```
      SUBROUTINE CONVT (NUM,L,N)
C
C  SUBROUTINE CONVT CONVERTS INTEGERS TO ALPHANUMERICS
C     FOR PRINTING
C
C  ASSUMES VALUE OF INTEGER IS POSITIVE
C
      DIMENSION L(5), JDIGIT(10)
C
      DATA JDIGIT/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/
      DATA JBLANK/1H /
C
      NI=NUM
      DO 5 I=1,N
      L(I)=JBLANK
    5 CONTINUE
C
      DO 10 K=1,N
      I=N-K+1
      NEXT=NI/10
      NDX=(NI-NEXT*10)+1
      L(I)=JDIGIT(NDX)
      IF (NEXT.LE.0) GO TO 15
      NI=NEXT
   10 CONTINUE
C
   15 RETURN
      END
```

```
      SUBROUTINE SAVLIN (T,C,N)
      COMMON /FRPLOT/ NIT(3),SAVCON(90,80),SAVTIM(80),JGRID(89,40),NT
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10
      DIMENSION C(91)
      DATA NFRST/1/
      IF (NFRST.EQ.1) GO TO 5
      IF (T.EQ.TOLD) RETURN
    5 IF (NT.LT.0) RETURN
      NFRST=2
      TOLD=T
      IF (NT.GT.80) RETURN
      IF (T.LT.SAVTIM(NT)) RETURN
      SAVTIM(NT)=T
      RTIM(NT)=T
      DO 10 I=1,N
   10 SAVCON(I,NT)=C(I)
      RDAT(NT)=RR1
      NT=NT+1
      RETURN
      END
```

```
      SUBROUTINE SPLNA (N,X,Y,J,D,C,W)
      DIMENSION X(10), Y(10), D(2), C(30), W(30)
C     ------------------------------------------------------------------
C             OVER THE INTERVAL X(I) TO X(I+1), THE INTERPOLATING
C             POLYNOMIAL
C                  Y=Y(I)+A(I)*Z+B(I)*Z**2+E(I)*Z**3
C             WHERE Z=(X-X(I))/(X(I+1)-X(I))
C             IS USED. THE COEFFICIENTS A(I),B(I) AND E(I) ARE COMPUTED
C             BY SPLNA AND STORED IN LOCATIONS C(3*I-2),C(3*I-1) AND
C             C(3*I) RESPECTIVELY.
C             WHILE WORKING IN THE ITH INTERVAL,THE VARIABLE Q WILL
C             REPRESENT Q=X(I+1) - X(I), AND Y(I) WILL REPRESENT
C             Y(I+1)-Y(I)
C     ------------------------------------------------------------------
C
      Q=X(2)-X(1)
      YI=Y(2)-Y(1)
      IF (J.EQ.2) GO TO 5
C     ------------------------------------------------------------------
C             IF THE FIRST DERIVATIVE AT THE END POINTS IS GIVEN,
C             A(1) IS KNOWN, AND THE SECOND EQUATION BECOMES
C             MERELY B(1)+E(1)=YI - Q*D(1).
C     ------------------------------------------------------------------
      C(1)=Q*D(1)
      C(2)=1.0
      W(2)=YI-C(1)
      GO TO 10
C     ------------------------------------------------------------------
C             IF THE SECOND DERIVATIVE AT THE END POINTS IS GIVEN
C             B(1) IS KNOWN, THE SECOND EQUATION BECOMES
C             A(1)+E(1)=YI-0.5*Q*Q*D(1). DURING THE SOLUTION OF
C             THE 3N-4 EQUATIONS,A1 WILL BE KEPT IN CELL C(2)
C             INSTEAD OF C(1) TO RETAIN THE TRIDIAGONAL FORM OF THE
C             COEFFICIENT MATRIX.
C     ------------------------------------------------------------------
    5 C(2)=0.0
      W(2)=0.5*Q*Q*D(1)
   10 M=N-2
      IF (M.LE.0) GO TO 20
C     ------------------------------------------------------------------
C             UPPER TRIANGULARIZATION OF THE TRIDIAGONAL SYSTEM OF
C             EQUATIONS FOR THE COEFFICIENT MATRIX FOLLOWS--
C     ------------------------------------------------------------------
      DO 15 I=1,M
      AI=Q
      Q=X(I+2)-X(I+1)
      H=AI/Q
      C(3*I)=-H/(2.0-C(3*I-1))
      W(3*I)=(-YI-W(3*I-1))/(2.0-C(3*I-1))
      C(3*I+1)=-H*H/(H-C(3*I))
```

```
      W(3*I+1)=(YI-W(3*I))/(H-C(3*I))
      YI=Y(I+2)-Y(I+1)
      C(3*I+2)=1.0/(1.0-C(3*I+1))
   15 W(3*I+2)=(YI-W(3*I+1))/(1.0-C(3*I+1))
C     ----------------------------------------------------------------
C             E(N-1) IS DETERMINED DIRECTLY FROM THE LAST EQUATION
C             OBTAINED ABOVE, AND THE FIRST OR SECOND DERIVATIVE
C             VALUE GIVEN AT THE END POINT.
C     ----------------------------------------------------------------
   20 IF (J.EQ.1) GO TO 25
      C(3*N-3)=(Q*Q*D(2)/2.0-W(3*N-4))/(3.0-C(3*N-4))
      GO TO 30
   25 C(3*N-3)=(Q*D(2)-YI-W(3*N-4))/(2.0-C(3*N-4))
   30 M=3*N-6
      IF (M.LE.0) GO TO 40
C     ----------------------------------------------------------------
C             BACK SOLUTION FOR ALL COEFFICENTS EXCEPT
C             A(1) AND B(1) FOLLOWS--
C     ----------------------------------------------------------------
      DO 35 II=1,M
      I=M-II+3
   35 C(I)=W(I)-C(I)*C(I+1)
   40 IF (J.EQ.1) GO TO 45
C     ----------------------------------------------------------------
C             IF THE SECOND DERIVATIVE IS GIVEN AT THE END POINTS,
C             A(1) CAN NOW BE COMPUTED FROM THE KNOWN VALUES OF
C             B(1) AND E(1). THEN A(1) AND B(1) ARE PUT INTO THEIR
C             PROPER PLACES IN THE C ARRAY.
C     ----------------------------------------------------------------
      C(1)=Y(2)-Y(1)-W(2)-C(3)
      C(2)=W(2)
      RETURN
   45 C(2)=W(2)-C(3)
      RETURN
      END
```

```
      SUBROUTINE DRIVES (N,T0,H0,Y0,TOUT,EPS,MF,INDEX,IA,JA)
      DIMENSION IA(1), JA(1), Y0(N)
      DIMENSION Y(91,6)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART
      COMMON /GEAR2/ YMAX(100)/GEAR3/ERROR(100)/GEAR4/W1(90,3)
      COMMON /GEAR5/ IW1(91,9)/GEAR6/W2(2000)/GEAR7/IW2(2000)
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,NZA,NPL,NPU,NZL,NZU,NZRO
      COMMON /INOUT/ INP,LOUT,ITAPE
      DATA NMX/90/,LENW2/2000/,LENIW2/2000/
      NGP=0
      IF (INDEX.EQ.4) GO TO 15
      IF (INDEX.EQ.0) GO TO 30
      IF (INDEX.EQ.2) GO TO 35
      IF (INDEX.EQ.-1) GO TO 40
      IF (INDEX.EQ.3) GO TO 45
      IF (INDEX.NE.1) GO TO 135
      IF (EPS.LE.0.) GO TO 120
      IF (N.LE.0) GO TO 125
      IF ((T0-TOUT)*H0.GE.0.) GO TO 130
      MITER=MF-10*(MF/10)
      IF ((MITER.NE.1).AND.(MITER.NE.2)) GO TO 15
      NP1=N+1
      NZA=IA(NP1)-1
      MAX=LENIW2/2
      IPTI2=MAX+1
      CALL SORDER (N,IA,JA,IW1,IW1(1,5),MAX,IW2,IW2(IPTI2),IER)
      IPTI2=NZA+1
      IF (IPTI2+NZA-1.GT.LENIW2) GO TO 145
      DO 5 I=1,NP1
    5 IW1(I,2)=IA(I)
      DO 10 I=1,NZA
   10 IW2(I)=JA(I)
      CALL NSCORD (N,IW1(1,2),IW2,IW1(1,3),IW2(IPTI2),IW1,IW1(1,5),IW1(1
     1,8))
      MAXPL=(LENIW2-NZA)/2
      IPTI3=IPTI2+MAXPL
      MAXPU=LENIW2-IPTI3+1
      CALL NSSFAC (N,IW1(1,2),IW2,MAXPL,IW1(1,3),IW2(IPTI2),IW1(1,4),MAX
     1PU,IW1(1,5),IW2(IPTI3),IW1(1,6),Y(1,6),IW1(1,9),Y,Y(1,2),Y(1,3),IW
     21(1,7),IW1(1,8),Y(1,4),Y(1,5),IER)
      NPL=IW1(N,4)
      NPU=IW1(N,6)
      NZL=IW1(N+1,3)
      NZU=IW1(N+1,5)
      IPTR2=NZA+1
      IPTR3=IPTR2+MAX0(NZA,NZL)
      IF (IPTR3+MAX0(NZA,NZU)-1.GT.LENW2) GO TO 145
   15 DO 20 I=1,N
      YMAX(I)=ABS(Y0(I))
```

```
      IF (YMAX(I).EQ.0.) YMAX(I)=1.E-10
   20 Y(I,1)=YO(I)
      NC=N
      T=TO
      H=HO
      NZRO=0
      TST=EPS*1.E-10
      DO 25 I=1,N
   25 IF (Y(I,1).GT.TST) NZRO=NZRO+1
      NZRO=MAXO(NZRO,1)
      NOLD=NZRO
      HMIN=ABS(HO)
      HMAX=ABS(TO-TOUT)*10.
      HMAX=AMIN1(HMAX,20.)
      EPSC=EPS
      MFC=MF
      JSTART=0
      NO=N
      NMX1=NMX+1
      EPSJ=SQRT(UROUND)
      NHCUT=0
      GO TO 50
   30 HMAX=ABS(TOUT-TOUTP)*10.
      HMAX=AMIN1(HMAX,20.)
      GO TO 80
   35 HMAX=ABS(TOUT-TOUTP)*10.
      HMAX=AMIN1(HMAX,20.)
      IF ((T-TOUT)*H.GE.0.) GO TO 150
      GO TO 85
   40 IF ((T-TOUT)*H.GE.0.) GO TO 140
      JSTART=-1
      NC=N
      EPSC=EPS
      MFC=MF
   45 CONTINUE
   50 CALL STIFFS (Y,NO,IA,JA,W1,NMX,IW1,NMX1)
      KGO=1-KFLAG
      GO TO (55,95,110,100),KGO
   55 CONTINUE
      D=0.
      NZRO=0
      DO 70 I=1,NC
      IF (Y(I,1).GE.0.) GO TO 65
      NGP=NGP+1
      DO 60 J=1,6
      K=(J-1)*N+I
   60 Y(K,1)=0.
   65 CONTINUE
      IF (Y(I,1).GT.TST) NZRO=NZRO+1
      AYI=ABS(Y(I,1))
```

```
      YMAX(I)=AMAX1(1.E-10,AYI)
   70 D=D+(AYI/YMAX(I))**2
      NZRO=MAX0(NZRO,1)
      IF (NZRO.NE.NOLD) JSTART=-1
      D=D*(UROUND/EPS)**2
      DO 75 II=1,NC
   75 YO(II)=Y(II,1)
      CALL SAVLIN (T,YO,N)
      IF (D.GT.FLOAT(N)) GO TO 115
      IF (INDEX.EQ.3) GO TO 150
      IF (INDEX.EQ.2) GO TO 85
   80 IF ((T-TOUT)*H.LT.0.) GO TO 45
      CALL INTERP (TOUT,Y,NO,YO)
      GO TO 160
   85 IF (T.GE.TOUT) GO TO 90
      IF (((T+H)-TOUT).LE.0.) GO TO 45
      H=(TOUT-T)*(1.+4.*UROUND)
      JSTART=-1
      GO TO 45
   90 JSTART=-1
      H=AMIN1(H,1.)
      GO TO 150
   95 CONTINUE
  100 IF (NHCUT.EQ.10) GO TO 105
      NHCUT=NHCUT+1
      HMIN=.1*HMIN
      H=.1*H
      JSTART=-1
      GO TO 45
  105 WRITE (LOUT,165)
      IF (KGO.EQ.4) WRITE (LOUT,180) T
      STOP
  110 WRITE (LOUT,170) T,H
      STOP
  115 WRITE (LOUT,175) T
      KFLAG=-2
      STOP
  120 WRITE (LOUT,185)
      STOP
  125 WRITE (LOUT,190)
      STOP
  130 WRITE (LOUT,195)
      STOP
  135 WRITE (LOUT,200) INDEX
      STOP
  140 WRITE (LOUT,205) T,TOUT,H
      STOP
  145 WRITE (LOUT,210)
      STOP
  150 TOUT=T
```

```
      DO 155 I=1,N
  155 YO(I)=Y(I,1)
      CALL SAVLIN (TOUT,YO,N)
  160 INDEX=KFLAG
      TOUTP=TOUT
      HO=HUSED
      IF (KFLAG.NE.0) HO=H
      RETURN
C
C
  165 FORMAT (//44H PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT//)
  170 FORMAT (//35H KFLAG = -2 FROM INTEGRATOR AT T = ,E16.8,5H  H =,E16
     1.8/52H  THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED//)
  175 FORMAT (//37H INTEGRATION HALTED BY DRIVER AT T = ,E16.8/56H  EPS
     1TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION/)
  180 FORMAT (//35H KFLAG = -3 FROM INTEGRATOR AT T = ,E16.8/45H  CORREC
     1TOR CONVERGENCE COULD NOT BE ACHIEVED/)
  185 FORMAT (//28H ILLEGAL INPUT.. EPS .LE. 0.//)
  190 FORMAT (//25H ILLEGAL INPUT.. N .LE. 0//)
  195 FORMAT (//36H ILLEGAL INPUT.. (TO-TOUT)*H .GE. 0.//)
  200 FORMAT (//24H ILLEGAL INPUT.. INDEX =,I5//)
  205 FORMAT (//44H INDEX = -1 ON INPUT WITH (T-TOUT)*H .GE. 0./4H T =,E
     116.8,9H   TOUT =,E16.8,6H   H =,E16.8)
  210 FORMAT (//42H INSUFFICIENT WORKING STORAGE IN IW2 OR W2//)
      END
```

```
      SUBROUTINE STIFFS (Y,NO,IA,JA,W1,NMX,IW1,NMX1)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS,UROUND,N,MF,KFLAG,JSTART
      COMMON /GEAR2/ YMAX(100)/GEAR3/ERROR(100)
      COMMON /GEAR6/ W2(2000)/GEAR7/IW2(2000)
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,IDUMMY(5),NZRO
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP
      DIMENSION Y(NO,1), IA(1), JA(1), W1(NMX,1), IW1(NMX1,1)
      DIMENSION EL(13), TQ(4), RT(3)
      DATA EL(2)/1./,OLDLO/1./
      KFLAG=0
      TOLD=T
      IF (JSTART.GT.0) GO TO 50
      IF (JSTART.NE.0) GO TO 10
      CALL DIFFUN (N,T,Y,W1)
      DO 5 I=1,N
    5 Y(I,2)=H*W1(I,1)
      METH=MF/10
      MITER=MF-10*METH
      NQ=1
      L=2
      IDOUB=3
      RMAX=1.E4
      RC=0.
      CRATE=1.
      HOLD=H
      MFOLD=MF
      NSTEP=0
      NSTEPJ=0
      NFE=1
      NJE=0
      IRET=3
      GO TO 15
   10 IF (MF.EQ.MFOLD) GO TO 25
      MEO=METH
      MIO=MITER
      METH=MF/10
      MITER=MF-10*METH
      MFOLD=MF
      IF (MITER.NE.MIO) IWEVAL=MITER
      IF (METH.EQ.MEO) GO TO 25
      IDOUB=L+1
      IRET=1
   15 CALL COSET (METH,NQ,EL,TQ,MAXDER)
      LMAX=MAXDER+1
      RC=RC*EL(1)/OLDLO
      OLDLO=EL(1)
