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GENKIN-I

A General Kinetics Code - Atmospheric Applications

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Introduction

This report describes a first version of a multipurpose, semi-automatic code for setting up and reliably solving large coupled sets of stiff, non-linear kinetic equations. The present code, GENKIN-I, is a product of a long period of kinetic theoretic and computational research and development spanning numerous application areas. This first version is dedicated primarily to atmospheric chemical kinetics.

Inasmuch as many of the forward-looking activities in applied physics are kinetic in nature, extensions of the basic elements of this capability to other application areas will undoubtedly be made as the needs occur.

A major feature of GENKIN-I is that it utilizes advanced variants^{1,2} of the basic GEAR method³ to stably and accurately solve large sets of stiff non-linear differential equations. From the beginning LLL's involvement and development of systematic methods for stiff systems has been intertwined with the present code.^{4,5} Another major feature of GENKIN-I is that, from a given reaction library, the user can "dial" arbitrary reaction sets that are then automatically compiled into an appropriate executable differential equation solution code. This eliminates tedious and error-prone hand coding of complex reaction networks. The present reaction library^{6,7} that interfaces with the general kinetics code emphasizes atmospheric chemical and radiative interaction processes. Evaluated rate data is incorporated wherever possible, and estimated rate data is supplied for unevaluated processes. Reaction libraries for other applications, such as gas lasers, ionic systems, combustion kinetics, coal and other fuel conversion processes,

and biological kinetics can be interfaced to the general kinetics code, as interest and program needs dictate. GENKIN-I has a number of flexibility features for altering reaction rate data from library values, graphical and tabular output arrays, and for solar flux evaluations at arbitrary latitude, longitude, time of year, and atmospheric composition. There are three major operation modes of GENKIN-I. The first applies to cases in which all reaction rate coefficients are constant in time. The other two modes are for cases with time varying reaction rate coefficients: A diurnal mode internally computes instantaneous solar flux values for a purely absorbing atmosphere at arbitrary altitude, latitude, month, day, local time, and atmospheric composition. The remaining mode allows the user to incorporate arbitrary time variations of temperature and/or pressure in chemical reaction rates as well as allowing the user to incorporate arbitrary time dependent sources, sinks, and entrainment factors.

It should be recognized that kinetics calculations are but one element of more general transport-kinetic theories. Thus, purely kinetics codes find their greatest utility as rapid-turnaround tools for in-depth studies of kinetic aspects of reaction networks, per se. Of course, kinetics calculations take on more rigorous physical modeling interpretations in systems where transport effects are not important.

I. Object of the Code

The kinetic evolution of a system of reactive species can be analytically described in terms of ordinary differential equations:

$$\frac{dy_i(t)}{dt} = R_i(y_j(t), \{QK(t)\}) + S_i(t) \quad i, j = 1, N, \quad (1)$$

where $y_i(t)$ is the number density (cm^{-3}) of the i^{th} specie at time, t . The reaction terms, $R_i(y_j(t), \{QK(t)\})$ are linear combinations of products of reaction rate coefficients belonging to the set $\{QK(t)\}$, times one, or more, of the $y(t)$'s. External sources and/or sinks are represented by $S_i(t)$. The object of this code is to set up and reliably solve non-linear sets of equations of the form given by (1) for atmospheric chemical species and their reaction processes.

Basically, the code operates in two stages, each having its own input deck. The first stage sets up the appropriate differential equations for user-specified reaction library numbers⁶ and generates other internal information needed by the (second) solution stage. Figure C-1 of Appendix C is a schematic representation of the more important elements of the overall code.

The input decks provided by the user are INRATE for the problem set-up stage and INSTIF for the problem solution stage. The setup program, CRNCIT, requires (in addition to INRATE) the presence of the library files CARLIB for a catalog of reaction processes, per se, and QKCOEFF for the corresponding reaction rate coefficients.* Execution of CRNCIT produces the output files OUTPRIN and CRACK1. OUTPRIN contains the compiled problem information for the user, and CRACK1 contains the compiled problem information required by the appropriate solution program option. There are presently three available solution program options, CRUNCH, DRUNCH, and ERUNCH, whose functions will be described in the next section. In addition to INSTIF, all solution program options require the presence of the file, CRACK1, generated in the setup

* Alteration options for the library rate coefficient values are described later.

stage. All solution program options produce tabular output files HSP0, HSP1, etc., DD80 graphs, and a controllee file, KINIT - of the solution program. The solution program option, DRUNCH, has an additional requirement. The file, NEWRDH containing microscopic radiative cross section data must be present at execution time.

II. Solution Program Options in Brief

The major factors that distinguish the solution program options are the inclusion or neglect of external sources and/or sinks, $S_i(t)$, and the time dependence or independence of the chemical and photochemical reaction rate coefficients, $\{QK(t)\}$. Briefly the option, CRUNCH, deals with problems for which $S_i(t) = 0$ and all chemical and photochemical reaction rate coefficients are constant. The option, DRUNCH, applies to diurnal problems with $S_i(t) = 0$. In this case all chemical reaction rate coefficients are taken to be constant, but photodissociation reaction rate coefficients are evaluated, in-line, for appropriate instantaneous solar flux values. The option ERUNCH is for cases in which $S_i(t)$ is non-zero and chemical rates are time dependent. Only for this ERUNCH option does the user have to provide the solution code with additional subroutines. ERUNCH is useful for entraining systems with time varying temperatures and/or pressures. It does not contain subroutines for calculating diurnal photodissociation rates.

III. Atmospheric Kinetic Theory - Selected Aspects

The basic atmospheric reaction processes considered in GENKIN-I are thermal chemical and photochemical interactions. Primary attention has been given to charge neutral species, but reactions of ionized species can also

be treated. Thus, for practical purposes the individual terms entering $R_i(y_i(t), \{QK(t)\})$ are so-called one, two, and three-body reaction processes. One-body reaction rates have the form $QK(t) y_i(t)$. Two-body rates have the form $QK(t) y_i(t) y_j(t)$, and three-body rates usually have the form $QK(t) y_i(t) y_j(t) y_k(t)$. GENKIN-I also treats pressure dependent rates of the form $QK(t)[y_i(t) y_j(t) y_k(t)/(\alpha(T(t)) + y_k(t))]$.

Thermal Chemical Rate Coefficients

These coefficients, $C(T(t))$, at temperature $T(t)$ are generally of the form

$$C(T(t)) = A[T(t)^B] e^{-C/T(t)}, \quad (2)$$

where A , B , and C are constant coefficients. The two and three-body rates are of the form $C(T(t)) y_i(t) y_j(t)$ and $C(T(t)) y_i(t) y_j(t) y_k(t)$, respectively. Chemical reaction rate coefficients that include the pressure dependence of $y_k(t)$ (cm^{-3}) have the form

$$C_{p(k)}(T(t)) = \frac{\{A[T(t)^B] e^{-C/T(t)}\} y_k(t)}{[DA(e^{-DC/T(t)}) + y_k(t)]}, \quad (3)$$

where A , B , C , DA and DC are constant coefficients. Thus, in the "high pressure" limit ($y_k(t) \gg DA(e^{-DC/T(t)})$) the three-body rate, $C_{p(k)}(T(t)) y_i(t) y_j(t) y_k(t)$, reduces to a true two-body rate; and in the low pressure limit ($y_k(t) \ll DA(e^{-DC/T(t)})$) a conventional three-body rate expression obtains.

Photodissociation Rate Coefficients

Photodissociation rates are considered as one-body reactions in GENKIN-I. These rates are of the form $J_{i \rightarrow j}(t) y_i(t)$, where $J_{i \rightarrow j}(t)$ is the photodissociation rate coefficient for specie i undergoing transition to specie j .