   20 FN=FLOAT(NZRO)
```

```
      EDN=FN*(TQ(1)*EPS)**2
      E=FN*(TQ(2)*EPS)**2
      EUP=FN*(TQ(3)*EPS)**2
      BND=FN*(TQ(4)*EPS)**2
      EPSOLD=EPS
      NOLD=NZRO
      GO TO (30,35,50),IRET
   25 IF (EPS.EQ.EPSOLD.AND.NZRO.EQ.NOLD) GO TO 30
      IRET=1
      GO TO 20
   30 IF (H.EQ.HOLD) GO TO 50
      RH=H/HOLD
      H=HOLD
      IREDO=3
      GO TO 40
   35 RH=AMAX1(RH,HMIN/ABS(H))
   40 RH=AMIN1(RH,HMAX/ABS(H),RMAX)
      R1=1.
      DO 45 J=2,L
      R1=R1*RH
      DO 45 I=1,N
   45 Y(I,J)=Y(I,J)*R1
      H=H*RH
      RC=RC*RH
      IDOUB=L+1
      IF (IREDO.EQ.0) GO TO 290
   50 IF (ABS(RC-1.).GT.0.3) IWEVAL=MITER
      IF (NSTEP.GE.NSTEPJ+20) IWEVAL=MITER
      T=T+H
      DO 55 J1=1,NQ
      DO 55 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 55 I=1,N
   55 Y(I,J)=Y(I,J)+Y(I,J+1)
   60 DO 65 I=1,N
   65 ERROR(I)=0.
      M=0
      CALL DIFFUN (N,T,Y,W1(1,2))
      NFE=NFE+1
      IF (IWEVAL.LE.0) GO TO 140
      IWEVAL=0
      RC=1.
      NJE=NJE+1
      NSTEPJ=NSTEP
      CON=-H*EL(1)
      ISV=M
      LSV=L
      NZ=IA(N+1)-1
      DO 70 I=1,NZ
   70 W2(I)=0.
```

```
      DO 125 IR=1,NR
      IF (KR(IR,1).EQ.0.OR.KR(IR,1).EQ.99) GO TO 125
      MT=ITYPE(IR)
      DO 85 I=1,MT
      IF (KR(IR,I).EQ.N+2) GO TO 85
      JX=I+1-I/3*3
      KX=I+2-I/2*3
      J=KR(IR,JX)
      K=KR(IR,KX)
      XJ=1.
      IF (J.EQ.0) GO TO 75
      XJ=Y(J,1)
      IF (J.EQ.N+2) XJ=SG
   75 XK=1.
      IF (K.EQ.0) GO TO 80
      XK=Y(K,1)
      IF (K.EQ.N+2) XK=SG
   80 RT(I)=R(IR)*XJ*XK
   85 CONTINUE
      DO 120 K=1,MT
      I=KR(IR,K)
      IF (I.EQ.N+2) GO TO 120
      DO 100 L=1,MT
      J=KR(IR,L)
      IF (J.EQ.N+2) GO TO 100
      M=IA(J)-1
   90 M=M+1
      IF (I-JA(M)) 90,95,90
   95 W2(M)=W2(M)-RT(L)
  100 CONTINUE
      DO 115 L=4,7
      J=KR(IR,L)
      M=IA(I)-1
      IF (J) 115,120,105
  105 M=M+1
      IF (J-JA(M)) 105,110,105
  110 W2(M)=W2(M)+RT(K)*SC(IR,L)
  115 CONTINUE
  120 CONTINUE
  125 CONTINUE
      DO 135 J=1,N
      KMIN=IA(J)
      KMAX=IA(J+1)-1
      DO 130 K=KMIN,KMAX
      W2(K)=W2(K)*CON
      IF (JA(K).EQ.J) W2(K)=W2(K)+1.-CON*DILUT
  130 CONTINUE
  135 CONTINUE
      CALL NSCORA (N,IA,JA,W2,IW1(1,2),W2(IPTR3),W2(IPTR2),IW1,IW1(1,7),
     1IW1(1,8))
```

```
      CALL NSNFAC (N,IW1(1,2),IW2,W2,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPT
     1R2),W1(1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1,IW1(1,7),IW1
     2(1,8),IER)
      M=ISV
      L=LSV
      IF (IER.NE.0) GO TO 160
  140 DO 145 I=1,N
      IF (M.LE.0) GO TO 145
      IF (-H*W1(I,2)*10..GT.Y(I,1)) GO TO 155
  145 W1(I,1)=H*W1(I,2)-(Y(I,2)+ERROR(I))
      CALL NSBSLV (N,IW1,IW1,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPTR2),W1(1
     1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1(1,2),W1,W2)
      D=0.
      DO 150 I=1,N
      ERROR(I)=ERROR(I)+W1(I,2)
      D=D+(W1(I,2)/YMAX(I))**2
  150 W1(I,1)=Y(I,1)+EL(1)*ERROR(I)
      IF (M.NE.0) CRATE=AMAX1(.9*CRATE,D/D1)
      IF ((D*AMIN1(1.,2.*CRATE)).LE.BND) GO TO 175
      D1=D
      M=M+1
      IF (M.EQ.3) GO TO 155
      CALL DIFFUN (N,T,W1,W1(1,2))
      GO TO 140
  155 NFE=NFE+2
      IF (IWEVAL.EQ.-1) GO TO 170
  160 T=TOLD
      RMAX=2.
      DO 165 J1=1,NQ
      DO 165 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 165 I=1,N
  165 Y(I,J)=Y(I,J)-Y(I,J+1)
      IF (ABS(H).LE.HMIN*1.00001) GO TO 285
      RH=.25
      IREDO=1
      GO TO 35
  170 IWEVAL=MITER
      GO TO 60
  175 IF (MITER.NE.0) IWEVAL=-1
      NFE=NFE+M
      D=0.
      DO 180 I=1,N
  180 D=D+(ERROR(I)/YMAX(I))**2
      IF (D.GT.E) GO TO 195
      KFLAG=0
      IREDO=0
      NSTEP=NSTEP+1
      HUSED=H
      NQUSED=NQ
```

```
      DO 185 J=1,L
      DO 185 I=1,N
  185 Y(I,J)=Y(I,J)+EL(J)*ERROR(I)
      IF (IDOUB.EQ.1) GO TO 205
      IDOUB=IDOUB-1
      IF (IDOUB.GT.1) GO TO 295
      IF (L.EQ.LMAX) GO TO 295
      DO 190 I=1,N
  190 Y(I,LMAX)=ERROR(I)
      GO TO 295
  195 KFLAG=KFLAG-1
      T=TOLD
      DO 200 J1=1,NQ
      DO 200 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 200 I=1,N
  200 Y(I,J)=Y(I,J)-Y(I,J+1)
      RMAX=2.
      IF (ABS(H).LE.HMIN*1.00001) GO TO 275
      IF (KFLAG.LE.-3) GO TO 265
      IREDO=2
      PR3=1.E+20
      GO TO 215
  205 PR3=1.E+20
      IF (L.EQ.LMAX) GO TO 215
      D1=0.
      DO 210 I=1,N
  210 D1=D1+((ERROR(I)-Y(I,LMAX))/YMAX(I))**2
      ENQ3=.5/FLOAT(L+1)
      PR3=((D1/EUP)**ENQ3)*1.4+1.4E-6
  215 ENQ2=.5/FLOAT(L)
      PR2=((D/E)**ENQ2)*1.2+1.2E-6
      PR1=1.E+20
      IF (NQ.EQ.1) GO TO 225
      D=0.
      DO 220 I=1,N
  220 D=D+(Y(I,L)/YMAX(I))**2
      ENQ1=.5/FLOAT(NQ)
      PR1=((D/EDN)**ENQ1)*1.3+1.3E-6
  225 IF (PR2.LE.PR3) GO TO 230
      IF (PR3.LT.PR1) GO TO 240
      GO TO 235
  230 IF (PR2.GT.PR1) GO TO 235
      NEWQ=NQ
      RH=1./PR2
      GO TO 255
  235 NEWQ=NQ-1
      RH=1./PR1
      GO TO 255
  240 NEWQ=L
```

```
      RH=1./PR3
      IF (RH.LT.1.1) GO TO 250
      DO 245 I=1,N
  245 Y(I,NEWQ+1)=ERROR(I)*EL(L)/FLOAT(L)
      GO TO 260
  250 IDOUB=10
      GO TO 295
  255 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1)) GO TO 250
      IF (NEWQ.EQ.NQ) GO TO 35
  260 NQ=NEWQ
      L=NQ+1
      IRET=2
      GO TO 15
  265 IF (KFLAG.EQ.-9) GO TO 280
      RH=10.**KFLAG
      RH=AMAX1(HMIN/ABS(H),RH)
      H=H*RH
      CALL DIFFUN (N,T,Y,W1)
      NFE=NFE+1
      DO 270 I=1,N
  270 Y(I,2)=H*W1(I,1)
      IWEVAL=MITER
      IDOUB=10
      IF (NQ.EQ.1) GO TO 50
      NQ=1
      L=2
      IRET=3
      GO TO 15
  275 KFLAG=-1
      GO TO 295
  280 KFLAG=-2
      GO TO 295
  285 KFLAG=-3
      GO TO 295
  290 RMAX=100.
  295 HOLD=H
      JSTART=NQ
      RETURN
      END
```

```
      SUBROUTINE COSET (METH,NQ,EL,TQ,MAXDER)
      DIMENSION PERTST(12,2,3), EL(13), TQ(4)
      DATA PERTST/1.,1.,2.,1.,.3158,.07407,.01391,.002182,.0002945,.0000
     13492,.000003692,.0000003524,1.,1.,.5,.1667,.04167,1.,1.,1.,1.,1.,1
     2.,1.,2.,12.,24.,37.89,53.33,70.08,87.97,106.9,126.7,147.4,168.8,19
     31.0,2.0,4.5,7.333,10.42,13.7,1.,1.,1.,1.,1.,1.,1.,12.0,24.0,37.89,
     453.33,70.08,87.97,106.9,126.7,147.4,168.8,191.0,1.,3.0,6.0,9.167,1
     52.5,1.,1.,1.,1.,1.,1.,1./
    5 MAXDER=5
      GO TO (10,15,20,25,30),NQ
   10 EL(1)=1.0
      GO TO 35
   15 EL(1)=6.6666666666667E-01
      EL(3)=3.3333333333333E-01
      GO TO 35
   20 EL(1)=5.4545454545455E-01
      EL(3)=EL(1)
      EL(4)=9.0909090909091E-02
      GO TO 35
   25 EL(1)=0.48
      EL(3)=0.7
      EL(4)=0.2
      EL(5)=0.02
      GO TO 35
   30 EL(1)=4.3795620437956E-01
      EL(3)=8.2116788321168E-01
      EL(4)=3.1021897810219E-01
      EL(5)=5.4744525547445E-02
      EL(6)=3.6496350364964E-03
   35 DO 40 K=1,3
   40 TQ(K)=PERTST(NQ,METH,K)
      TQ(4)=.5*TQ(2)/FLOAT(NQ+2)
      RETURN
      END
```

```
      SUBROUTINE NSCORA (N,IA,JA,A,IAP,JAWORK,AWORK,C,IR,ICT)
      INTEGER IA(1),JA(1),IAP(1),JAWORK(1),C(1),IR(1),ICT(1)
      REAL A(1),AWORK(1)
      DO 5 K=1,N
      ICK=C(K)
    5 IR(ICK)=K
      JMIN=1
      DO 15 K=1,N
      ICK=C(K)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IF (JMIN.GT.JMAX) GO TO 15
      IAINK=IA(ICK)-1
      DO 10 J=JMIN,JMAX
      IAINK=IAINK+1
      JAOUTJ=JA(IAINK)
      JAOUTJ=IR(JAOUTJ)
      JAWORK(J)=JAOUTJ
   10 AWORK(J)=A(IAINK)
   15 JMIN=JMAX+1
      DO 20 I=1,N
   20 ICT(I)=IAP(I)
      JMIN=1
      DO 30 I=1,N
      ICK=C(I)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IF (JMIN.GT.JMAX) GO TO 30
      DO 25 J=JMIN,JMAX
      JAOUTJ=JAWORK(J)
      ICTJ=ICT(JAOUTJ)
      A(ICTJ)=AWORK(J)
      ICT(JAOUTJ)=ICTJ+1
   25 CONTINUE
   30 JMIN=JMAX+1
      RETURN
      END
```

```
      SUBROUTINE NSNFAC (N,IA,JA,A,IL,JL,ISL,L,D,IU,JU,ISU,U,X,IRL,JRL,I
     1ER)
      INTEGER IA(1),JA(1),IL(1),JL(1),ISL(1)
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1)
      REAL A(1),L(1),D(1),U(1),X(1)
      REAL LKI
      IER=0
      DO 5 K=1,N
      IRL(K)=IL(K)
    5 JRL(K)=0
      DO 90 K=1,N
      X(K)=0.
      I1=0
      IF (JRL(K).EQ.0) GO TO 15
      I=JRL(K)
   10 I2=JRL(I)
      JRL(I)=I1
      I1=I
      X(I)=0.
      I=I2
      IF (I.NE.0) GO TO 10
   15 JMIN=ISU(K)
      JMAX=JMIN+IU(K+1)-IU(K)-1
      IF (JMIN.GT.JMAX) GO TO 25
      DO 20 J=JMIN,JMAX
      JUJ=JU(J)
   20 X(JUJ)=0.
   25 JMIN=IA(K)
      JMAX=IA(K+1)-1
      DO 30 J=JMIN,JMAX
      JAJ=JA(J)
   30 X(JAJ)=A(J)
      I=I1
      IF (I.EQ.0) GO TO 50
   35 IRLI=IRL(I)
      LKI=-X(I)
      L(IRLI)=-LKI
      JMIN=IU(I)
      JMAX=IU(I+1)-1
      IF (JMIN.GT.JMAX) GO TO 45
      ISUB=ISU(I)-1
      DO 40 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   40 X(JUJ)=X(JUJ)+LKI*U(J)
   45 I=JRL(I)
      IF (I.NE.0) GO TO 35
   50 IF (X(K).EQ.0.) GO TO 95
      DK=1./X(K)
      D(K)=DK
```

```
      IF (K.EQ.N) GO TO 90
      JMIN=IU(K)
      JMAX=IU(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 60
      ISUB=ISU(K)-1
      DO 55 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   55 U(J)=X(JUJ)*DK
   60 CONTINUE
      I=I1
      IF (I.EQ.0) GO TO 85
   65 IRL(I)=IRL(I)+1
      I1=JRL(I)
      IF (IRL(I).GE.IL(I+1)) GO TO 80
      ISLB=IRL(I)-IL(I)+ISL(I)
      J=JL(ISLB)
   70 IF (I.GT.JRL(J)) GO TO 75
      J=JRL(J)
      GO TO 70
   75 JRL(I)=JRL(J)
      JRL(J)=I
   80 I=I1
      IF (I.NE.0) GO TO 65
   85 ISLK=ISL(K)
      IF (IRL(K).GE.IL(K+1)) GO TO 90
      J=JL(ISLK)
      JRL(K)=JRL(J)
      JRL(J)=K
   90 CONTINUE
      RETURN
   95 IER=K
      RETURN
      END
```

```
      SUBROUTINE NSBSLV (N,R,C,IL,JL,ISL,L,D,IU,JU,ISU,U,X,B,Y)
      DIMENSION R(1), IL(1), JL(1), IU(1), JU(1), C(1), ISL(1), ISU(1)
      DIMENSION L(1), X(1), B(1), U(1), Y(1), D(1)
      INTEGER R,RK,C,CK
      REAL L
      DO 5 K=1,N
      RK=R(K)
    5 Y(K)=B(RK)
      DO 15 K=1,N
      JMIN=IL(K)
      JMAX=IL(K+1)-1
      YK=-D(K)*Y(K)
      Y(K)=-YK
      IF (JMIN.GT.JMAX) GO TO 15
      ISLB=ISL(K)-1
      DO 10 J=JMIN,JMAX
      ISLB=ISLB+1
      JLJ=JL(ISLB)
   10 Y(JLJ)=Y(JLJ)+YK*L(J)
   15 CONTINUE
      K=N
      DO 30 I=1,N
      SUM=-Y(K)
      JMIN=IU(K)
      JMAX=IU(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 25
      ISUB=ISU(K)-1
      DO 20 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   20 SUM=SUM+U(J)*Y(JUJ)
   25 Y(K)=-SUM
      CK=C(K)
      X(CK)=-SUM
   30 K=K-1
      RETURN
      END
```

```
      SUBROUTINE YSMER (A,K,A1)
      INTEGER A,A1(2)
      COMMON /INOUT/ INP,LOUT,ITAPE
      WRITE (LOUT,5) A,K,A1(1),A1(2)
      RETURN
C
C
C
    5 FORMAT (1X,A10,I6,2A10)
      END
```

```
      SUBROUTINE INTERP (TOUT,Y,NO,YO)
      COMMON /GEAR1/ T,H,DUMMY(4),N,IDUMMY(2),JSTART
      DIMENSION YO(NO), Y(NO,1)
      DO 5 I=1,N
    5 YO(I)=Y(I,1)
      L=JSTART+1
      S=(TOUT-T)/H
      S1=1.
      DO 15 J=2,L
      S1=S1*S
      DO 10 I=1,N
   10 YO(I)=YO(I)+S1*Y(I,J)
   15 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SPARS (IA,JA,N)
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT
      DIMENSION IA(N), JA(N)
      DO 5 I=1,N
    5 IA(I)=1
      KT=0
      IA(N+1)=1
      JA(1)=0
      DO 70 IR=1,NR
      IF (KR(IR,1).EQ.N+2) GO TO 70
      IF (KR(IR,1).EQ.0.OR.KR(IR,1).EQ.99) GO TO 70
      MT=ITYPE(IR)
      DO 65 K=1,MT
      I=KR(IR,K)
      IF (KR(IR,K).EQ.N+2) GO TO 65
      DO 30 L=1,MT
      J=KR(IR,L)
      IF (KR(IR,L).EQ.N+2) GO TO 30
      K1=IA(J)
      K2=IA(J+1)-1
      IF (K1.GT.K2) GO TO 15
      DO 10 M=K1,K2
   10 IF (I.EQ.JA(M)) GO TO 30
   15 DO 20 M=J,N
   20 IA(M+1)=IA(M+1)+1
      KT=KT+1
      KD=KT-K2
      K2=K2+1
      DO 25 M=1,KD
   25 JA(KT+2-M)=JA(KT+1-M)
      JA(K2)=I
   30 CONTINUE
      K1=IA(I)
      DO 60 L=4,7
      K2=IA(I+1)-1
      J=KR(IR,L)
      IF (KR(IR,L).EQ.N+2) GO TO 60
      IF (J) 60,65,35
   35 IF (K1.GT.K2) GO TO 45
      DO 40 M=K1,K2
      IF (J.EQ.JA(M)) GO TO 60
   40 CONTINUE
   45 DO 50 M=I,N
   50 IA(M+1)=IA(M+1)+1
      KT=KT+1
      KD=KT-K2
      K2=K2+1
      DO 55 M=1,KD
   55 JA(KT+2-M)=JA(KT+1-M)
```

```
      JA(K2)=J
   60 CONTINUE
   65 CONTINUE
   70 CONTINUE
      DO 80 I=1,N
      K1=IA(I)+1
      K2=IA(I+1)-1
      IF (K1.GT.K2) GO TO 80
      MT=K2-K1+1
      DO 75 K=1,MT
      DO 75 M=K1,K2
      IF (JA(M).GT.JA(M-1)) GO TO 75
      J=JA(M-1)
      JA(M-1)=JA(M)
      JA(M)=J
   75 CONTINUE
   80 CONTINUE
      M=N
      DO 95 I=1,M
      IF (IA(I+1).GT.IA(I)) GO TO 95
      NM=I+1
      NN=N+1
      KMIN=IA(NM)
      KMAX=IA(NN)
      DO 85 J=KMIN,KMAX
      KM=KMAX+KMIN-J
   85 JA(KM)=JA(KM-1)
      KNOW=IA(I)
      JA(KNOW)=I
      DO 90 LL=NM,NN
   90 IA(LL)=IA(LL)+1
   95 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SORDER (N,IA,JA,P,Q,MAX,V,L,IER)
      INTEGER IA(1),JA(1),P(1),Q(1),V(1),L(1)
      INTEGER S,SFS,PI,PJ,PK,VI,VJ,VK,QVK,DTHR,DMIN
      IER=0
      DO 5 S=1,MAX
    5 L(S)=S+1
      SFS=1
      L(MAX)=0
      DO 10 K=1,N
      P(K)=K
      Q(K)=K
      V(K)=1
   10 L(K)=0
      SFS=SFS+N
      DO 50 K=1,N
      JMIN=IA(K)
      JMAX=IA(K+1)-1
      IF (JMIN.GT.JMAX+1) GO TO 145
      KDIAG=0
      DO 45 J=JMIN,JMAX
      VJ=JA(J)
      IF (VJ.NE.K) GO TO 15
      KDIAG=1
      GO TO 45
   15 LLK=K
   20 LK=LLK
      LLK=L(LK)
      IF (LLK.EQ.0) GO TO 25
      IF (V(LLK)-VJ) 20,30,25
   25 LLK=SFS
      IF (LLK.EQ.0) GO TO 150
      SFS=L(SFS)
      V(K)=V(K)+1
      V(LLK)=VJ
      L(LLK)=L(LK)
      L(LK)=LLK
   30 LLK=VJ
   35 LK=LLK
      LLK=L(LK)
      IF (LLK.EQ.0) GO TO 40
      IF (V(LLK)-K) 35,45,40
   40 LLK=SFS
      IF (LLK.EQ.0) GO TO 150
      SFS=L(SFS)
      V(VJ)=V(VJ)+1
      V(LLK)=K
      L(LLK)=L(LK)
      L(LK)=LLK
   45 CONTINUE
      IF (KDIAG.EQ.0) GO TO 160
```

```
 50 CONTINUE
    J=0
    DTHR=0
    DMIN=N
    I=0
 55 I=I+1
    IF (I.GT.N) GO TO 140
    JMIN=MAXO(J+1,I)
    IF (JMIN.GT.N) GO TO 70
 60 DO 65 J=JMIN,N
    VI=P(J)
    IF (V(VI).LE.DTHR) GO TO 75
    IF (V(VI).LT.DMIN) DMIN=V(VI)
 65 CONTINUE
 70 DTHR=DMIN
    DMIN=N
    JMIN=I
    GO TO 60
 75 PJ=P(I)
    P(J)=PJ
    Q(PJ)=J
    PI=VI
    P(I)=PI
    Q(PI)=I
    LI=VI
 80 LI=L(LI)
    IF (LI.EQ.0) GO TO 105
    VK=V(LI)
    LLK=VK
    LJ=VI
 85 LJ=L(LJ)
    IF (LJ.EQ.0) GO TO 100
    VJ=V(LJ)
    IF (VJ.EQ.VK) GO TO 85
 90 LK=LLK
    LLK=L(LK)
    IF (LLK.EQ.0) GO TO 95
    IF (V(LLK)-VJ) 90,85,95
 95 LLK=SFS
    IF (LLK.EQ.0) GO TO 155
    SFS=L(SFS)
    V(VK)=V(VK)+1
    V(LLK)=VJ
    L(LLK)=L(LK)
    L(LK)=LLK
    GO TO 85
100 IF (V(VK).GT.V(VI)) GO TO 80
    I=I+1
    QVK=Q(VK)
    PI=P(I)
```

```
      P(QVK)=PI
      Q(PI)=QVK
      P(I)=VK
      Q(VK)=I
      GO TO 80
  105 LI=VI
  110 IF (L(LI).EQ.0) GO TO 135
      LI=L(LI)
      VK=V(LI)
      LLK=VK
      QVK=MIN0(Q(VK),I)
  115 LK=LLK
      LLK=L(LK)
      IF (LLK.EQ.0) GO TO 120
      VJ=V(LLK)
      IF (Q(VJ).GT.QVK) GO TO 115
      V(VK)=V(VK)-1
      L(LK)=L(LLK)
      L(LLK)=SFS
      SFS=LLK
      LLK=LK
      GO TO 115
  120 IF (Q(VK).LE.I) GO TO 130
      IF (V(VK).LE.DTHR) GO TO 125
      IF ((DTHR.LT.V(VK)).AND.(V(VK).LT.DMIN)) DMIN=V(VK)
      GO TO 110
  125 J=MIN0(Q(VK)-1,J)
      DTHR=V(VK)
      GO TO 110
  130 L(LK)=SFS
      SFS=L(VK)
      GO TO 110
  135 L(LI)=SFS
      SFS=L(VI)
      GO TO 55
  140 RETURN
  145 CALL YSMER (3HROW,K,13H OF A IS NULL)
      GO TO 165
  150 CALL YSMER (3HROW,K,16H EXCEEDS STORAGE)
      GO TO 165
  155 CALL YSMER (6HVERTEX,VI,16H EXCEEDS STORAGE)
      GO TO 165
  160 CALL YSMER (6HCOLUMN,K,19H.. DIAGONAL MISSING)
  165 IER=1
      RETURN
      END
```

```
      SUBROUTINE NSSFAC (N,IA,JA,MAXPL,IL,JL,ISL,MAXPU,IU,JU,ISU,P,V,IRA
     1,JRA,IRAC,IRL,JRL,IRU,JRU,IER)
      INTEGER IA(1),JA(1),IRA(1),JRA(1),IL(1),JL(1),ISL(1)
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1),IRU(1),JRU(1)
      INTEGER P(1),V(1),IRAC(1)
      INTEGER VI,VJ,VK,PK,PPK,PI,CEND,REND
      IER=0
      DO 5 K=1,N
      IRAC(K)=0
      JRA(K)=0
      JRL(K)=0
    5 JRU(K)=0
      DO 10 K=1,N
      IAK=IA(K)
      IF (IAK.GT.IA(K+1)) GO TO 200
      IF (JA(IAK).GT.K) GO TO 10
      JAIAK=JA(IAK)
      JRA(K)=IRAC(JAIAK)
      IRAC(JAIAK)=K
   10 IRA(K)=IAK
      JLPTR=0
      IL(1)=1
      JUPTR=0
      IU(1)=1
      DO 195 K=1,N
      P(1)=1
      V(1)=N+1
      LSFS=2
      VJ=IRAC(K)
      IF (VJ.EQ.0) GO TO 30
   15 PPK=1
   20 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 20,220,25
   25 P(PK)=LSFS
      V(LSFS)=VJ
      P(LSFS)=PPK
      LSFS=LSFS+1
      VJ=JRA(VJ)
      IF (VJ.NE.0) GO TO 15
   30 LASTI=0
      I=K
   35 I=JRU(I)
      IF (I.EQ.0) GO TO 60
      PPK=1
      JMIN=IRL(I)
      JMAX=ISL(I)+IL(I+1)-IL(I)-1
      IF (LASTI.GT.I) GO TO 40
      LASTI=I
      LASTID=JMAX-JMIN
```

```
      IF (JL(JMIN).NE.K) LASTID=LASTID+1
   40 IF (JMIN.GT.JMAX) GO TO 35
      DO 55 J=JMIN,JMAX
      VJ=JL(J)
   45 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 45,55,50
   50 P(PK)=LSFS
      V(LSFS)=VJ
      P(LSFS)=PPK
      PPK=LSFS
      LSFS=LSFS+1
   55 CONTINUE
      GO TO 35
   60 PI=P(1)
      IF (V(PI).NE.K) GO TO 225
      IF (LASTI.EQ.0) GO TO 65
      IF (LASTID.NE.LSFS-3) GO TO 65
      IRLL=IRL(LASTI)
      ISL(K)=IRLL+1
      IF (JL(IRLL).NE.K) ISL(K)=ISL(K)-1
      IL(K+1)=IL(K)+LASTID
      IRL(K)=ISL(K)
      GO TO 80
   65 ISL(K)=JLPTR+1
      PI=P(1)
      PI=P(PI)
      VI=V(PI)
   70 IF (VI.GT.N) GO TO 75
      JLPTR=JLPTR+1
      IF (JLPTR.GT.MAXPL) GO TO 230
      JL(JLPTR)=VI
      PI=P(PI)
      VI=V(PI)
      GO TO 70
   75 IRL(K)=ISL(K)
      IL(K+1)=IL(K)+JLPTR-ISL(K)+1
   80 P(1)=1
      V(1)=N+1
      LSFS=2
      JMIN=IRA(K)
      JMAX=IA(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 100
      DO 95 J=JMIN,JMAX
      VJ=JA(J)
      PPK=1
   85 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 85,205,90
   90 P(PK)=LSFS
```

```
      V(LSFS)=VJ
      P(LSFS)=PPK
   95 LSFS=LSFS+1
  100 LASTI=0
      I=K
  105 I=JRL(I)
      IF (I.EQ.0) GO TO 130
      PPK=1
      JMIN=IRU(I)
      JMAX=ISU(I)+IU(I+1)-IU(I)-1
      IF (LASTI.GT.I) GO TO 110
      LASTI=I
      LASTID=JMAX-JMIN
      IF (JU(JMIN).NE.K) LASTID=LASTID+1
  110 IF (JMIN.GT.JMAX) GO TO 105
      DO 125 J=JMIN,JMAX
      VJ=JU(J)
  115 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 115,125,120
  120 P(PK)=LSFS
      V(LSFS)=VJ
      P(LSFS)=PPK
      PPK=LSFS
  125 LSFS=LSFS+1
      GO TO 105
  130 PI=P(1)
      IF (V(PI).NE.K) GO TO 210
      IF (LASTI.EQ.0) GO TO 135
      IF (LASTID.NE.LSFS-3) GO TO 135
      IRUL=IRU(LASTI)
      ISU(K)=IRUL+1
      IF (JU(IRUL).NE.K) ISU(K)=ISU(K)-1
      IU(K+1)=IU(K)+LASTID
      IRU(K)=ISU(K)
      GO TO 150
  135 ISU(K)=JUPTR+1
      PI=P(1)
      PI=P(PI)
      VI=V(PI)
  140 IF (VI.GT.N) GO TO 145
      JUPTR=JUPTR+1
      IF (JUPTR.GT.MAXPU) GO TO 215
      JU(JUPTR)=VI
      PI=P(PI)
      VI=V(PI)
      GO TO 140
  145 IRU(K)=ISU(K)
      IU(K+1)=IU(K)+JUPTR-ISU(K)+1
  150 I=K
```

```
155 I1=JRL(I)
    CEND=ISL(I)+IL(I+1)-IL(I)
    IF (IRL(I).GE.CEND) GO TO 160
    IRLI=IRL(I)
    J=JL(IRLI)
    JRL(I)=JRL(J)
    JRL(J)=I
160 I=I1
    IF (I.EQ.0) GO TO 165
    IRL(I)=IRL(I)+1
    GO TO 155
165 I=K
170 I1=JRU(I)
    REND=ISU(I)+IU(I+1)-IU(I)
    IF (IRU(I).GE.REND) GO TO 175
    IRUI=IRU(I)
    J=JU(IRUI)
    JRU(I)=JRU(J)
    JRU(J)=I
175 I=I1
    IF (I.EQ.0) GO TO 180
    IRU(I)=IRU(I)+1
    GO TO 170
180 I=IRAC(K)
    IF (I.EQ.0) GO TO 195
185 I1=JRA(I)
    IRA(I)=IRA(I)+1
    IF (IRA(I).GE.IA(I+1)) GO TO 190
    IRAI=IRA(I)
    IF (JA(IRAI).GT.I) GO TO 190
    JAIRAI=JA(IRAI)
    JRA(I)=IRAC(JAIRAI)
    IRAC(JAIRAI)=I
190 I=I1
    IF (I.NE.0) GO TO 185
195 CONTINUE
    ISL(N)=JLPTR
    ISU(N)=JUPTR
    RETURN
200 CALL YSMER (3HROW,K,13H OF A IS NULL)
    GO TO 235
205 CALL YSMER (3HROW,K,20H HAS DUPLICATE ENTRY)
    GO TO 235
210 CALL YSMER (3HROW,K,17H HAS A NULL PIVOT)
    GO TO 235
215 CALL YSMER (3HROW,K,19H EXCEEDS JU STORAGE)
    GO TO 235
220 CALL YSMER (3HCOL,K,20H HAS DUPLICATE ENTRY)
    GO TO 235
225 CALL YSMER (3HCOL,K,17H HAS A NULL PIVOT)
```

```
      GO TO 235                                           U  201
  230 CALL YSMER (3HCOL,K,19H EXCEEDS JL STORAGE)         U  202
  235 IER=1                                               U  203
      RETURN                                              U  204
      END                                                 U  205-
```

```
      SUBROUTINE NSCORD (N,IA,JA,IAWORK,JAWORK,C,IR,ICT)
      INTEGER IA(1),JA(1),IAWORK(1),JAWORK(1),C(1),IR(1),ICT(1)
      DO 5 I=1,N
    5 ICT(I)=0
      IAWORK(1)=1
      DO 15 K=1,N
      ICK=C(K)
      JMIN=IAWORK(K)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IAWORK(K+1)=JMAX+1
      IF (JMIN.GT.JMAX) GO TO 15
      IAINK=IA(ICK)-1
      DO 10 J=JMIN,JMAX
      IAINK=IAINK+1
      JAOUTJ=JA(IAINK)
      JAOUTJ=IR(JAOUTJ)
      JAWORK(J)=JAOUTJ
   10 ICT(JAOUTJ)=ICT(JAOUTJ)+1
   15 CONTINUE
      IA(1)=1
      DO 20 I=1,N
      IA(I+1)=IA(I)+ICT(I)
   20 ICT(I)=IA(I)
      DO 30 I=1,N
      JMIN=IAWORK(I)
      JMAX=IAWORK(I+1)-1
      IF (JMIN.GT.JMAX) GO TO 30
      DO 25 J=JMIN,JMAX
      JAOUTJ=JAWORK(J)
      ICTJ=ICT(JAOUTJ)
      JA(ICTJ)=I
   25 ICT(JAOUTJ)=ICTJ+1
   30 CONTINUE
      RETURN
      END
```

```
      BLOCK DATA ALPHA1
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER
      COMMON /APLOT/ JVERT(52,2),JBLANK,JSTAR,JPLUS,JBAR
      COMMON /GEAR1/ T,GUESS,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST,
     1IPH(30),QM(100),PM(100),PSTOP
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10
      DATA IGO(1)/4HMORE/,IGO(2)/4HCONT/,IGO(3)/4HPLOT/,IGO(4)/4H    /,I
     1BLANK/4H    /,MBLANK/4HM   /,JINTER/4HINTV/
      DATA JVERT/12*4H    ,4H C  ,4H O  ,4H N  ,4H C  ,4H E  ,4H N  ,4H
     1T  ,4H R  ,4H A  ,4H T  ,4H I  ,4H O  ,4H N  ,4H    ,4H P  ,4H P
     2,4H M  ,75*4H    /
      DATA JBLANK/4H    /,JSTAR/1H*/,JPLUS/1H+/,JBAR/1HI/
      DATA ITEMP/4HTEMP/,TEMEND/0.0/,PSTOP/0.0/,IN10/1/
      DATA UROUND/7.5E-15/
      END
```