Most models assume (as do we) that the solar flux can be obtained from a one-dimensional solution of the purely absorbing radiative transfer equation, with the sun as the only source.* Generally, $J_{i \rightarrow j}(t)$ also has parametric dependences upon a particular altitude, z_p , as well as on the month, day, latitude, longitude, and atmospheric composition $N_j(t)$, all denoted by P . With this in mind our photodissociation rate coefficients are evaluated according to the following expressions:

$$J_{i \rightarrow j}(z_p, P, t) \equiv \int_{\text{all } \lambda} d\lambda \sigma_T^i[\lambda, T(z_p)] Q_\lambda(i \rightarrow j) I_\lambda(z_p, N_j(t), P, t) \quad , \quad (4)$$

Where $I_\lambda(z_p, N_j(t), P, t) d\lambda \equiv$ radiation intensity (photons $\text{cm}^{-2} \text{sec}^{-1}$) in the wavelength interval $d\lambda$ about λ , at altitude z_p and time t for the parameters P , and $\sigma_D^i[j, \lambda, T(z_p)] \equiv$ microscopic cross-section (cm^2) for photodissociation of the i^{th} type of specie to produce the j^{th} type of specie at temperature $T(z_p)$. The often-used quantum yield, $Q_\lambda(i \rightarrow j)$, is the ratio of $\sigma_D^i[j, \lambda, T(z_p)]$ to the total absorption cross section, $\sigma_T^i[\lambda, T(z_p)]$. The radiation intensity obtained from a one-dimensional solution of the purely absorbing radiative transfer equation, with the sun as the only source is

$$I_\lambda(z_p, N_j(t), P, t) = I_\lambda(\infty) \exp[-\tau(z_p, N_j(t), P, t)] \quad . \quad (5)$$

The optical depth, τ , is defined by

$$\tau(z_p, N_j(t), P, t) \equiv \int_{z_p}^{\infty} dz \sum_j N_j(z, t) \sigma_T^j[\lambda, T(z)] \sec \theta(P, t) \quad (6)$$

where $\theta(P, t)$ is the solar zenith angle at time t for the month, day, latitude, and longitude specified by the parameters, P . See Appendix A for

* In a separate paper⁸ this assumption is examined

zenith angle formulae. Appendix B gives a table of the individual photo-dissociation processes ($i \rightarrow j$), the wavelength bins ($\Delta\lambda, \lambda$) and values of the solar flux values outside the earth's atmosphere (extrapolated to 1 A.U.), $I_\lambda(\infty)$, used in GENKIN-I. The fully time dependent, instantaneous expressions (4)-(6) are incorporated in the diurnal option, DRUNCH. But for the constant rate coefficient option, CRUNCH, it is necessary to use some form of photo-dissociation rates that are constant. Most often, daily averaged values are used, which are defined at altitude, z_p , by

$$\langle J_{i \rightarrow j}(z_p, P, t) \rangle \equiv \int_{\text{all } \lambda} d\lambda \sigma_T^i[\lambda, T(z_p)] Q_\lambda(i \rightarrow j) \langle I_\lambda(z_p, N_j, P) \rangle, \quad (7)$$

where the daily averaged solar flux has been defined by

$$\langle I_\lambda(z_p, N_j, P) \rangle \equiv \left[\int_{t_1}^{t_1 + t_d} dt I_\lambda(z_p, N_j(t), P, t) \right] / t_d, \quad (8)$$

with

$$t_d \equiv 86400 \text{ seconds/day} \quad (9) \quad (9)$$

In the absence of temperature dependent data, $\sigma_T^i(\lambda, T(z_p))$ was treated as a time independent quantity in (7). A separate code is available⁹ for computing $\langle I_\lambda(z_p, N_i, P) \rangle$ and the $\langle J_{i \rightarrow j}(z_p, P, t) \rangle$ for the processes contained in the GENKIN-I reaction library, CARLIB.

Finally, the atmospheric composition profiles, denoted by $N_j(z, t)$ in Eq. (6), are required in order to evaluate the above radiative quantities. Unless the user specifies his own profiles, the diurnal option of GENKIN-I automatically incorporates column density data for O_2 and O_3 given in

Appendix C. The O_2 data as well as atmospheric temperature and density profiles is taken from the U.S. Standard Atmosphere¹⁰. The O_3 column densities are rather variable in the atmosphere. Our choice of values for O_3 column densities in GENKIN-I is arbitrarily taken from data suggested by J. Chang.¹¹

For stratospheric applications, which have been emphasized to date, it is necessary to treat the high resolution Schumann-Runge bands of O_2 (175nm-205nm) with special care because of the important "window" at about 200 nm. The radiation intensity at altitude z_p is given, to a first approximation, in this spectral interval by

$$I_{\lambda}(z_p, P, t) = I_{\lambda}(\infty) \exp \left\{ - \int_{z_p}^{\infty} dz \left[N_{O_2}(z, t) \sigma_T^{O_2}[\lambda, T(z)] + N_{O_3}(z, t) \sigma_T^{O_3}[\lambda, T(z)] \right] \sec \theta(P, t) \right\} \quad (9)$$

Solar flux data for $I_{\lambda}(\infty)$ is resolved only over fairly broad spectral "bins" of wavelength width Δ ; so one uses "group-averaged" radiation intensities, $I_{\Delta}(z_p, P, t)$, defined by

$$I_{\Delta}(z_p, P, t) = \Phi_{\Delta}(\infty) R_{O_2, O_3}(\Delta, z_p, P, t) \quad (10)$$

where the O_2 , O_3 reduction factor is defined by

$$R_{O_2, O_3}(\Delta, z_p, P, t) \equiv \frac{1}{\Delta} \int_{\Delta} d\lambda \exp \left\{ - \int_{z_p}^{\infty} dz \left[N_{O_2}(z, t) \sigma_T^{O_2}[\lambda, T(z)] + N_{O_3}(z, t) \sigma_T^{O_3}[\lambda, T(z)] \right] \sec \theta(P, t) \right\} \quad (11)$$

and

$$\phi_{\Delta}(\infty) = \int_{\Delta} d\lambda I_{\lambda}(\infty) = I_{\Delta}(\infty) \cdot \Delta \quad (12)$$

The fact that available ozone absorption cross section data is temperature independent and only resolved over bins, Δ , comparable to the solar flux data* allows R_{O_2, O_3} to be factored as

$$R_{O_2, O_3}(\Delta, z_p, P, t) = R_{O_2}(\Delta, z_p, P, t) R_{O_3}(\Delta, z_p, P, t) \quad (13)$$

with

$$R_{O_3}(\Delta, z_p, P, t) \equiv \exp \left[-\sigma_T^{O_3}(\Delta) \cdot N_{O_3}(z_p, P, t) \right] \quad (14)$$

$$N_{O_3}(z_p, P, t) \equiv \int_{z_p}^{\infty} dz N_{O_3}(z, t) \sec \theta(P, t) \quad (15)$$

$\equiv$ ozone column density (cm^{-2})

and

$$R_{O_2}(\Delta, z_p, P, t) \equiv \frac{1}{\Delta} \int_{\Delta} d\lambda \exp \left[- \int_{z_p}^{\infty} dz N_{O_2}(z, t) \sigma_T^{O_2}[\lambda, T(z)] \sec \theta(P, t) \right] \quad (16)$$

The O_2 photodissociation rate is given by

$$J_{O_2 \rightarrow O}(z_p, P, t) = \sum_{\text{all } \Delta} J_{O_2 \rightarrow O}(\Delta, z_p, P, t) \quad (17)$$

* We use Ackerman's¹² (1970) data for $\phi_{\Delta}(\infty)$. See Appendix B

where

$$J_{O_2}(\Delta, z_p, P, t) = I_{\Delta}(\infty) R_{O_2}(\Delta, z_p, P, t) \int_{\Delta} d\lambda \sigma_T^{O_2}[\lambda, T(z_p)] Q_{\lambda}(O_2 \rightarrow O) \\ \times \exp \left[- \int_{z_p}^{\infty} dz N_{O_2}(z, t) \sigma_T^{O_2}[\lambda, T(z)] \sec \theta(P, t) \right] . \quad (18)$$

The ozone absorption coefficient assumes relatively large values at wavelengths greater than about 210 nm, and the O_2 Schumann-Runge band absorption (super-imposed on an underlying continuum) is known to be relatively large at wavelengths shorter than about 195 nm. The strength and position of this lower cutoff is of central importance to ultraviolet (u.v.) solar fluxes and to photodissociation rates. Because there may be literally hundreds of O_2 spectral lines (having peaks very much greater in magnitude than the valleys) in a bin, Δ , in the Schumann-Runge band region, and because this absorption spectrum is temperature dependent, there is an obvious need for a careful evaluation of $R_{O_2}(\Delta, z_p, P, t)$ for temperature-dependent atmospheres as a function of altitude and solar zenith angle. To date this need has been met best by R. D. Hudson¹³, whose work is incorporated in this code at a constant temperature, T_c , at all altitudes. That is,

$$R_{O_2}(\Delta, z_p, P, t) \approx \frac{1}{\Delta} \int_{\Delta} d\lambda \exp \left[- \sigma_T^{O_2}(\sigma, T_c) \int_{z_p}^{\infty} dz \right. \\ \left. \times N_{O_2}(z, t) \sec \theta(P, t) \right] \quad (19)$$

or

$$R_{O_2}(\Delta, z_p, P, t) = \frac{1}{\Delta} \int_{\Delta} d\lambda \exp - \left[\sigma_T^{O_2}(\lambda, T_c) N_{O_2}(z_p, P, t) \right] \quad (20)$$

and

$$J_{O_2 \rightarrow O}(\Delta, z_p, P, t) = I_{\Delta}(\infty) R_{O_3}(\Delta, z_p, P, t) \int_{\Delta} d\lambda \sigma_T^{O_2}(\lambda, T_c) \\ \times Q_{\lambda}(O_2 \rightarrow O) \exp - \left[\sigma_T^{O_2}(\lambda, T_c) N_{O_2}(z_p, P, t) \right] \quad (21)$$

This section can be concluded with a few remarks concerning multi-specie treatment of bands.