Appendix B

INPUT DATA--CHEMK FORMAT

APPENDIX B
INPUT DATA--CHEMK FORMAT

69		SAVE		.000324					
1	NO2			NO	O			1.000E+00	
2	O			O3				4.400E+06	
3	NO	O3		NO2				2.39E+01	1450.0
4	NO2	O3		NO3				4.800E-02	2450.0
5	NO2	O		NO				1.340E+04	
6	OH	O3		HO2				7.700E+01	1000.0
7	HO2	O3		OH				8.000E+00	1525.0
8	OH	NO2		HNO3				1.400E+04	
9	OH	CO		HO2	CO2			4.400E+02	
10	NO	NO		NO2	NO2			1.500E-04	
11	NO	NO3		NO2	NO2			2.800E+04	
12	NO2	NO3	H2O					1.560E-03	-10600.0
13	NO	HO2		NO2	OH			1.200E+04	
14	HO2	HO2						1.800E+04	
15	O	PAR		MEO2	OH			2.000E+01	
16	OH	PAR		MEO2				1.500E+03	
17	O	OLE		MEO2	ACO3	X		2.700E+03	
18	O	OLE		CARB	PAR			2.700E+03	
19	OH	OLE		RAO2				4.200E+04	
20	O3	OLE		CARB	CRIG			8.000E-03	
21	O3	OLE		CARB	MCRG	X		8.000E-03	
22	O	ETH		MEO2	HO2	CO		6.000E+02	
23	O	ETH		CARB	PAR			6.000E+02	
24	OH	ETH		RBO2				1.200E+04	
25	O3	ETH		CARB	CRIG			2.400E-03	
26	NO	ACO3		NO2	MEO2	CO2		3.800E+03	
27	NO	RBO2		NO2	CARB	CARB	HO2	1.200E+04	
28	NO	RAO2		NO2	CARB	CARB	HO2	1.200E+04	
29	NO	MEO2		NO2	CARB	MEO2	X	4.000E+03	
30	NO	MEO2		NO2	CARB	HO2		8.000E+03	
31	NO	MEO2		NRAT				5.000E+02	
32	O3	RBO2		CARB	CARB	HO2		5.000E+00	
33	O3	RAO2		CARB	CARB	HO2		2.000E+02	
34	O3	MEO2		CARB	HO2			5.000E+00	
35	OH	CARB		HO2	CO			9.500E+03	
36	OH	CARB		ACO3	X			9.500E+03	
37	CARB			QQ				1.000E+00	
38	QQ			HO2	HO2	CO		1.000E+02	
39	QQ			MEO2	X	HO2	CO	1.000E+02	
40	CARB			CO				3.500E-01	
41	PAR	X						1.000E+05	
42	NO2	ACO3		PAN				2.000E+03	
43	PAN			ACO3	NO2			2.800E-02	12500.0
44	HO2	ACO3						4.000E+03	
45	HO2	MEO2						4.000E+03	
46	NO	CRIG		NO2	CARB			1.200E+04	
47	NO2	CRIG		NO3	CARB			8.000E+03	
48	CARB	CRIG						2.000E+03	
49	NO	MCRG		NO2	CARB	PAR		1.200E+04	
50	NO2	MCRG		NO3	CARB	PAR		8.000E+03	
51	CARB	MCRG						2.000E+03	
52	CRIG			CO				6.700E+02	
53	CRIG							8.400E+02	
54	CRIG			HO2	HO2	CO2		9.000E+01	
55	MCRG							1.500E+02	
56	MCRG			MEO2	OH	CO		8.400E+02	
57	MCRG			MEO2	HO2	CO2		4.250E+02	
58	MCRG			CARB	HO2	HO2	CO	8.500E+01	
59	OH	ARO		HO2	Y	Y	Y	6.000E+03	
60	OH	ARO		HO2	CLY	X		1.600E+03	
61	OH	ARO		OH	CLY	W		1.500E+04	
62	CARB	W						1.000E+03	

```
 63  NO    Y          NO   CARB PAR         8.000E+01
 64  NO    Y          NO2  AERO             1.500E+01
 65  NO3   Y          CARB CARB             3.500E+04
 66  O3    Y          AERO                  6.000E-01
 67  OH    GLY        HO2  GC   CO          1.000E+04
 68  GC               Y    Y    Y           1.000E+02
 69  GLY              ME02 HO2  GC          2.026E-01
MORE
 70        SAVE       .000324
  1  NO2              NO   O               .3
 37  CARB             OO                   .00064
 40  CARB             CO                   .00032
 29  NO    ME02       NO2  CARB ME02 X     2770.
 30  NO    ME02       NO2  CARB HO2        9230.
 69  GLY              ME02 HO2  GC         .072
 71  RX               OH                   .03
 72                   CO                   .003
 73  O3                                    .001
 70  H20                                   -.000324
EC-237
 10                             60.        60.
NO          NO2        OLE      PAR        ARO        CARB       H20
RX          CO         ETH
.377        .106       .09      7.35       .177       .1012      24000.
.004        .9         .875
            360.       303.2
PLOT
EC-237
      3          0.00 0.20 0.40 0.60 0.80  0.         .8         0.         400.
O3    25 O
0.          .002       15.        .002       30.        .01        45.        .042
60.         .11        75.        .188       90.        .264       105.       .335
120.        .391       135.       .452       150.       .511       165.       .557
180.        .594       195.       .62        210.       .64        225.       .65
240.        .655       255.       .65        270.       .645       285.       .635
300.        .628       315.       .613       330.       .603       345.       .594
360.        .584
NO    25 N
0.          .377       15.        .272       30.        .169       45.        .083
60.         .04        75.        .024       90.        .018       105.       .013
120.        .011       135.       .01        150.       .007       165.       .007
180.        .006       195.       .006       210.       .006       225.       .006
240.        .006       255.       .006       270.       .005       285.       .005
300.        .005       315.       .005       330.       .005       345.       .005
360.        .005
NO2   25 2
0.          .106       15.        .198       30.        .29        45.        .353
60.         .368       75.        .35        90.        .324       105.       .297
120.        .268       135.       .234       150.       .205       165.       .171
180.        .142       195.       .117       210.       .096       225.       .07
240.        .074       255.       .068       270.       .063       285.       .05
300.        .039       315.       .038       330.       .037       345.       .037
360.        .036
                         BLANK CARD
                         BLANK CARD
```

APPENDIX C
INPUT DATA--EPA FORMAT

Appendix C

INPUT DATA--EPA FORMAT

70	1	SAVE		.000324						
NO2			1		NO		O		1.000E+00	
O			2		O3				4.400E+06	
NO	O3		3		NO2				2.390E+01	1450.
NO2	O3		4		NO3				4.800E-02	2450.
NO2	O		5		NO				1.340E+04	
OH	O3		6		HO2				7.700E+01	1000.
HO2	O3		7		OH				5.000E+00	1525.
OH	NO2		8		HNO3				1.400E+04	
OH	CO		9		HO2		CO2		4.400E+02	
NO	NO		10	2.	NO2				1.500E-04	
NO	NO3		11	2.	NO2				2.800E+04	
NO2	NO3	H2O	12						1.560E-03	-10600.
NO	HO2		13		NO2		OH		1.200E+04	
HO2	HO2		14						1.500E+04	
O	PAR		15		MEO2		OH		2.000E+01	
OH	PAR		16		MEO2				1.500E+03	
O	OLE		17		MEO2		ACO3	X	2.700E+03	
O	OLE		18		CARB		PAR		2.700E+03	
OH	OLE		19		RAO2				4.200E+04	
O3	OLE		20		CARB		CRIG		8.000E-03	
O3	OLE		21		CARB		MCRC	X	8.000E-03	
O	ETH		22		MEO2		HO2	CO	6.000E+02	
O	ETH		23		CARB		PAR		6.000E+02	
OH	ETH		24		RBO2				1.200E+04	
O3	ETH		25		CARB		CRIG		2.400E-03	
NO	ACO3		26		NO2		MEO2	CO2	3.800E+03	
NO	RBO2		27		NO2	2.	CARB	HO2	1.200E+04	
NO	RAO2		28		NO2	2.	CARB	HO2	1.200E+04	
NO	MEO2		29		NO2		CARB	PP	4.000E+03	
PP			30		MEO2		X		1.000E+05	
NO	MEO2		31		NO2		CARB	HO2	8.000E+03	
NO	MEO2		32		NRAT				5.000E+02	
O3	RBO2		33	2.	CARB		HO2		5.000E+00	
O3	RAO2		34	2.	CARB		HO2		2.000E+02	
O3	MEO2		35		CARB		HO2		5.000E+00	
OH	CARB		36		HO2		CO		9.500E+03	
OH	CARB		37		ACO3		X		9.500E+03	
CARB			38		QQ		CO		1.000E+00	
QQ			39	2.	HO2				1.000E+02	
QQ			40		MEO2		X	HO2	1.000E+02	
CARB			41		CO				3.500E-01	
PAR	X		42						1.000E+05	
NO2	ACO3		43		PAN				2.000E+03	
PAN			44		ACO3		NO2		2.800E-02	12500.
HO2	ACO3		45						4.000E+03	
HO2	MEO2		46						4.000E+03	
NO	CRIG		47		NO2		CARB		1.200E+04	
NO2	CRIG		48		NO3		CARB		8.000E+03	
CARB	CRIG		49						2.000E+03	
NO	MCRC		50		NO2		CARB	PAR	1.200E+04	
NO2	MCRC		51		NO3		CARB	PAR	8.000E+03	
CARB	MCRC		52						2.000E+03	
CRIG			53		CO				6.700E+02	
CRIG			54						2.400E+02	
CRIG			55	2.	HO2		CO2		9.000E+01	
MCRC			56						1.500E+02	
MCRC			57		MEO2		OH	CO	3.400E+02	
MCRC			58		MEO2		HO2	CO2	4.250E+02	
MCRC			59		CARB	2.	HO2	CO	8.500E+01	
OH	ARO		60		HO2	3.	Y		6.800E+03	
OH	ARO		61		HO2		GLY	X	1.600E+03	
OH	ARO		62		OH		GLY	V	1.500E+04	
CARB	W		63						1.000E+05	
NO	Y		64		NO		CARB	PAR	8.000E+01	
NO	Y		65		NO2		AERO		1.500E+01	
NO3	Y		66	2.	CARB				8.500E+04	
O3	Y		67		AERO				6.000E-01	
OH	GLY		68		HO2		CC	CO	1.000E+04	
CC			69	3.	Y				1.000E+02	
GLY			70		MEO2		HO2	CC	2.025E-01	

```
MORE
 74    1    SAVE           .000324
NO2                   1         NO             0                        .3
CARB                 38         OO             CO                       .00064
CARB                 41         CO                                      .00032
NO      MEO2         29         NO2            CARB          PP        2770.
NO      MEO2         31         NO2            CARB          HO2       9230.
GLY                  70         MEO2           HO2           CC         .072
RX                   71         OH                                      .03
                     72         CO                                       .003
O3                   73                                                  .001
H2O                  74                                                -.000324
EC-237
 10                                        60.          60.
NO            NO2           OLE            PAR          ARO           CARB          H2O
RX            CO            ETH
.377          .106          .09            7.35         .177          .1012         24000.
.004          .9            .875
              360.          303.2
PLOT
EC-237
      3            0.00 0.20 0.40 0.60 0.80  0.         .8            0.            400.
O3    25 0
0.            .002          15.            .002         30.           .01           45.           .042
60.           .11           75.            .188         90.           .264          105.          .235
120.          .391          135.           .452         150.          .511          165.          .557
180.          .594          195.           .62          210.          .64           225.          .65
240.          .655          255.           .65          270.          .645          285.          .635
300.          .628          315.           .613         330.          .603          345.          .594
360.          .584
NO    25 N
0.            .377          15.            .272         30.           .169          45.           .083
60.           .04           75.            .024         90.           .018          105.         -.013
120.          .011          135.           .01          150.          .007          165.          .007
180.          .006          195.           .006         210.          .006          225.          .006
240.          .006          255.           .006         270.          .005          285.          .005
300.          .005          315.           .005         330.          .005          345.          .005
360.          .005
NO2   25 2
0.            .106          15.            .198         30.           .29           45.           .353
60.           .368          75.            .35          90.           .324          105.          .297
120.          .268          135.           .234         150.          .205          165.          .171
180.          .142          195.           .117         210.          .096          225.          .07
240.          .074          255.           .068         270.          .063          285.          .05
300.          .039          315.           .038         330.          .037          345.          .037
360.          .036
                        BLANK CARD
                        BLANK CARD
```

APPENDIX D
OUTPUT DATA

(using EPA input format for the chemical reactions)

APPENDIX D
OUTPUT DATA

THE REACTIONS													RATE CONSTANT	ACT. ENERGY (K)
1	NO2					=	NO	+	O				1.000E+00	-0.
2	O					=	O3						4.400E+06	-0.
3	NO	+	O3			=	NO2						2.690E+01	1.450E+03
4	NO2	+	O3			=	NO3						4.800E-03	2.450E+03
5	NO2	+	O			=	NO						1.340E+04	-0.
6	OH	+	O3			=	HO2						7.700E+01	1.000E+03
7	HO2	+	O3			=	OH						6.000E+00	1.528E+03
8	OH	+	NO2			=	HNO3						1.400E+04	-0.
9	OH	+	CO			=	HO2	+	CO2				4.400E+02	-0.
10	NO	+	NO			=	2 NO2						1.600E-04	-0.
11	NO	+	NO3			=	2 NO2						3.800E+04	-0.
12	NO2	+	NO3	+	H2O	=							1.860E-03	-1.060E+04
13	NO	+	HO2			=	NO2	+	OH				1.200E+04	-0.
14	HO2	+	HO2			=							1.500E+04	-0.
15	O	+	PAR			=	MEO2	+	OH				2.000E+01	-0.
16	OH	+	PAR			=	MEO2						1.600E+03	-0.
17	O	+	OLE			=	MEO2	+	ACO3	+	X		3.700E+03	-0.
18	O	+	OLE			=	CARB	+	PAR				3.700E+03	-0.
19	OH	+	OLE			=	RAO2						4.200E+04	-0.
20	O3	+	OLE			=	CARB	+	CRIG				8.000E-03	-0.
21	O3	+	OLE			=	CARB	+	MCRG	+	X		8.000E-03	-0.
22	O	+	ETH			=	MEO2	+	HO2	+	CO		6.000E+03	-0.
23	O	+	ETH			=	CARB	+	PAR				6.000E+03	-0.
24	OH	+	ETH			=	RBO2						1.200E+04	-0.
25	O3	+	ETH			=	CARB	+	CRIG				2.400E-03	-0.
26	NO	+	ACO3			=	NO2	+	MEO2	+	CO2		8.800E+03	-0.
27	NO	+	RBO2			=	NO2	+	2 CARB	+	HO2		1.200E+04	-0.
28	NO	+	RAO2			=	NO2	+	2 CARB	+	HO2		1.200E+04	-0.
29	NO	+	MEO2			=	NO2	+	CARB	+	PP		4.000E+03	-0.
30	PP					=	MEO2	+	X				1.600E+05	-0.
31	NO	+	MEO2			=	NO2	+	CARB	+	HO2		8.000E+03	-0.

32	NO	+	MEO2	=	NRAT					5.000E+02	-0.
33	O3	+	RRO2	=	2 CARB	+	HO2			5.000E+00	-0.
34	O3	+	RAO2	=	2 CARB	+	HO2			2.000E+02	-0.
35	O3	+	MEO2	=	CARB	+	HO2			5.000E+00	-0.
36	OH	+	CARB	=	HO2	+	CO			9.500E+03	-0.
37	OH	+	CARB	=	ACO3	+	X			9.500E+03	-0.
38	CARB			=	QQ	+	CO			1.000E+00	-0.
39	QQ			=	2 HO2					1.000E+02	-0.
40	QQ			=	MEO2	+	X	+	HO2	1.000E+02	-0.
41	CARB			=	CO					3.500E-01	-0.
42	PAR	+	X	=						1.000E+05	-0.
43	NO2	+	ACO3	=	PAN					2.000E+03	-0.
44	PAN			=	ACO3	+	NO2			2.800E-02	1.250E+04
45	HO2	+	ACO3	=						4.000E+03	-0.
46	HO2	+	MEO2	=						4.000E+03	-0.
47	NO	+	CRIG	=	NO2	+	CARB			1.200E+04	-0.
48	NO2	+	CRIG	=	NO3	+	CARB			8.000E+03	-0.
49	CARB	+	CRIG	=						2.000E+03	-0.
50	NO	+	MCRG	=	NO2	+	CARB	+	PAR	1.200E+04	-0.
51	NO2	+	MCRG	=	NO3	+	CARB	+	PAR	8.000E+03	-0.
52	CARB	+	MCRG	=						2.000E+03	-0.
53	CRIG			=	CO					6.700E+02	-0.
54	CRIG			=						2.400E+02	-0.
55	CRIG			=	2 HO2	+	CO2			9.000E+01	-0.
56	MCRG			=						1.500E+02	-0.
57	MCRG			=	MEO2	+	OH	+	CO	3.400E+02	-0.
58	MCRG			=	MEO2	+	HO2	+	CO2	4.250E+02	-0.
59	MCRG			=	CARB	+	2 HO2	+	CO	8.500E+01	-0.
60	OH	+	ARO	=	HO2	+	3 Y			6.000E+03	-0.
61	OH	+	ARO	=	HO2	+	GLY	+	X	1.600E+03	-0.
62	OH	+	ARO	=	OH	+	GLY	+	W	1.500E+04	-0.
63	CARB	+	W	=						1.000E+05	-0.

64	NO	+	Y	=	NO	+	CARB	+	PAR	8.000E+01	-0.
65	NO	+	Y	=	NO2	+	AERO			1.500E+01	-0.
66	NO3	+	Y	=	2 CARB					8.500E+04	-0.
67	O3	+	Y	=	AERO					6.000E-01	-0.
68	OH	+	GLY	=	HO2	+	CC	+	CO	1.000E+04	-0.
69	CC			=	8 Y					1.000E+02	-0.
70	GLY			=	MEO2	+	HO2	+	CO	2.025E-01	-0.

THE REACTIONS

											RATE CONSTANT	ACT. ENERGY (K)
1	NO2			=	NO	+	O				3.000E-01	-0.
38	CARB			=	QQ	+	CO				6.400E-04	-0.
41	CARB			=	CO						3.200E-04	-0.
29	NO	+	MEO2	=	NO2	+	CARB	+	PP		2.770E+03	-0.
31	NO	+	MEO2	=	NO2	+	CARB	+	HO2		9.230E+03	-0.
70	GLY			=	MEO2	+	HO2	+	CC		7.200E-02	-0.
71	RX			=	OH						3.000E-02	-0.
72				=	CO						3.000E-03	-0.
73	O3			=							1.000E-03	-0.
74	H2O			=							-3.240E-04	-0.