It is well recognized that some atmospheric trace species have spectral bands that lie in the O_2 Schumann-Runge band region. For cases where these other species have non-negligible individual optical depths, compared to O_2 , the computation of the solar flux and of photodissociation rates becomes greatly complicated. For now the total microscopic optical depth (summed over all species) at all high-resolution integration points, λ_k , must be computed in-line for the specific model atmosphere of interest. To date, this more complex computation has been done in only one instance of which we're aware. That is the case of NO bands examined by Cieslik and Nicolet.¹⁴

Another candidate for more detailed treatment is NH_3 , perhaps, in primeval atmospheres. Also SO_2 and CO have bands in the 200 nm region. The point of importance to users of our codes is that there is presently no treatment of spectral bands in the solar flux attenuation calculations except for O_2 .

IV. Code Description and Information for Users

The code description will be divided into two major segments of similar form - one segment is devoted to the set-up stage and the other to the solution stage. In each segment input instructions will be given first, including definition of the variables. Then a detailed description of the major code functions and options will follow, and finally the output description will be given.

A. The Set-Up Program

The heart of the setup stage is a program named CRNCIT. This program is available only as a binary controllee deck. The successful execution of CRNCIT requires an input file, INRATE, made up by the user and the library files CARLIB and QKCOEFF to be present.

CRNCIT is executed under "ORDER" by typing (on the teletype):

CRNCIT / T V
Formats for "INRATE"

There are twelve types of input cards to be used in the order that follows, except as deletions may be allowed. No terminator card is required.

Type 1 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	NRCHEM
-----	--------

Type 2 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	ICHEM
-----	-------

Type 3 Format (4I4, E12.5)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	NG
5-8	NFINE
9-12	KDEC

Type 3 cont.

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

13-16	ISDEC
-------	-------

17-28	YDEC
-------	------

Type 4 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	NPIC1
-----	-------

Type 5 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	NPRIN
-----	-------

Type 6 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	NRATE
-----	-------

Type 7 Format (20I4)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	NRK(1)
-----	--------

5-8	NRK(2)
-----	--------

.	.
---	---

.	.
---	---

etc.	etc.
------	------

Type 8 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-4	NELIM
-----	-------

Type 9 Format (8A10) (left adjusted)

<u>Columns</u>	<u>Variable Name</u>
----------------	----------------------

1-10	ENAM(1)
------	---------

11-20	ENAM(2)
-------	---------

.	.
---	---

etc	etc
-----	-----

Type 10 Format (2E12.5)

<u>Columns</u>	<u>Variable Name</u>
1-12	ALT
13-24	TEMP

Type 11 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
1 4	NCHANGE

Type 12 Format (I4, E20.13, I4)

<u>Columns</u>	<u>Variable Name</u>
1-4	K
5-24	RMULT
25-28	IREPLACE

Definition of "INRATE" Variables

NRCHEM $\equiv$ Mode indicator for solution code options. It operates in tandem with ICHEM. The option designations are given in connection with ICHEM.

ICHEM $\equiv$ Mode indicator for solution code options, as listed below:

"CRUNCH" is selected for {NRCHEM = 0, ICHEM = 0}

"ERUNCH" is selected for {NRCHEM = 0, ICHEM $\neq$ 0}

"DRUNCH" is selected for {NRCHEM $\neq$ 0, ICHEM = arbitrary}

NG $\equiv$ Number of species to be graphed in plot routines of the solution code. The default value is zero.

- NFINE ≡ Number of single days over which solutions are to be graphed and tabulated with "fine" resolution when the diurnal option is selected. The default value is one.
- KDEC ≡ Number of solution points graphed and tabulated per decade of the independent time variable, t . The default value is two.
- ISDEC ≡ Power of the first decade to be shown on solution graphs. The default value is one.
- YDEC ≡ A fractional value of the maximum solution magnitude occurring in the problem solution history. This fraction determines the lower limit of solution magnitudes shown on graphs.
- NPIC1 ≡ Number of solution points in the internal graph and table storage array, TX, of the solution code. The minimum default value is 100, and the maximum default value is 400.
- NPRIN ≡ Maximum number of lines to appear in solution output tables. The default value is 50.
- NRATE ≡ Number of reactions in the reaction set to be read in. The maximum allowable value is presently 100.
- NRK(I) ≡ Set of library reaction numbers for the reaction set to be read in ($I = \text{NRATE}$). These reaction numbers with their associated reaction processes and the rate coefficient values are listed in compendia prepared by Duewer and Gelinas.⁶ If NRK(I) is not in the library range an output message to that effect is issued. The code will internally put NRK(I) into sequential numerical order, regardless of input ordering.

- NELIM $\equiv$ Number of species that are to be held fixed by the solution routine. That is, these species are given zero derivative and, therefore, are not included as time varying species in the set of differential equations being solved by the solution program. The default value is zero.
- ENAM(I) $\equiv$ The appropriate library compendium names of species to be held fixed ($I = 1, \text{NELIM}$).
- ALT $\equiv$ Problem altitude (km). The default value is zero. The code internally computes the air density and temperature at this specified altitude.
- TEMP $\equiv$ Problem temperature ($^{\circ}\text{K}$). The default value is an internally computed temperature at the altitude, ALT.
- NCHANGE $\equiv$ Number of reaction rate coefficients, QK, for which the internally computed library values will be altered. The default value is zero.
- K $\equiv$ Library reaction number of the rate coefficient to be altered. If the entry K is not in the specified reaction set (NRK(I)), an output message is issued. If the entry K appears more than once, an output message is issued, and the problem terminates.
- RMULT $\equiv$ Alteration parameter for reaction number K. The use of this parameter is described in the definition of IREPLACE, directly below.

IREPLACE = Replacement mode indicator for alteration of the internally computed value of the reaction rate coefficient, RQK(K), for library reaction number K.

- (a) IREPLACE = 0 replaces RQK(K) with the value of RQK(K)*RMULT
- (b) IREPLACE > 0 replaces RQK(K) with the value of RMULT.

Major Options and Functions of CRNCIT

The program CRNCIT is composed of five major subroutines whose functions will be described in their logical order. Recall that CRNCIT has two main outputs - one is a description (in file OUTPRIN) of the compiled problem to the user, and the other is a coded description (in file CRACK1) of the compiled problem for use in the solution code (CRUNCH, DRUNCH, or ERUNCH).

After the input file INRATE is read, a test is made immediately to insure that all the library reaction numbers, NRK(I) for I = 1, NRATE, are indeed in the reaction library files CARLIB and QKCOEFF. The problem is terminated if a default is encountered at this stage. From here the following sequence of subroutine calls is made:

BUSTER

Given the reaction set specified by the library reaction numbers, NRK(I), I = 1, NRATE, the subroutine BUSTER searches and decodes the appropriate segments of the library file CARLIB. The CARLIB file simply contains a listing in chemical form, of one reaction per line along with its library

number. For example lines 29 and 30 of CARLIB appear as:

corresponding to reactions 29 and 30 listed in the LLL reaction library compendia.⁶ The symbols +, -, =, and : used in CARLIB formats are delimiters for the symbolic logic in BUSTER. As the specified reactions are scanned by BUSTER, a tally of species and their production and loss reactions is compiled in a form which is later used to compile the reaction system in differential equation form for the chosen solution code option. Information is also stored which allows a compilation of correct analytic expressions for the specie derivative Jacobian elements, $\frac{\delta \left(\frac{dy_i(t)}{dt} \right)}{\delta y_j(t)}$, which can later be used in sensitivity analysis and by the differential equation solution routines. If a faulty format is encountered in the scan of CARLIB, an error message is issued by BUSTER.

SHUFFLE

The subroutine SHUFFLE simply moves to the bottom of the species and derivative arrays those elements (ENAM(I), I = 1, NELIM) which have been specified to be held constant. There is no need to include constant species in the set of differential equations to be integrated. So the number of time dependent species, NEQN, is simply deduced for later use by the solution routines as

$$\text{NEQN} = \text{NSP} - \text{NELIM} \quad , \quad (22)$$

where NSP is the total number of time varying, plus constant, species in the selected reaction set. The maximum number of species that can be accommodated in present code versions is 50. It is not difficult to increase this

number when needs arise. But it is necessary to use large core memory (LCM) when NSP and other parameters exceed their presently set maximum.

DEOUT

This is simply an output routine which lists for the user his compiled problem information in the file OUTPRIN.

QKCALC

Given the reaction rate library numbers, QKCALC performs a number of operations. It evaluates the appropriate rate coefficients for thermal chemical reaction processes according to Eqs. (2) and (3) above. The coefficients A, B, C, DA, and DC are stored in the library file QKCOEFF. When the diurnal solution option is chosen, QKCALC also identifies the radiative rates to be used in the diurnal subroutines of the solution code. The rate alterations that are specified by NCHANGE, K, RMULT, and IREPLACE are made for both chemical and photochemical processes and the coded information needed by the solution code is stored into the file CRACK1. If the diurnal option is not chosen, the user must provide constant reaction rates for radiative (photodissociation) reactions from independent sources. If this is not done, the default rate values for radiative reaction specified in the NRK(I) array are zero in the solution option CRUNCH and ERUNCH.

JACOB

This subroutine generates, in coded form, the exact analytic expressions for all Jacobian analytic elements, $\delta(dy_i(t)/dt)/\delta y_j(t)$. These elements

are useful in two ways. First, they are a qualitative guide to the sensitivity of the i^{th} type of species to the j^{th} type of species. These elements are used explicitly in an associated sensitivity code which will be forthcoming shortly. Second, the differential equation solution routine² that is used in GENKIN-I is an implicit numerical method in which the analytic Jacobian expressions may sometimes be used to good advantage.

B. The Solution Program

The solution program has the three options CRUNCH, ERUNCH, and DRUNCH mentioned in Section II. The program options are available either as individual binary controllee decks or as FORTRAN coded decks. The successful execution of the above mentioned options requires an input file, INSTIF, and the compiled program information file, CRACK1. The radiative data file, NEWRDH, is required (in addition to INSTIF and CRACK1) for executing DRUNCH. At present all solution options are dimensioned for a maximum of fifty species and one hundred reaction processes. The execution commands under ORDER are the following:

CRUNCH - The FORTRAN deck is executed as:

```
ORDER CRUNCH / T V
```

The binary controllee is named KINITC. It is executed as:

```
KINITC / T V
```

DRUNCH - The FORTRAN deck is executed as:

```
ORDER DRUNCH / T V
```

The binary controllee is named KINITD. It is executed as:

```
KINITD / T V
```


ERUNCH - The ERUNCH version allows the user to merge to the basic ERUNCH program with his own subroutine, DIFFCOR(NDM,T,Z,DY), which alters the species derivatives for time dependent rate coefficients due to temperature and pressure variations and for external sources and sinks. The functions TFUN(T) and ZMFUN(T) must be provided by the user and merged to ERUNCH for the time variation of temperature and pressure, respectively. The arguments of DIFFCOR are defined in the text which follows for ERUNCH. The merged ERUNCH program is executed as follows:

```
ORDER ERUNCH / T V .
```

After execution of ERUNCH a complete binary controllee file, KINITE is created. KINITE can be executed for subsequent runs by the command

```
KINITE / T V .
```

There are numerous operations and input features that are common to all of the solution options. Thus, all of the possible types of input cards for INSTIF will be given below. Then, in later detailed descriptions of each of the solution options, the appropriate combinations of input cards for the specific options will be indicated.

Type 1 Format (4E20.13)

<u>Columns</u>	<u>Variable Name</u>
1-20	YFLOOR(1)
21-40	YFLOOR(2)
.	.
.	.
.	.
etc	etc

Type 2 Format (6E12.5) - used only for diurnal mode

<u>Columns</u>	<u>Variable Name</u>
1-12	COL02
13-24	COL03
25-36	COLN02

Type 3 Format (3I6, 3E12.5) - used only for diurnal mode

<u>Columns</u>	<u>Variable Name</u>
1-6	MYEAR
7-12	MONTH
13-18	MDAY
19-30	TIME
31-42	DLAT
43-54	DLONG

Type 4 Format (I4)

<u>Columns</u>	<u>Variable Name</u>
1-4	NINP

Type 5 Format (A10, E20.13)

<u>Columns</u>	<u>Variable Name</u>
1-10	NSPEC
11-30	CONC

Type 6 Format (3E12.4, I4) - used only for CRUNCH and ERUNCH modes

<u>Columns</u>	<u>Variable Name</u>
1-12	TEND
13-24	DINOW
25-36	EPS
37-40	MF

Type 7 Format (2E12.4, I4) - used only for diurnal mode

<u>Columns</u>	<u>Variable Name</u>
1-12	DTNOW
13-24	EPS
25-28	MF

Type 8 Format (8A10)

<u>Columns</u>	<u>Variable Name</u>
1-10	NGRAPH(1)
11-20	NGRAPH(2)
.	.
.	.
.	.
etc	etc

Type 9 Format (I6) - used only in diurnal mode

<u>Columns</u>	<u>Variable Name</u>
1-6	NRDAY

Type 10 Format (E12.5, I4) - used only in diurnal mode

<u>Columns</u>	<u>Variable Name</u>
1-12	DDAY
13-16	NCOAR

Definition of "INSTIF" Variables

YFLOOR(I) $\equiv$ Non-zero "floor values" used for error control of the solutions, $YU(1)$, ($1 = 1, NEQN$). The number of differential equations being solved is $NEQN = NSP - NELIM$, where NSP is the total number of species in the reaction system, and $NELIM$ is the number of species

held constant. Recall that NELIM is specified by the user in "INRATE"; its default value is zero. The user must verify the value for NEQN from the output file, OUTPRIN, of the set-up stage.

The data cards for the correct number (NEQN) of non-zero YFLOOR values must be provided by the user. Failure to provide these entries will usually give a format error default for "INSTIF". Guidelines for choosing values of YFLOOR(I) will be discussed under the section, SOLUTION METHOD, that follows the present section.

- COL02 $\equiv$ Column density of O_2 (no./cm²). In case of default, a value is computed internally from the data of the U.S. Standard Atmosphere.¹⁰
- COL03 $\equiv$ Column density of O_3 (no./cm²). In case of default, a value is computed from internally stored data.
- COLN02 $\equiv$ Column density of NO_2 (no./cm²). The default value is zero.
- MYEAR $\equiv$ Calendar year; e.g. 1974. This is used as an initial value for the diurnal mode. The default value is zero.
- MONTH $\equiv$ Number of calendar month, e.g. 1 $\rightarrow$ January, 2 $\rightarrow$ February, etc. This is used as an initial value for the diurnal mode. A default of zero or greater than 12 calls EXIT and prints a message.

- MDAY ≡ Number of the day in the month to be used as a starting value for the diurnal mode. A default of zero, or of too large a value calls EXIT and prints a message.
- TIME ≡ Greenwich time in seconds past midnight of MDAY. This is used as an initial value for the diurnal mode. The default value is zero. A default of greater than 86400 seconds, or a negative value, calls EXIT and prints a message.
- DLAT ≡ Degrees north latitude (0° to 90°). DLAT (and DLONG) is used to compute the solar zenith angle for photodissociation rates.
- DLONG ≡ Degrees longitude (0° to $\pm 180^\circ$). West longitude is positive, and east is negative. Local time is input by setting DLONG = 0.
- NINP ≡ Number of initial concentrations (no./cm³) to be read in. The default value is zero. This card must be included, even when NINP = 0.
- NSPEC ≡ Name of specie in reaction set for which an initial concentration, CONC, is to be read (left adjusted). If NSPEC does not correspond to a species in the reaction system, an error message is issued and the problem is exited.
- CONC ≡ initial concentration (no./cm³) of specie, NSPEC.
- TEND ≡ ending time of solution history (seconds).

DTNOW $\equiv$ initial time increment, Δt , (seconds) to be used by solution routine.

EPS $\equiv$ local truncation error to be satisfied by solution method.

MF $\equiv$ method flag for solution method options. A standard choice is MF = 22. See the section entitled SOLUTION METHOD.

NGRAPH(I) $\equiv$ names of species (left adjusted) to be graphed for (I = 1, NG), where NG was specified in the set-up stage. If NGRAPH(I) does not correspond to a specie in the reaction set, being solved, an error message is printed, and the problem is exited.

NRDAY $\equiv$ the total number of days to be run by the diurnal mode.

DDAY $\equiv$ the time increment (hours) between plot points for "coarse" diurnal graphs.

NCOAR $\equiv$ the number of days for which species concentrations are plotted on a single "coarse" graph frame of the diurnal mode. For instance NCOAR = 3 would give "coarse" graphs with 3 days of solution, information plotted per "coarse" graph.

SOLUTION METHOD

An LLL variant^{1,2} of the basic Gear method³ is used in GENKIN-I to integrate the compiled set of differential equations. A number of the variables provided by INSTIF are used as control parameters by the solution subroutine.

The variables, YFLOOR(I), (I = 1, NEQN) are used internally for controlling the local truncation error of the solutions, Y0(I). Non-zero values

must be specified for all YFLOOR(I), (I = 1, NEQN). As the name of the variable implies, "floor values" are needed to control especially those variables whose values may approach very small magnitudes at any time in the solution history. It is quite common for decaying components to approach small values that constitute noise. Clearly, it is not desirable to pay the price of precise error control on noisy components.