EC-237

INITIAL CONCENTRATION

NO	NO2	OLE	PAR	ARO	CARB	H2O	RX	CO	ETH
3.770E-01	1.060E-01	9.000E-02	7.350E+00	1.770E-01	1.012E-01	2.400E+04	4.000E-03	9.000E-01	8.750E-01

THE TEMPERATURE OF THE CELL WAS = 3.03E+02 AND THE ERROR TOLERANCE = 1.00E-02

THE OVERALL DILUTION RATE WAS 8.24E-04

THE RATE CONSTANTS USED WERE

3.000E-01	4.400E+06	2.898E+01	5.527E-02	1.840E+04	8.156E+01	5.459E+00	1.400E+04	4.400E+02	1.500E-04
3.800E+04	8.476E-04	1.200E+04	1.500E+04	2.000E+01	1.500E+03	2.700E+03	2.700E+03	4.200E+04	8.000E-08
8.000E-03	6.000E+02	6.000E+02	1.200E+04	2.400E-03	3.800E+03	1.200E+04	1.200E+04	2.770E+03	1.000E+05
9.230E+03	5.000E+02	5.000E+00	2.000E+02	5.000E+00	9.500E+03	9.500E+03	6.400E-04	1.000E+02	1.000E+02
3.200E-04	1.000E+05	2.000E+03	8.749E-02	4.000E+03	4.000E+03	1.200E+04	8.000E+03	2.000E+03	1.200E+04
8.000E+03	2.000E+03	6.700E+02	2.400E+02	9.000E+01	1.500E+02	3.400E+03	4.250E+03	8.500E+01	6.000E+05
1.600E+03	1.500E+04	1.000E+05	8.000E+01	1.560E+01	8.500E+04	6.000E-01	1.000E+04	1.000E+02	1.080E-02
3.000E-02	8.000E-03	1.000E-03	-3.240E-04						

TI[illegible] IN[illegible]L	NO2 H2O ETH AERO	NO PAR RB02 CC	O HE02 PP RX	O3 OLE NRYT TEMP	NO3 AC03 GQ M	OH X PAN	HO2 CARB ARO	HNO3 RA02 Y	CO CRIG GLY	CO2 MCRG W
0.	1.060E-01	3.770E-01	0.	0.	0.	0.	0.	0.	9.000E-01	0.
1.0[illegible]-10	2.400E+04	7.350E+00	0.	9.000E-02	0.	0.	1.012E-01	0.	0.	0.
	8.750E-01	0.	0.	0.	0.	0.	1.770E-01	0.	0.	0.
	0.	0.	4.000E-03	3.032E+02	2.401E+04					
NET RA[illegible]S	-3.179E-02	3.164E-02	3.100E-02	0.	0.	1.200E-04	0.	0.	2.806E-03	0.
	0.	-2.381E-03	0.	-2.916E-05	0.	0.	-1.299E-04	0.	0.	0.
	-2.835E-04	0.	0.	0.	6.477E-05	0.	-5.735E-03	0.	0.	0.
	0.	0.	-1.213E-04	0.	3.163E-02					

THE R[illegible]CTION RATES ARE

3.1[illegible]-02	0.	0.	0.	0.	0.	0.	0.	0.	2.13E-05
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3.2[illegible]-05	0.	0.	0.	0.	0.	0.	6.48E-05	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
1.20[illegible]-04	3.00E-03	0.	-7.78E+00						

TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RO2 CC	O MEO2 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAN	HO2 CARB ARO	HNO3 RAO2 Y	CO CRIC GLY	CO2 MCRC W
6.000E+01	3.902E-01	5.123E-03	2.636E-08	8.206E-03	1.263E-06	9.331E-08	8.434E-06	2.287E-02	1.006E+00	1.122E-02
6.026E+00	2.400E+04	7.121E+00	3.718E-06	6.601E-03	5.980E-07	1.231E-09	3.430E-01	4.053E-07	3.680E-08	[illegible]
	7.927E-01	1.421E-06	3.918E-09	4.363E-03	1.097E-06	4.801E-03	1.809E-01	2.683E-04	1.166E-02	[illegible]
	1.097E-03	1.360E-06	6.458E-04	3.032E+02	3.401E+04					
ET RATES	-3.523E-04	-4.683E-04	-1.076E-08	5.497E-03	7.507E-03	-3.342E-08	1.830E-03	5.023E-04	3.288E-03	[illegible]
	-1.002E-05	-3.724E-03	2.876E-08	-3.762E-04	8.930E-07	-4.006E-08	3.808E-03	2.743E-06	-6.851E-08	-6.731E-08
	-1.326E-03	1.204E-03	-5.936E-06	6.023E-05	1.143E-08	1.897E-04	-3.672E-04	1.990E-05	9.319E-05	2.433E-07
	2.159E-04	1.128E-08	-1.988E-05	0.	6.740E-03					

THE REACTION RATES ARE

1.17E-01	1.17E-01	1.09E-01	1.77E-03	1.39E-04	6.25E-07	2.43E-06	5.10E-04	4.46E-03	3.94E-07
1.01E-03	1.00E-05	3.34E-03	4.43E-07	3.70E-06	9.97E-04	4.73E-06	4.73E-06	2.59E-04	4.33E-03
4.33E-05	1.26E-05	1.26E-05	8.88E-04	1.56E-04	1.17E-04	8.74E-04	2.49E-04	3.06E-04	3.92E-04
1.29E-03	6.96E-05	5.03E-07	6.63E-06	1.12E-06	3.04E-04	3.04E-04	3.20E-04	1.10E-04	1.10E-04
1.10E-04	8.76E-04	4.67E-04	3.76E-04	1.30E-08	5.91E-08	2.26E-03	1.18E-04	2.52E-03	4.92E-06
2.50E-03	5.49E-06	2.47E-03	8.83E-06	3.31E-06	1.20E-06	2.72E-06	3.40E-06	6.80E-07	[illegible]
3.23E-03	2.11E-04	2.11E-04	4.13E-04	2.06E-04	1.19E-05	1.32E-03	1.09E-03	1.37E-04	[illegible]
1.94E-03	3.00E-03	8.21E-03	-7.70E+00						

TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RO3 CC	O MEO2 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAN	HO2 CARB ARO	HNO3 RAO2 Y	CO CRIC GLY	CO2 MCRC W
1.200E+02	3.429E-01	8.941E-03	2.833E-08	3.814E-01	2.793E-05	1.112E-07	8.839E-05	5.446E-02	1.299E+00	2.100E-02
4.339E+00	2.400E+04	6.878E+00	1.831E-05	3.927E-03	2.900E-06	2.043E-09	8.834E-01	1.017E-06	1.517E-07	2.433E-08
	6.981E-01	8.809E-06	4.546E-09	8.792E-03	1.867E-06	2.558E-02	1.290E-01	5.107E-04	1.563E-02	3.683E-09
	2.396E-02	1.862E-06	1.037E-04	3.032E+02	2.401E+04					
ET RATES	-2.158E-03	1.239E-06	-1.712E-08	5.186E-03	1.984E-05	-1.029E-05	8.336E-06	5.160E-04	3.831E-03	1.792E-04
	-1.930E-04	-4.863E-03	8.178E-06	-4.403E-04	1.421E-06	5.681E-09	4.364E-03	-3.011E-08	-1.260E-07	-8.506E-08
	-1.816E-03	3.182E-06	-1.123E-06	7.900E-05	1.400E-08	5.100E-04	-3.660E-04	-5.277E-06	4.687E-05	5.446E-08
	1.776E-04	6.849E-09	-3.206E-06	0.	5.338E-03					

THE REACTION RATES ARE

1.03E-01	1.03E-01	8.86E-03	7.23E-03	1.07E-04	3.46E-06	7.99E-03	8.34E-04	6.35E-03	[illegible]
7.00E-03	1.93E-04	4.12E-03	2.31E-05	3.21E-06	1.15E-03	2.32E-06	2.82E-06	1.07E-04	[illegible]
1.22E-04	9.78E-06	9.78E-06	9.31E-04	6.39E-04	9.05E-05	9.13E-04	1.09E-04	4.53E-04	[illegible]
1.51E-03	8.19E-05	1.62E-05	7.76E-03	3.49E-05	6.16E-04	6.16E-04	3.73E-04	1.07E-04	[illegible]
1.07E-04	1.40E-03	1.99E-03	1.47E-03	4.43E-07	2.01E-06	1.63E-03	4.16E-04	1.77E-04	[illegible]
6.67E-05	2.01E-05	1.02E-04	3.64E-03	1.37E-03	3.65E-06	8.27E-06	1.03E-05	2.07E-06	[illegible]
2.30E-05	2.13E-04	3.13E-04	1.37E-04	6.83E-03	5.00E-04	1.17E-04	1.74E-05	1.86E-04	[illegible]
3.17E-06	3.00E-03	3.01E-04	-7.70E+00						

TIME INTERVAL	NO2 / H2O / ETH / AERO	NO / PAR / RBO2 / CC	O / MEO2 / PP / RX	O3 / OLE / NRAT / TEMP	NO3 / ACO3 / QQ / M	OH / X / PAN	HO2 / CARB / ARO	HNO3 / RAO2 / Y	CO / CRIG / GLY	CO2 / MCRG / W
[illegible]	2.003E-01	2.864E-03	1.366E-03	6.353E-01	7.998E-05	1.065E-07	1.070E-04	7.935E-02	1.843E+00	3.294E-03
[illegible]	2.400E+04	6.500E+00	5.258E-05	1.777E-02	1.095E-05	2.487E-09	8.214E-01	5.018E-07	2.294E-07	2.113E-08
	5.847E-01	2.022E-03	4.186E-09	1.347E-02	2.629E-06	6.397E-02	1.085E-01	2.463E-04	1.680E-02	2.148E-09
	3.100E-02	2.006E-06	1.698E-05	3.032E+02	2.401E+04					
NET RATES	-2.572E-03	8.724E-05	-6.326E-08	3.099E-03	1.468E-05	-1.130E-06	5.627E-06	2.789E-04	4.247E-03	2.118E-04
	-3.263E-04	-4.785E-03	6.356E-06	-2.687E-04	1.144E-05	-1.753E-07	3.209E-03	8.051E-09	-1.166E-07	-1.072E-07
	-1.852E-03	1.978E-06	-1.425E-06	7.093E-05	1.031E-08	6.914E-04	-3.012E-04	-1.627E-06	-1.066E-08	1.032E-07
	9.420E-05	-2.195E-09	-5.149E-07	0.	1.869E-03					

THE REACTION RATES ARE

[illegible]	6.01E-02	4.73E-02	7.01E-03	3.67E-03	5.62E-06	3.74E-04	3.05E-04	7.37E-08	1.23E-09
[illegible]	3.26E-04	3.71E-03	1.74E-01	1.80E-06	1.07E-03	6.56E-07	6.56E-07	8.10E-05	9.03E-05
[illegible]	4.79E-06	4.79E-06	7.61E-01	8.92E-04	1.19E-04	6.95E-04	1.72E-03	4.17E-04	4.19E-04
[illegible]	7.53E-05	6.43E-03	6.37E-03	1.67E-04	8.47E-04	8.47E-04	5.26E-04	2.63E-04	2.63E-04
2.63E-04	1.64E-03	4.39E-03	3.68E-03	4.72E-06	2.27E-05	7.89E-06	3.68E-04	3.77E-04	7.26E-07
3.39E-03	3.47E-05	1.54E-04	5.51E-03	2.06E-03	3.17E-06	7.18E-06	8.98E-06	1.80E-06	7.06E-03
[illegible]	1.77E-04	1.76E-04	2.12E-05	1.06E-03	6.90E-04	9.39E-05	1.83E-05	2.01E-04	1.82E-04
5.09E-07	3.00E-03	6.35E-04	-7.70E+00						

TIME INTERVAL	NO2 / H2O / ETH / AERO	NO / PAR / RBO2 / CC	O / MEO2 / PP / RX	O3 / OLE / NRAT / TEMP	NO3 / ACO3 / QQ / M	OH / X / PAN	HO2 / CARB / ARO	HNO3 / RAO2 / Y	CO / CRIG / GLY	CO2 / MCRG / W
[illegible]	7.959E-02	9.527E-04	5.425E-09	7.100E-01	9.841E-05	7.010E-08	1.667E-04	8.829E-02	1.796E+00	4.869E-02
8.250E+00	2.400E+04	6.323E+00	9.441E-05	7.105E-03	3.875E-03	1.968E-09	9.567E-01	1.046E-07	2.468E-07	1.147E-08
	4.860E-01	2.718E-05	2.496E-09	1.683E-02	3.061E-06	9.980E-02	9.412E-02	1.880E-04	1.448E-02	1.034E-09
	3.623E-02	1.666E-06	2.759E-06	3.032E+02	2.401E+04					
NET RATES	-1.421E-03	-1.986E-05	-2.908E-08	-1.379E-04	-2.499E-06	-1.769E-06	2.043E-07	4.931E-05	4.100E-03	2.080E-04
	-1.593E-04	-3.945E-03	2.003E-06	-1.051E-04	3.975E-05	-1.835E-07	1.363E-03	2.827E-08	-2.466E-08	-1.208E-08
	-1.408E-03	3.045E-07	-4.673E-07	3.952E-05	4.372E-09	3.990E-04	-1.796E-04	-7.339E-07	-6.176E-05	4.778E-08
	5.867E-05	-1.273E-09	-8.368E-08	0.	-1.182E-03					

THE REACTION RATES ARE

2.39E-02	2.39E-02	1.78E-02	3.16E-03	5.79E-06	4.11E-06	6.54E-04	7.81E-05	6.54E-05	1.36E-10
2.63E-03	1.59E-04	1.91E-03	4.17E-04	6.86E-07	6.65E-04	1.04E-07	1.04E-07	2.09E-05	4.09E-08
4.09E-03	1.58E-06	1.58E-06	4.09E-01	8.38E-04	1.40E-04	3.11E-04	1.84E-06	2.49E-04	2.50E-04
8.30E-04	4.50E-05	9.77E-05	1.94E-03	3.39E-04	6.37E-04	6.37E-01	6.12E-04	3.06E-04	3.06E-04
[illegible]	1.24E-03	6.17E-03	5.74E-03	2.50E-05	6.30E-05	2.82E-06	1.67E-04	4.72E-04	1.31E-07
7.31E-06	2.20E-05	1.65E-04	5.92E-05	2.22E-03	1.72E-06	3.90E-06	4.80E-06	9.75E-07	3.96E-05
1.06E-03	9.90E-05	9.89E-03	4.52E-06	2.26E-06	5.44E-04	6.81E-05	1.02E-05	1.67E-04	1.56E-04
8.20E-08	3.00E-03	7.19E-04	-7.78E+00						

TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RHO2 CG	O HEO3 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH K PAN	HO2 CARB ARO	HNO3 RAO2 Y	CO CRIG GLY	CO2 MGLY W
3.000E+03	2.364E-03	2.098E-04	1.543E-09	6.539E-01	6.033E-03	3.603E-08	1.046E-04	8.871E-03	2.032E+00	5.706E-02
4.336E+00	2.400E+04	6.113E+00	1.071E-04	3.142E-03	1.439E-04	1.313E-09	1.001E+00	3.625E-08	2.093E-07	5.149E-09
	4.133E-01	3.734E-03	1.102E-09	1.037E-03	3.204E-06	1.141E-01	8.602E-03	1.610E-04	1.043E-02	4.748E-10
	3.937E-03	1.163E-06	4.868E-07	3.032E+02	2.401E+04					
NET RATES	-4.673E-04	-8.774E-06	-2.665E-09	-1.784E-03	-1.803E-06	-2.179E-08	-4.169E-07	-1.706E-05	3.767E-03	1.959E-04
	-2.770E-03	-3.119E-08	5.089E-07	-3.073E-05	3.907E-05	-8.280E-08	2.431E-04	3.638E-09	1.764E-08	2.931E-07
	-9.698E-04	-3.040E-08	-9.272E-08	1.892E-03	7.016E-10	6.102E-06	-9.931E-05	1.312E-06	-6.721E-03	7.736E-0[illegible]
	5.100E-03	-4.894E-09	-1.303E-08	0.	-2.233E-03					

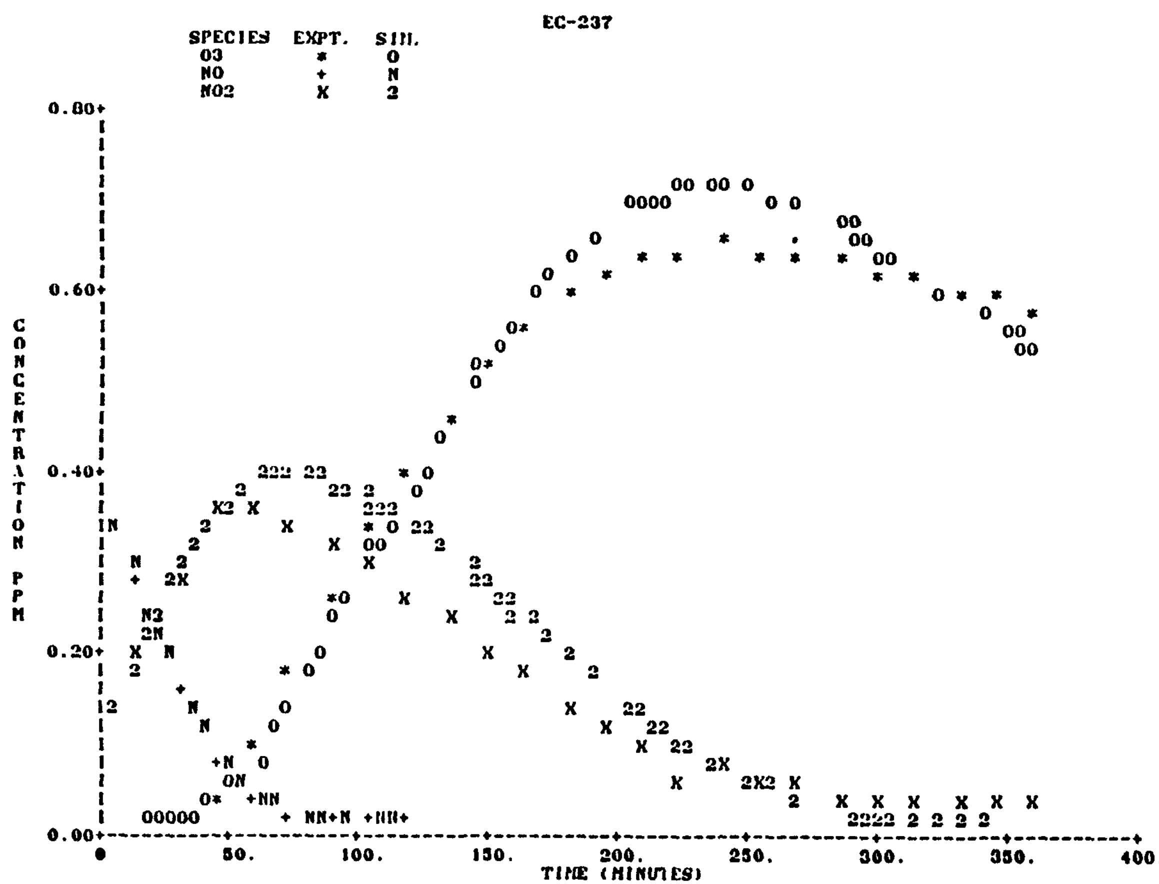
THE REACTION RATES ARE

6.79E-03	6.79E-03	4.92E-03	8.17E-04	4.60E-07	1.96E-06	6.88E-04	1.17E-05	3.39E-03	1.26E-11
4.90E-04	2.78E-05	6.42E-04	5.11E-04	1.09E-07	3.38E-04	1.31E-08	1.31E-08	4.06E-06	1.64E-03
1.64E-05	3.03E-07	3.03E-07	1.04E-04	6.51E-04	1.61E-04	9.47E-05	1.26E-07	1.10E-04	1.10E-04
3.67E-04	1.99E-05	8.89E-03	4.73E-06	4.48E-04	3.51E-04	3.51E-04	6.41E-04	3.20E-04	3.20E-04
3.20E-04	8.03E-04	6.60E-03	6.56E-03	1.08E-04	1.01E-04	7.28E-07	3.79E-05	4.19E-04	1.79E-08
9.32E-07	1.03E-05	1.40E-04	5.02E-05	1.88E-05	7.72E-07	1.75E-06	2.19E-06	4.38E-07	1.90E-05
5.07E-06	4.70E-03	4.75E-03	1.40E-06	7.00E-07	3.40E-04	6.31E-05	3.04E-06	1.16E-04	1.13E-04
1.37E-08	3.90E-03	6.53E-04	-7.78E+00						

TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RHO2 CC	O HEO3 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAN	HO2 CARB ARO	HNO3 RAO2 Y	CO CRIG GLY	CO2 MGLY W
3.600E+03	9.249E-03	1.356E-04	6.308E-10	5.423E-01	3.466E-03	2.366E-08	1.760E-04	8.733E-02	2.250E+00	6.924E-02
5.517E+00	3.400E+04	5.945E+00	1.634E-04	1.610E-03	8.244E-04	1.035E-09	9.978E-01	1.460E-08	1.570E-07	2.203E-09
	3.662E-01	2.396E-03	6.141E-10	1.801E-03	3.193E-06	1.074E-01	8.116[illegible]03	2.212E-04	6.933E-03	2.888[illegible]-10
	4.280E-02	7.652E-07	7.491E-08	3.032E+03	2.401E+04					
NET RATES	-4.383E-08	-4.622E-07	-3.498E-11	-1.726E-03	-1.941E-07	3.199E-09	-1.033E-07	-2.823E-08	9.830E-03	1.833E-04
	-4.640E-06	-3.749E-03	1.162E-07	-1.618E-05	1.373E-06	-3.819E-10	-2.710E-04	-1.060E-10	5.201E-09	4.375E-10
	-6.994E-04	-4.624E-08	-4.022E-09	4.979E-06	-8.664E-10	-2.077E-04	-6.960E-05	-3.080E-07	-4.609E-03	1.827E-10
	5.836E-03	-5.098E-09	-3.272E-09	0.	-2.075E-03					

THE REACTION RATES ARE

3.77E-03	2.77E-03	1.91E-03	2.77E-04	7.81E-08	1.05E-06	5.21E-04	3.06E-06	2.34E-03	2.76E-12
9.37E-05	4.64E-06	2.07E-04	4.63E-04	7.49E-08	2.11E-04	2.75E-09	2.75E-09	1.61E-06	7.02E-06
7.02E-06	1.39E-07	1.39E-07	1.04E-04	4.77E-04	1.67E-04	3.90E-05	2.38E-08	6.14E-05	6.14E-05
2.03E-04	1.11E-05	6.80E-03	1.58E-06	4.43E-04	2.24E-04	2.24E-04	6.39E-04	3.19E-04	3.19E-04
3.19E-04	6.15E-04	6.00E-03	6.17E-03	2.28E-04	1.15E-04	2.56E-07	1.17E-05	3.14E-04	3.72E-09
1.69E-07	4.36E-06	1.05E-04	3.78E-05	1.42E-05	3.43E-07	7.77E-07	9.71E-07	1.94E-07	1.15E-05
3.07E-06	2.08E-03	2.08E-03	9.00E-07	4.50E-07	1.91E-04	7.20E-05	1.64E-06	7.65E-05	7.49E-05
2.35E-09	3.00E-03	5.42E-04	-7.78E+00						


EC-237
SPECIES EXPT. SIM.
O3 * O
NO + N
NO2 X 2
CONCENTRATION PPM
0.00
0.20
0.40
0.60
0.80
50.
100.
150.
200.
250.
300.
350.
400.
TIME (MINUTES)

APPENDIX E

EXAMPLE USE OF VARIABLE PHOTOLYSIS AND PRINT OPTIONS

APPENDIX E

EXAMPLE USE OF VARIABLE PHOTOLYSIS AND PRINT OPTIONS

```
 33   1                                      14   60    7                 1
          1          12          17          18         19         24         25
.016       .13        .29         .39         .46        .5         .52
.33        .52        .5          .46         .39        .29        .13
 016
NO2                  1        NO           O                       1.
O                    2        O3                                   4400000.
.3     NO            3        NO2                                  23.8        1450.
NO2    O3            4        NO3                                  .0474       2450.
NO2    O             5        NO                                   13000.
NO3    NO            62.      NO2                                  28000.
NO2    NO3           7        N2O5                                 3910.       -861.
N2O5                 8        NO2          NO3                     6.85        10320.
N2O5                 92.      HNO3                                 .02
NO     NO2           102.     HONO                                 .0000003
HONO   HONO          11       NO           NO2                     .000015
HONO                 12       OH           NO                      .18
OH     NO2           13       HNO3                                 16000.
OH     NO            14       HONO                                 16000.
HO2    NO            15       NO2          OH                      12000.
HO2    HO2           16       HOOH                                 7400.
HOOH                 172.     OH                                   .00079
O3                   18       O1D                                  .0027
O3                   19       O                                    .069
O1D                  20       O                                       4.45E10 -97.4
O1D                  212.     OH                                       6.8E09
OH     O3            22       HO2                                  76.9        1000.
O3     HO2           23       OH                                   2.93        580.
HCHO                 24                                            .0046
HCHO                 252.     HO2                                  .003
HCHO   OH            26       HO2                                  14000.
MEO2   NO            28       MEO          NO2                     12000.
MEO                  29       HCHO         HO2                     200000.
MEO    NO2           30                                            15000.
MEO    NO2           31       HCHO         HONO                    4400.
MEO2   HO2           32                                            7400.
REACTIVITY 1000 PPMC METHANE
  3                                     60.        60.
NO          NO2          CH4
.1          .1           1000.
            840.         303.        .01
PLOT
REACTIVITY 1000 PPMC METHANE
      1         0.00 0.40 0.80 1.20 1.40 0.          1.6        0.          880.
O3      0
            BLANK CARD
            BLANK CARD
```

REACTIONS					=					RATE CONSTANT	ACT. ENERGY (K)
1	NO2				=		NO	+	O	1.000E+00	-0.
2	O				=		O3			4.400E+06	-0.
3	O3	+	NO		=		NO2			2.300E+01	1.450E+03
4	NO2	+	O3		=		NO3			4.740E-02	2.450E+03
5	NO2	+	O		=		NO			1.300E+04	-0.
6	NO3	+	NO		=	2	NO2			2.800E+04	-0.
7	NO2	+	NO3		=		N2O5			3.910E+03	-8.610E+02
8	N2O5				=		NO2	+	NO3	6.850E+00	1.032E+04
9	N2O5				=	2	HNO3			2.000E-02	-0.
10	NO	+	NO2		=	2	HONO			3.000E-07	-0.
11	HONO	+	HONO		=		NO	+	NO2	1.500E-05	-0.
12	HONO				=		OH	+	NO	1.800E-01	-0.
13	OH	+	NO2		=		HNO3			1.600E+04	-0.
14	OH	+	NO		=		HONO			1.600E+04	-0.
15	HO2	+	NO		=		NO2	+	OH	1.200E+04	-0.
16	HO2	+	HO2		=		HOOH			7.400E+03	-0.
17	HOOH				=	2	OH			7.900E-04	-0.
18	O3				=		O1D			2.700E-03	-0.
19	O3				=		O			6.900E-02	-0.
20	O1D				=		O			4.450E+10	-9.740E+01
21	O1D				=	2	OH			6.800E+09	-0.
22	OH	+	O3		=		HO2			7.690E+01	1.000E+03
23	O3	+	HO2		=		OH			2.930E+00	5.800E+02
24	HCHO				=					4.600E-03	-0.
25	HCHO				=	2	HO2			8.000E-03	-0.
26	HCHO	+	OH		=		HO2			1.400E+04	-0.
27	CH4	+	OH		=		MEO2			1.110E+01	1.710E+03
28	MEO2	+	NO		=		MEO	+	NO2	1.200E+04	-0.
29	MEO				=		HCHO	+	HO2	2.000E+05	-0.
30	MEO	+	NO2		=					1.500E+04	-0.
31	MEO	+	NO2		=		HCHO	+	HONO	4.400E+03	-0.
32	MEO2	+	HO2		=					7.400E+03	-0.