The YFLOOR(I) array allows the user to specify a magnitude for each solution component, Y0(I), below which a measure of local truncation error control is relinquished. Any bit of knowledge the user has of likely magnitudes of solution components, the better he can select values for YFLOOR(I). In atmospheric applications, species concentrations may range from roughly 10^{-4} cm^{-3} for very reactive trace species to roughly $1. \times 10^{12} \text{ cm}^{-3}$ for less reactive trace species. Floor values of $1. \times 10^{-20}$ for all components usually suffice for constant rate coefficient (CRUNCH) problems. But diurnal (DRUNCH) and other time varying rate coefficient (ERUNCH) problems may require some amount of testing with larger values on pathological components. (Recall that the Y0(I) and YFLOOR(I) array elements are identified by chemical species name in OUTPRIN of the set-up program.)

The other control variables provided by INSTIF are TEND, the final solution time (seconds), DTNOW, the initial time increment, Δt , (seconds) to be used by the integration method, EPS, the local truncation error (that is maintained for each integration cycle, by definition), and the numerical integration method flag, MF.

The parameter TEND is not required by the diurnal option because it is computed internally from the number of days to be run, NRDAY. All problems automatically terminate when the integration time extends beyond TEND.

The parameter DTNOW should deliberately be chosen a very small value, because the solution method is self-starting at first order. Subsequently the order, JSTART, of the integration method and DTNOW are automatically adjusted for efficient solution, minimizing the impact of an initially small DTNOW.

The local truncation error, EPS, should be assigned ranges of values, perhaps for 10^{-2} to 10^{-6} , to determine the reproducibility of solutions of various types of problems, versus EPS. See reference 15 for control strategies.

The parameter MF takes values obtained from the expression

$$MF = (10 * METH + MITER)$$

where METH is the basic integration method indicator. It takes values:

METH = 1 means modified Adams method

METH = 2 means modified backward differentiation method

MITER is the iteration method indicator. It takes values:

MITER = 0 means functional iteration (no partial derivatives needed)

MITER = 1 means chord method with an analytic Jacobian generated by GENKIN-I.

MITER = 2 means chord method with a Jacobian calculated by finite differences

MITER = 3 means chord method with a Jacobian replaced by a diagonal approximation based on a directional derivative.

Every user is well-advised to read References 1 and 2, which gives a detailed view of the solution method and its options.

In the event that a problem cannot be satisfactorily integrated to completion, the termination flag, KFLAG, is printed with the following meaning:

KFLAG = -1 means the requested error could not be achieved with an internally generated minimum Δt .

KFLAG = -2 means the requested error is too small to be handled for this problem.

KFLAG = -3 means the corrector convergence could not be achieved with an internally generated minimum Δt .

In many cases adjustment of EPS, DTNOW, and some or all of the YFLOOR(I) values can alleviate these types of termination. But, again, the user should examine the reproducibility of solutions over ranges of these control parameters to establish some confidence limits on the results obtained. Finally, if the time increment Δt is so small that it is noise relative to the problem time, t , a message is printed, but the problem is not exited.

MAJOR OPTIONS AND FUNCTIONS OF CRUNCH

The INSTIF input for CRUNCH is comprised of only the following types of input cards: types 1, 4, 5, 6, and 8.

Only the files INSTIF and CRACK1 are required for execution. As these files are read, default messages are printed if format or logic errors are encountered. Corrective measures for the more obvious defaults have been indicated in the previous text. Any other difficulties should be brought to the attention of the authors.

The integration of the reaction system runs serially from $t = 0$. to $t = \text{TEND}$. The output files are described in a later section with an example.

MAJOR OPTIONS AND FUNCTIONS OF ERUNCH

The INSTIF input for ERUNCH is comprised of only the following types of input cards: types 1, 4, 5, 6, 8, and any additional input that the user may call for in his subroutine DIFFCOR(NDM, T, Z, DY) and functions TFUN(T) and ZMFUN(T). All input is read on tape 2. The user is expected to construct his read statements in DIFFCOR, TFUN, and ZMFUN so that repeated calls to those routines in the solution sequence do not attempt unwarranted repetitive input reads. If DIFFCOR is a dummy routine (made up of only a RETURN and an END card) and TFUN and ZMFUN are also dummies, ERUNCH simply becomes an inefficient CRUNCH calculation. The subroutine DIFFCOR(NDM, T, Z, DY) is designed to alter the species derivatives otherwise calculated in subroutine DIFFUN. Recall that the differential equations calculated in DIFFUN were compiled initially in CRNCIT with no external sources and sinks.

The user should also familiarize himself with the COMMON and CLICHE structure of the MAIN subroutine of ERUNCH. Again the file CRACK1 is required for execution as well as INSTIF. The integration of the system runs serially from $t = 0$ to $t = \text{TEND}$. The output files and an example are given in a later section.

MAJOR OPTIONS AND FUNCTIONS OF DRUNCH

The solution option, DRUNCH, integrates the selected reaction system day by day for a user specified number of days. Internally evaluated, instantaneous photodissociation rates are used unless otherwise specified in INRATE. DRUNCH computes internally its starting time and its finishing

time, TEND, for each day. In addition to INSTIF and CRACK1, the file NEWRDH containing microscopic radiative data is required for execution. The INSTIF input for DRUNCH is comprised of only the following types of input cards: types 1, 2, 3, 4, 5, 7, 8, 9, and 10.

The logic of the DRUNCH option may give an output message concerning the TX array which is unique to DRUNCH. That is, the time value of TX(NPIC1) must exceed TEND when "fine days" are calculated and graphed one day at a time. For "coarse days", which are graphed NCOAR days per graph, TX(NPIC1) must span (NCOAR+1) days. A message will be printed when these conditions are not met. Any and/or all of the following measures will correct the difficulty:

- 1) increase the value of NPIC1
- 2) increase the value of ISDEC
- 3) decrease the value of KDEC
- 4) if the difficulty occurs in the "coarse day" segment, increasing DDAY and/or decreasing NCOAR will also help.

The numerical solution of systems with rapidly time varying photodissociation rates (internally computed in DRUNCH) can be very demanding on running time costs. The user must simply develop his base of experience for these pathologies. Manipulation of the control parameters YFLOOR(I), EPS, etc. is the suggested course for ameliorating this type of difficulty at the present time. The output files and an example are given in the next major section.

EXAMPLES

In this section, illustrative examples are presented for the options discussed above. Output information will be presented and further described in a reasonable amount of detail.

The basic example consists of four reactions and three atmospheric species. It is the very simple, but classic, Chapman mechanism for atmospheric ozone kinetics:

where the reaction library numbers are given by R88, R89, R93, and R103.

1. CRUNCH

The input deck INRATE contains the following information:

Card 1:	NRCHEM = 0	(Col. 4)
Card 2:	ICHEM = 0	(Col. 4)
Card 3:	NG = 2	(Col. 4)
	NFINE = 2	(Col. 8) ... NFINE has no meaning in CRUNCH and ERUNCH
	KDEC = 7	(Col. 12)
	ISDEC = -4	(Cols. 15, 16)
	YDEC = 1.E-10	(Cols. 17-28)
Card 4:	NPIC1 = 800	(Cols. 2-4)
Card 5:	NPRIN = 125	(Cols. 2-4)

Card 6: NRATE = 4 (Col. 4)

Card 7: NRK(1) = 88 (Cols. 2-4)
NRK(2) = 89 (Cols. 7-8)
NRK(3) = 93 (Cols. 11-12)
NRK(4) = 103 (Cols. 15-16)

Card 8: NELIM = 1 (Col. 4)

Card 9: ENAM(1) = 02 (Cols. 1-2)

Card 10: ALT = 35. (Cols. 1-12)
TEMP = 0. (Cols. 13-24)

Card 11: NCHANGE = 3 (Col. 4)

Card 12: K = 89 (Cols. 3-4)
RMULT = 4.66E-16 (Cols. 5-24)
IREPLACE = 1 (Col. 28)

Card 13: K = 93 (Cols. 3-4)
RMULT = 5.E-11 (Cols. 5-24)
IREPLACE = 1 (Col. 28)

Card 14: K = 103 (Cols. 2-4)
RMULT = 2.5E-04 (Cols. 5-24)
IREPLACE = 1 (Col. 28)

The output file OUTPRIN appears below.

THIS IS A CHEMISTRY RUN

GRAPH INFORMATION FOLLOWS

NG= 2 NFINE= 2 KDEC= 7 ISDEC= -4 YDEC= 1.00000E-10

THE NO. OF POINTS IN THE TX ARRAY IS 800

THE MAXIMUM NUMBER OF LINES IN PRINTOUT TABLES IS 125

THE NO. OF RATES TO BE READ IS 4

THE INPUT RATES FOLLOW

88 89 93 103

THE NO. OF SPECIES NOT FOLLOWED BY THE DIFFERENTIAL EQUATIONS IS 1

THE SPECIES NOT TRACKED ARE AS FOLLOWS

02

USER SHOULD VERIFY THAT UNTRACKED SPECIES APPEAR AT END OF SPECIES LIST BELOW

ALTITUDE(METERS)= 3.50000E+04 TEMPERATURE(K)= 2.36513E+02

UNORDERED RATES FOLLOW

88 89 93 103

ORDERED RATES FOLLOW

88 89 93 103

THE CHEMICAL EQUATIONS FOLLOW

0 + 02 = 03 : R88

0 + 03 = 202 : R89

02 = 0 + 0 : R93

03 = 0 + 02 : R103

END

A DESCRIPTION OF THE D. E. SUBROUTINE FOLLOWS

THE NUMBER OF EQUATIONS IS 2

SPECIES AND THEIR INDEX FOLLOWS

1 0

2 03

3 02

1
THE DIFFERENTIAL EQUATIONS ARE

$$D(0)/DT = 2 * QK(3) * 02 + QK(4) * 03 - QK(2) * 0 * 03 - QK(1) * 0 * 02$$

$$D(03)/DT = QK(1) * 0 * 02 - QK(4) * 03 - QK(2) * 0 * 03$$

SPECIES PER RATE FOLLOW

RATE NUMBER	1	SPECIES	1	3
RATE NUMBER	2	SPECIES	1	2
RATE NUMBER	3	SPECIES	3	
RATE NUMBER	4	SPECIES	2	

RATES PER DERIVATIVE FOLLOW

DERIVATIVE NUMBER IS	1
RATES	1 2 3 4

DERIVATIVE NUMBER IS	2
RATES	1 2 4

COEFFICIENTS OF THE RATES FOLLOW

DERIVATIVE NUMBER IS	1
COEF.	-1. -1. 2. 1.

DERIVATIVE NUMBER IS	2
COEF.	1. -1. -1.

ZM = 1.75980E+17 (CM-3)

LIBRARY RATE NO. 88 , WHICH IS QK(1), IS DEPENDENT ON ZM

THE NO. OF RATES TO BE CHANGED IS 3 THE RATES FOLLOW

K	RMULT	IREP
89	4.66000000000000E-16	1
93	5.00000000000000E-11	1
103	2.50000000000000E-04	1

QK NO.	LIB. NO.	QK
1	88	1.6267812916936E-16
2	89	4.66000000000000E-16
3	93	5.00000000000000E-11
4	103	2.50000000000000E-04

THE NO. OF RADIATIVE RATES IS 0

JACOBIAN OUTPUT FOLLOWS

NO. OF COMPONENTS = 1

The input deck INSTIF contains the following information:

Card 1:	YFLOOR(1) = 1.E-20	(Cols. 1-20)
	YFLOOR(2) = 1.E-20	(Cols. 21-40)
Card 2:	NINP = 3	(Col. 4)
Card 3:	NSPEC = 03	(Cols. 1-2)
	CONC = 1.E + 12	(Cols. 11-30)
Card 4:	NSPEC = 0	(Col. 1)
	CONC = 1.E + 06	(Cols. 11-30)
Card 5:	NSPEC = 02	(Cols. 1-2)
	CONC = 3.7E + 16	(Cols. 11-30)
Card 6:	TEND = 8.E + 08	(Cols. 1-12)
	DINOW = 1.E-19	(Cols. 13-24)
	EPS = 1.E-04	(Cols. 25-36)
	MF = 22	(Cols. 39-40)
Card 7:	NGRAPH(1) = 03	(Cols. 1-2)
	NGRAPH(2) = 0	(Col. 11)

The tabular output from file HSPO appears directly below.

NG OR NPIC1 OR NPL EXCEEDS CODE LIMITS

NSP= 3 NEQN= 2 NRATE= 4 NPIC1=400 NG= 2 NPL= 50

THIS IS AN EPISODE RUN

ALTITUDE(METERS)= 3.50000E+04

FLOOR VALUES FOLLOW

1.000000000000000E-20 1.000000000000000E-20

SPECIES FROM CHEMIT

0 03 02

THE NUMBER OF INPUT INITIAL VALUES = 3

03 1.000000000000000E+12
0 1.000000000000000E+06
02 3.700000000000000E+16

GEAR INPUT

TEND= 8.00000E+08 DT= 1.00000E-19 EPS= 1.00000E-04 MF= 22

THE DIFFERENTIAL EQUATIONS ARE

$D(0)/DT = 2 * QK(3) * 02 + QK(4) * 03 - QK(2) * 0 * 03 - QK(1) * 0 * 02$

$D(03)/DT = QK(1) * 0 * 02 - QK(4) * 03 - QK(2) * 0 * 03$

GRAPH INFORMATION

NG= 2 NFINE= 2 KDEC= 7 ISDEC= -4

THE MAXIMUM NO. OF DECADES IN GRAPHS IS SET BY 1.00000E-10

03 IS GRAPH NUMBER 1

0 IS GRAPH NUMBER 2

1

QK TABLE

1	1.62678E-16
2	4.66000E-16
3	5.00000E-11
4	2.50000E-C4

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
2.78E-08	1.02E+06	1.00E+12	3.70E+16
6.75E-08	1.06E+06	1.00E+12	3.70E+16
1.07E-07	1.10E+06	1.00E+12	3.70E+16
1.47E-07	1.13E+06	1.00E+12	3.70E+16
1.87E-07	1.17E+06	1.00E+12	3.70E+16
2.26E-07	1.20E+06	1.00E+12	3.70E+16
2.66E-07	1.24E+06	1.00E+12	3.70E+16
2.78E-07	1.25E+06	1.00E+12	3.70E+16
6.75E-07	1.60E+06	1.00E+12	3.70E+16
1.07E-06	1.94E+06	1.00E+12	3.70E+16
1.47E-06	2.29E+06	1.00E+12	3.70E+16
1.87E-06	2.63E+06	1.00E+12	3.70E+16
2.26E-06	2.96E+06	1.00E+12	3.70E+16
2.66E-06	3.30E+06	1.00E+12	3.70E+16
2.78E-06	3.40E+06	1.00E+12	3.70E+16
6.75E-06	6.58E+06	1.00E+12	3.70E+16
1.07E-05	9.51E+06	1.00E+12	3.70E+16
1.47E-05	1.22E+07	1.00E+12	3.70E+16
1.87E-05	1.47E+07	1.00E+12	3.70E+16
2.26E-05	1.70E+07	1.00E+12	3.70E+16
2.66E-05	1.90E+07	1.00E+12	3.70E+16
2.78E-05	1.96E+07	1.00E+12	3.70E+16
6.75E-05	3.25E+07	1.00E+12	3.70E+16
1.07E-04	3.78E+07	1.00E+12	3.70E+16
1.47E-04	4.01E+07	1.00E+12	3.70E+16
1.87E-04	4.14E+07	1.00E+12	3.70E+16
2.26E-04	4.23E+07	1.00E+12	3.70E+16
2.66E-04	4.33E+07	1.00E+12	3.70E+16
2.78E-04	4.37E+07	1.00E+12	3.70E+16
6.75E-04	4.59E+07	1.00E+12	3.70E+16
1.07E-03	4.52E+07	1.00E+12	3.70E+16
1.47E-03	4.48E+07	1.00E+12	3.70E+16
1.87E-03	3.85E+07	1.00E+12	3.70E+16
2.26E-03	4.13E+07	1.00E+12	3.70E+16
2.66E-03	4.21E+07	1.00E+12	3.70E+16
2.78E-03	4.21E+07	1.00E+12	3.70E+16
6.75E-03	4.21E+07	1.00E+12	3.70E+16
1.07E-02	4.22E+07	1.00E+12	3.70E+16
1.47E-02	4.22E+07	1.00E+12	3.70E+16
1.87E-02	4.22E+07	1.00E+12	3.70E+16
2.26E-02	4.22E+07	1.00E+12	3.70E+16
2.66E-02	4.22E+07	1.00E+12	3.70E+16
2.78E-02	4.22E+07	1.00E+12	3.70E+16
6.75E-02	4.22E+07	1.00E+12	3.70E+16
1.07E-01	4.22E+07	1.00E+12	3.70E+16