Output Results

```
                         REACTIVITY 1000 PPMC METHANE
INITIAL CONCENTRATION
            NO          NO2          CH4
         1.000E-01   1.000E-01   1.000E+03
THE TEMPERATURE OF THE CELL WAS = 3.03E+02 AND THE ERROR TOLERANCE = 1.00E-02
THE RATE CONSTANTS USED WERE
         1.000E+00   4.400E+06   2.879E+01   5.429E-02   1.300E+04   2.000E+04   5.728E+03   1.218E+01   2.000E-02   5.000E-07
         1.300E-05   1.800E-01   1.600E+04   1.600E+04   1.200E+04   7.400E+03   7.900E-04   2.700E-03   6.900E-02   4.426E+10
         6.000E+09   8.120E+01   3.026E+00   4.600E-03   3.000E-03   1.400E+04   1.220E+01   1.200E+04   2.000E+05   1.500E+04
         4.400E+03   7.400E+03

THE PHOTOLYSIS REACTIONS ARE
            1          12          17          18          19          24          25
THE PHOTOLYSIS RATIOS OF EACH OF THE REACTIONS ABOVE ARE
        1.000E+00   1.800E-01   7.900E-04   2.700E-03   6.900E-02   4.600E-03   3.000E-03

THE NO2 PHOTOLYSIS NUMBERS IN INTERVALS OF  60 TIME UNITS ARE
     1.600E-02   1.300E-01   2.900E-01   3.900E-01   4.600E-01   5.000E-01   5.200E-01   5.300E-01   5.200E-01   5.000E-01
     4.60 [illegible]-01   3.900E-01   2.900E-01   1.300E-01   1.600E-02
```

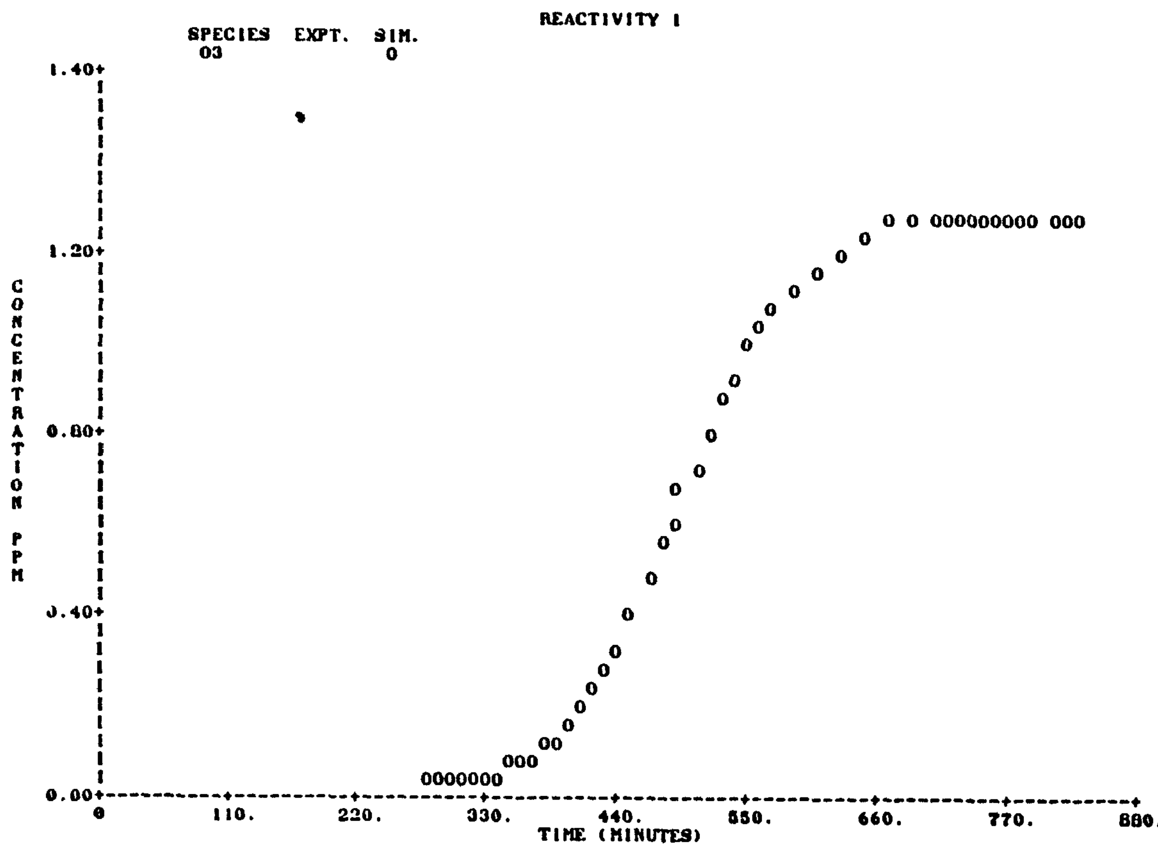
Output Results (Continued)

[illegible]	NO2 HOOH	NO O1D	O HCHO	O3 CH4	NO3 MEO2	N2O5 MEO	HNO3 TEMP	HONO M	OH	HO2
0. 1.[illegible]	1.600E-01 0.	1.000E-01 0.	0. 0.	0. 1.000E+03	0. 0.	0. 0.	0. 3.030E+02	0. 1.000E+03	0.	0.
6.[illegible] 3.[illegible]	9.329E-02 2.244E-13	1.047E-01 3.127E-17	2.025E-09 3.924E-05	4.551E-03 1.000E+03	8.020E-09 1.641E-09	2.344E-07 1.022E-11	5.302E-06 3.030E+02	4.444E-06 1.000E+03	1.690E-10	1.651E-09
1.[illegible] 3.793E+00	9.070E-02 2.012E-11	1.092E-01 1.427E-16	6.023E-09 4.579E-04	9.301E-03 1.000E+03	1.497E-08 1.221E-08	4.165E-07 7.930E-11	5.960E-05 3.030E+02	3.064E-05 1.000E+03	1.311E-09	1.272E-08
1.[illegible] 1.[illegible]	9.025E-02 3.494E-10	1.093E-01 2.561E-16	8.075E-09 2.200E-03	1.243E-02 1.000E+03	1.988E-08 4.205E-08	5.502E-07 2.790E-10	2.098E-04 3.030E+02	9.503E-05 1.000E+03	4.614E-09	4.647E-08
2.[illegible] 1.[illegible]	9.688E-02 4.490E-09	1.017E-01 4.108E-16	1.025E-08 7.586E-03	1.689E-02 1.000E+03	3.113E-08 1.409E-07	9.237E-07 8.533E-10	1.069E-03 3.030E+02	2.414E-04 1.000E+03	1.412E-08	1.579E-07
3.[illegible] 4.[illegible]	1.176E-01 5.230E-08	7.818E-02 7.631E-16	1.359E-08 2.164E-02	2.886E-02 1.000E+03	8.394E-08 4.688E-07	3.019E-06 2.177E-09	3.540E-03 3.030E+02	4.731E-04 1.000E+03	3.609E-08	5.442E-07
[illegible] 2.[illegible]	1.403E-01 7.787E-07	4.000E-02 2.002E-15	1.813E-08 5.076E-02	7.283E-02 9.999E+02	5.216E-07 1.890E-06	2.365E-05 4.475E-09	1.052E-02 3.030E+02	5.625E-04 1.000E+03	7.441E-08	2.302E-06
4.[illegible] 4.516E+00	1.509E-01 2.409E-05	1.372E-02 6.114E-15	2.076E-08 1.043E-01	2.182E-01 9.999E+02	4.784E-06 1.141E-05	2.296E-04 9.289E-09	2.701E-02 3.030E+02	4.421E-04 1.000E+03	1.847E-07	1.454E-05
4.[illegible] 8.022E+00	1.301E-01 1.130E-03	3.832E-03 1.552E-14	2.012E-08 2.000E-01	5.644E-01 9.997E+02	3.606E-05 7.164E-05	1.444E-03 1.644E-08	5.958E-02 3.030E+02	3.165E-04 1.001E+03	2.771E-07	9.388E-05

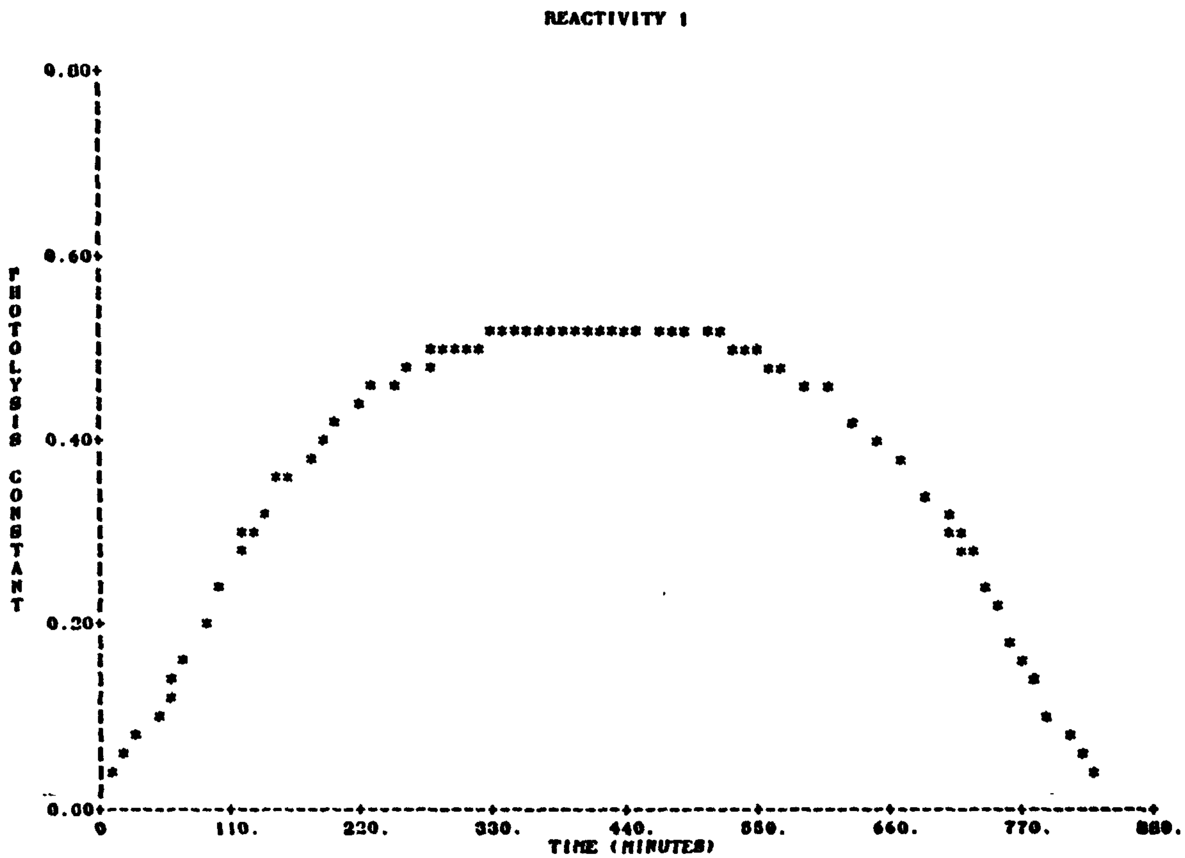
Output Results (Continued)

TIME LAT ANG	HO2 HOOH	NO O1D	O HCHO	O3 CH4	NO3 MEO2	N2O5 MEO	HNO3 TEMP	HONO M	OH	NO2
[illegible]E+03 6.[illegible]E+00	9.397E-03 1.003E-03	1.311E-03 3.403E-14	1.839E-08 3.731E-01	9.390E-01 9.998E+03	1.111E-04 1.420E-04	3.201E-03 1.277E-08	9.311E-02 3.030E+02	1.414E-04 1.001E+03	2.262E-07	1.730E-04
6.[illegible]E+03 2.[illegible]0E-01	6.048E-03 2.436E-02	7.973E-04 3.810E-14	1.879E-08 2.909E-01	1.188E+00 9.994E+03	1.886E-04 1.013E-04	3.972E-03 8.610E-09	1.170E-01 3.030E+02	6.566E-05 1.001E+03	1.627E-07	1.860E-04
6.600E+03 2.[illegible]0E+01	5.027E-03 3.833E-03	4.388E-04 2.605E-14	1.244E-08 2.831E-01	1.261E+00 9.993E+03	3.739E-04 2.099E-04	4.216E-03 5.498E-09	1.346E-01 3.030E+02	3.380E-05 1.001E+03	1.123E-07	1.698E-04
7.200E+03 1.230E+[illegible]0	3.867E-03 4.000E-02	2.101E-04 1.983E-14	8.436E-09 2.709E-01	1.298E+00 9.992E+02	4.007E-04 2.307E-04	4.472E-03 2.998E-09	1.487E-01 3.030E+02	1.729E-05 1.001E+03	6.880E-08	1.318E-04
7.[illegible]0E+03 1.[illegible]E+00	1.801E-03 5.173E-03	3.390E-05 8.839E-15	3.242E-09 2.567E-01	1.286E+00 9.993E+03	1.118E-03 3.360E-04	6.174E-03 6.821E-10	1.624E-01 3.030E+02	7.622E-06 1.001E+03	2.286E-08	8.858E-06
8.[illegible]0E+03 [illegible]70E-01	2.162E-03 5.191E-03	1.676E-07 1.139E-15	3.876E-10 2.409E-01	1.270E+00 9.992E+03	6.347E-03 6.961E-04	4.219E-03 6.999E-12	1.769E-01 3.030E+03	4.079E-06 1.001E+03	1.976E-09	3.7[illegible]E-06

Output Results (Continued)



Output Results (Continued)



Output Results (Concluded).

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

Mechanisms that describe the formation of photochemical smog are developed using a computer modeling technique directed toward the simulation of data collected in two smog chambers: an indoor chamber and a dual outdoor chamber. The results of simulating 164 different experiments are presented in Vol. 1. Individual compounds for which specific experiments were simulated and mechanisms developed include the following: formaldehyde, acetaldehyde, ethylene, propylene, butane, and toluene. Experiments in both chambers were simulated for all these compounds. The mechanisms reported describe the decay of the precursor organic compound, formation and decay of secondary organic compounds, conversion of nitrogen oxides, formation of nitrates, and the appearance and decay of ozone. Special emphasis is given to the chemistry of toluene. Also included is a study of a generalized smog-based or carbon-bond mechanism developed in a previous study. Volume 2 contains the user's manual and coding for a chemical kinetics computer program, CHEMK.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
* Air pollution		13B
* Reaction kinetics		07D
* Photochemical reactions		07E
* Test chambers		14B
* Mathematical models		12A
* Computerized simulation		09B

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS *(This Report)* UNCLASSIFIED	21. NO. OF PAGES 113
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