1.47E-01	4.22E+07	1.00E+12	3.70E+16
1.87E-01	4.22E+07	1.00E+12	3.70E+16
2.26E-01	4.23E+07	1.00E+12	3.70E+16
2.66E-01	4.23E+07	1.00E+12	3.70E+16
2.78E-01	4.23E+07	1.00E+12	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
2.78E-08	2.48E+08	-2.44E+08	0.
6.75E-08	2.47E+08	-2.44E+08	0.
1.07E-07	2.47E+08	-2.43E+08	0.
1.47E-07	2.47E+08	-2.43E+08	0.
1.87E-07	2.47E+08	-2.43E+08	0.
2.26E-07	2.46E+08	-2.43E+08	0.
2.66E-07	2.46E+08	-2.43E+08	0.
2.78E-07	2.46E+08	-2.42E+08	0.
6.75E-07	2.44E+08	-2.40E+08	0.
1.07E-06	2.42E+08	-2.38E+08	0.
1.47E-06	2.40E+08	-2.36E+08	0.
1.87E-06	2.38E+08	-2.34E+08	0.
2.26E-06	2.36E+08	-2.32E+08	0.
2.66E-06	2.34E+08	-2.30E+08	0.
2.78E-06	2.33E+08	-2.30E+08	0.
6.75E-06	2.14E+08	-2.10E+08	0.
1.07E-05	1.96E+08	-1.93E+08	0.
1.47E-05	1.80E+08	-1.77E+08	0.
1.87E-05	1.65E+08	-1.62E+08	0.
2.26E-05	1.52E+08	-1.48E+08	0.
2.66E-05	1.39E+08	-1.35E+08	0.
2.78E-05	1.36E+08	-1.32E+08	0.
6.75E-05	5.78E+07	-5.41E+07	0.
1.07E-04	2.59E+07	-2.22E+07	0.
1.47E-04	1.21E+07	-8.45E+06	0.
1.87E-04	4.57E+06	-9.05E+05	0.
2.26E-04	-9.94E+05	4.65E+06	0.
2.66E-04	-6.77E+06	1.04E+07	0.
2.78E-04	-9.07E+06	1.27E+07	0.
6.75E-04	-2.28E+07	2.65E+07	0.
1.07E-03	-1.84E+07	2.21E+07	0.
1.47E-03	-1.59E+07	1.96E+07	0.
1.87E-03	2.19E+07	-1.82E+07	0.
2.26E-03	4.80E+06	-1.14E+06	0.
2.66E-03	4.38E+05	3.22E+06	0.
2.78E-03	1.27E+04	3.65E+06	0.
6.75E-03	1.56E+02	3.66E+06	0.
1.07E-02	1.52E+02	3.66E+06	0.
1.47E-02	1.52E+02	3.66E+06	0.
1.87E-02	1.52E+02	3.66E+06	0.
2.26E-02	1.52E+02	3.66E+06	0.
2.66E-02	1.52E+02	3.66E+06	0.
2.78E-02	1.52E+02	3.66E+06	0.
6.75E-02	1.52E+02	3.66E+06	0.
1.07E-01	1.52E+02	3.66E+06	0.
1.47E-01	1.52E+02	3.66E+06	0.
1.87E-01	1.52E+02	3.66E+06	0.
2.26E-01	1.52E+02	3.66E+06	0.

2.66E-01	1.52E+02	3.66E+06	0.
2.78E-01	1.52E+02	3.66E+06	0.

TIME(HR) QQ TABLE

2.78E-08	6.17E+06	4.78E+02	1.85E+06	2.50E+08
6.75E-08	6.38E+06	4.94E+02	1.85E+06	2.50E+08
1.07E-07	6.59E+06	5.10E+02	1.85E+06	2.50E+08
1.47E-07	6.81E+06	5.27E+02	1.85E+06	2.50E+08
1.87E-07	7.02E+06	5.43E+02	1.85E+06	2.50E+08
2.26E-07	7.23E+06	5.60E+02	1.85E+06	2.50E+08
2.66E-07	7.44E+06	5.76E+02	1.85E+06	2.50E+08
2.78E-07	7.50E+06	5.81E+02	1.85E+06	2.50E+08
6.75E-07	9.61E+06	7.44E+02	1.85E+06	2.50E+08
1.07E-06	1.17E+07	9.05E+02	1.85E+06	2.50E+08
1.47E-06	1.38E+07	1.06E+03	1.85E+06	2.50E+08
1.87E-06	1.58E+07	1.22E+03	1.85E+06	2.50E+08
2.26E-06	1.78E+07	1.38E+03	1.85E+06	2.50E+08
2.66E-06	1.99E+07	1.54E+03	1.85E+06	2.50E+08
2.78E-06	2.05E+07	1.58E+03	1.85E+06	2.50E+08
6.75E-06	3.96E+07	3.07E+03	1.85E+06	2.50E+08
1.07E-05	5.72E+07	4.43E+03	1.85E+06	2.50E+08
1.47E-05	7.34E+07	5.69E+03	1.85E+06	2.50E+08
1.87E-05	8.84E+07	6.84E+03	1.85E+06	2.50E+08
2.26E-05	1.02E+08	7.90E+03	1.85E+06	2.50E+08
2.66E-05	1.15E+08	8.87E+03	1.85E+06	2.50E+08
2.78E-05	1.18E+08	9.15E+03	1.85E+06	2.50E+08
6.75E-05	1.96E+08	1.52E+04	1.85E+06	2.50E+08
1.07E-04	2.28E+08	1.76E+04	1.85E+06	2.50E+08
1.47E-04	2.42E+08	1.87E+04	1.85E+06	2.50E+08
1.87E-04	2.49E+08	1.93E+04	1.85E+06	2.50E+08
2.26E-04	2.55E+08	1.97E+04	1.85E+06	2.50E+08
2.66E-04	2.60E+08	2.02E+04	1.85E+06	2.50E+08
2.78E-04	2.63E+08	2.03E+04	1.85E+06	2.50E+08
6.75E-04	2.76E+08	2.14E+04	1.85E+06	2.50E+08
1.07E-03	2.72E+08	2.11E+04	1.85E+06	2.50E+08
1.47E-03	2.70E+08	2.09E+04	1.85E+06	2.50E+08
1.87E-03	2.32E+08	1.79E+04	1.85E+06	2.50E+08
2.26E-03	2.49E+08	1.93E+04	1.85E+06	2.50E+08
2.66E-03	2.53E+08	1.96E+04	1.85E+06	2.50E+08
2.78E-03	2.54E+08	1.96E+04	1.85E+06	2.50E+08
6.75E-03	2.54E+08	1.96E+04	1.85E+06	2.50E+08
1.07E-02	2.54E+08	1.96E+04	1.85E+06	2.50E+08
1.47E-02	2.54E+08	1.96E+04	1.85E+06	2.50E+08
1.87E-02	2.54E+08	1.96E+04	1.85E+06	2.50E+08
2.26E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
2.66E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
2.78E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
6.75E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
1.07E-01	2.54E+08	1.97E+04	1.85E+06	2.50E+08
1.47E-01	2.54E+08	1.97E+04	1.85E+06	2.50E+08
1.87E-01	2.54E+08	1.97E+04	1.85E+06	2.51E+08
2.26E-01	2.54E+08	1.98E+04	1.85E+06	2.51E+08
2.66E-01	2.55E+08	1.98E+04	1.85E+06	2.51E+08
2.78E-01	2.55E+08	1.98E+04	1.85E+06	2.51E+08

TIME(HR) QK TABLE

2.78E-08	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-08	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-01	1.63E-16	4.66E-16	5.00E-11	2.50E-04

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
6.75E-01	4.25E+07	1.01E+12	3.70E+16

1.07E+00	4.27E+07	1.01E+12	3.70E+16
1.47E+00	4.29E+07	1.02E+12	3.70E+16
1.87E+00	4.32E+07	1.02E+12	3.70E+16
2.26E+00	4.34E+07	1.03E+12	3.70E+16
2.66E+00	4.36E+07	1.03E+12	3.70E+16
2.78E+00	4.37E+07	1.04E+12	3.70E+16
6.75E+00	4.58E+07	1.09E+12	3.70E+16
1.07E+01	4.80E+07	1.14E+12	3.70E+16
1.47E+01	5.02E+07	1.19E+12	3.70E+16
1.87E+01	5.23E+07	1.25E+12	3.70E+16
2.26E+01	5.45E+07	1.30E+12	3.70E+16
2.66E+01	5.66E+07	1.35E+12	3.70E+16
2.78E+01	5.73E+07	1.36E+12	3.70E+16
6.75E+01	7.86E+07	1.88E+12	3.70E+16
1.07E+02	9.95E+07	2.38E+12	3.70E+16
1.47E+02	1.20E+08	2.87E+12	3.70E+16
1.87E+02	1.40E+08	3.35E+12	3.70E+16
2.26E+02	1.59E+08	3.80E+12	3.70E+16
2.66E+02	1.77E+08	4.24E+12	3.70E+16
2.78E+02	1.82E+08	4.37E+12	3.70E+16
6.75E+02	3.13E+08	7.53E+12	3.70E+16
1.07E+03	3.72E+08	8.95E+12	3.70E+16
1.47E+03	3.94E+08	9.49E+12	3.70E+16
1.87E+03	4.02E+08	9.67E+12	3.70E+16
2.26E+03	4.05E+08	9.74E+12	3.70E+16
2.66E+03	4.06E+08	9.76E+12	3.70E+16
2.78E+03	4.06E+08	9.76E+12	3.70E+16
6.75E+03	4.06E+08	9.77E+12	3.70E+16
1.07E+04	4.06E+08	9.77E+12	3.70E+16
1.47E+04	4.06E+08	9.77E+12	3.70E+16
1.87E+04	4.06E+08	9.77E+12	3.70E+16
2.26E+04	4.06E+08	9.77E+12	3.70E+16
2.66E+04	4.06E+08	9.77E+12	3.70E+16
2.78E+04	4.06E+08	9.77E+12	3.70E+16
6.75E+04	4.06E+08	9.77E+12	3.70E+16
1.07E+05	4.06E+08	9.77E+12	3.70E+16
1.47E+05	4.06E+08	9.77E+12	3.70E+16
1.87E+05	4.06E+08	9.77E+12	3.70E+16
2.22E+05	4.06E+08	9.77E+12	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
6.75E-01	1.52E+02	3.66E+06	0.
1.07E+00	1.52E+02	3.66E+06	0.
1.47E+00	1.52E+02	3.66E+06	0.
1.87E+00	1.52E+02	3.66E+06	0.
2.26E+00	1.52E+02	3.66E+06	0.
2.66E+00	1.52E+02	3.66E+06	0.
2.78E+00	1.52E+02	3.66E+06	0.
6.75E+00	1.52E+02	3.65E+06	0.
1.07E+01	1.52E+02	3.65E+06	0.
1.47E+01	1.51E+02	3.64E+06	0.
1.87E+01	1.51E+02	3.64E+06	0.
2.26E+01	1.51E+02	3.63E+06	0.
2.66E+01	1.51E+02	3.63E+06	0.
2.78E+01	1.51E+02	3.63E+06	0.

6.75E+01	1.47E+02	3.56E+06	0.
1.07E+02	1.46E+02	3.48E+06	0.
1.47E+02	1.41E+02	3.38E+06	0.
1.87E+02	1.40E+02	3.26E+06	0.
2.26E+02	1.45E+02	3.14E+06	0.
2.66E+02	1.32E+02	3.00E+06	0.
2.78E+02	1.42E+02	2.96E+06	0.
6.75E+02	2.28E+02	1.50E+06	0.
1.07E+03	6.16E+02	5.96E+05	0.
1.47E+03	5.30E+01	2.13E+05	0.
1.87E+03	-1.58E+01	7.38E+04	0.
2.26E+03	-2.22E+01	2.54E+04	0.
2.66E+03	1.93E+01	8.89E+03	0.
2.78E+03	2.54E+01	6.52E+03	0.
6.75E+03	7.74E+03	-7.75E+03	0.
1.07E+04	-1.05E-03	-2.82E+00	0.
1.47E+04	2.75E-04	-8.93E-01	0.
1.87E+04	1.60E-03	-1.55E-01	0.
2.26E+04	4.88E-04	-2.50E-02	0.
2.66E+04	0.	3.47E-02	0.
2.78E+04	-3.05E-05	3.89E-02	0.
6.75E+04	0.	-4.58E-05	0.
1.07E+05	0.	1.53E-05	0.
1.47E+05	-3.05E-05	4.58E-05	0.
1.87E+05	-1.53E-05	3.05E-05	0.
2.22E+05	1.53E-05	0.	0.

TIME(HR) QQ TABLE

6.75E-01	2.56E+08	2.00E+04	1.85E+06	2.52E+08
1.07E+00	2.57E+08	2.02E+04	1.85E+06	2.54E+08
1.47E+00	2.59E+08	2.04E+04	1.85E+06	2.55E+08
1.87E+00	2.60E+08	2.06E+04	1.85E+06	2.56E+08
2.26E+00	2.61E+08	2.08E+04	1.85E+06	2.57E+08
2.66E+00	2.62E+08	2.10E+04	1.85E+06	2.59E+08
2.78E+00	2.63E+08	2.11E+04	1.85E+06	2.59E+08
6.75E+00	2.76E+08	2.33E+04	1.85E+06	2.72E+08
1.07E+01	2.89E+08	2.55E+04	1.85E+06	2.85E+08
1.47E+01	3.02E+08	2.79E+04	1.85E+06	2.98E+08
1.87E+01	3.15E+08	3.04E+04	1.85E+06	3.11E+08
2.26E+01	3.28E+08	3.29E+04	1.85E+06	3.24E+08
2.66E+01	3.41E+08	3.56E+04	1.85E+06	3.37E+08
2.78E+01	3.45E+08	3.64E+04	1.85E+06	3.41E+08
6.75E+01	4.73E+08	6.88E+04	1.85E+06	4.70E+08
1.07E+02	5.99E+08	1.10E+05	1.85E+06	5.95E+08
1.47E+02	7.21E+08	1.60E+05	1.85E+06	7.18E+08
1.87E+02	8.40E+08	2.18E+05	1.85E+06	8.37E+08
2.26E+02	9.54E+08	2.81E+05	1.85E+06	9.51E+08
2.66E+02	1.06E+09	3.49E+05	1.85E+06	1.06E+09
2.78E+02	1.10E+09	3.71E+05	1.85E+06	1.09E+09
6.75E+02	1.88E+09	1.10E+06	1.85E+06	1.88E+09
1.07E+03	2.24E+09	1.55E+06	1.85E+06	2.24E+09
1.47E+03	2.37E+09	1.74E+06	1.85E+06	2.37E+09
1.87E+03	2.42E+09	1.81E+06	1.85E+06	2.42E+09
2.26E+03	2.44E+09	1.84E+06	1.85E+06	2.43E+09
2.66E+03	2.44E+09	1.85E+06	1.85E+06	2.44E+09
2.78E+03	2.44E+09	1.85E+06	1.85E+06	2.44E+09
6.75E+03	2.45E+09	1.85E+06	1.85E+06	2.44E+09

1.07E+04	2.45E+09	1.85E+06	1.85E+06	2.44E+09
1.47E+04	2.45E+09	1.85E+06	1.85E+06	2.44E+09
1.87E+04	2.45E+09	1.85E+06	1.85E+06	2.44E+09
2.26E+04	2.45E+09	1.85E+06	1.85E+06	2.44E+09
2.66E+04	2.45E+09	1.85E+06	1.85E+06	2.44E+09
2.78E+04	2.45E+09	1.85E+06	1.85E+06	2.44E+09
6.75E+04	2.45E+09	1.85E+06	1.85E+06	2.44E+09
1.07E+05	2.45E+09	1.85E+06	1.85E+06	2.44E+09
1.47E+05	2.45E+09	1.85E+06	1.85E+06	2.44E+09
1.87E+05	2.45E+09	1.85E+06	1.85E+06	2.44E+09
2.22E+05	2.45E+09	1.85E+06	1.85E+06	2.44E+09

TIME(HR) QK TABLE

6.75E-01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+00	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+00	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+00	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E+00	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E+00	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E+00	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E+00	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E+01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E+01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E+01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E+01	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E+02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E+02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E+02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E+02	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E+03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E+03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E+03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E+03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E+04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E+04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E+04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E+04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.22E+05	1.63E-16	4.66E-16	5.00E-11	2.50E-04

The graphical DD80 output appears below. The name of DD80 files begins with "DX" when generated.

03

* 1 0

* 2

DD80 Output for CRUNCH Example

2. ERUNCH

The input deck INRATE is identical to that of the CRUNCH example above, except for card 2.

Card 2: ICHEM = 1 (Col. 4)

The file OUTPRIN is essentially the same as given for the CRUNCH example.

The input deck INSTIF is identical to that of the CRUNCH example above, except for Card 8, which is to be read by DIFFCOR for the general, arbitrary example described by the routines that follow:

Card 8: S03 = 1.E + 11 (Cols. 1-12)

A general, arbitrary example is described by the routines given below.

(Other examples of ERUNCH applications appear in reference 15.)

```
SUBROUTINE DIFFCOR(NDM,T,Z,DY)
```

```
DATA(IRD = 0)
```

```
IF(IRD .NE. 0) GO TO 1
```

```
READ(2,2) S03
```

```
2 FORMAT(E12.5)
```

```
IRD = 1
```

```
WRITE(3,3) S03
```

```
3 FORMAT(11,34H THE 03 SOURCE STRENGTH MAXIMUM IS , E12.5 , 11)
```

```
c There are 3.1536 E + 07 seconds/year
```

```
c DY(2) is the ozone derivative
```

```
1 W = 6.2832/(3.1536 E + 07)
```

```
DY(2) = DY(2) + SIN(W * T)
```

```
RETURN
```

```
END
```

```
FUNCTION TFUN(T)
```

```
TFUN = 36.5 + 200. *(EXP(-T/10000.))
```

```
RETURN
```

```
END
```

```

FUNCTION ZMFUN(T)
ZMFUN = 1.E + 17*(0.76 + EXPF(-T/(1.E + 07)))
RETURN
END

```

It is, of course, a trivial exercise to also verify that ERUNCH reduces to CRUNCH by using a dummy SUBROUTINE DIFFCOR(NDUM,T,Z,DY) (which is comprised only of a RETURN and END card) and the following function routines:

```

FUNCTION ZMFUN(T)
USE KIN1
ZMFUN = ZM
RETURN
END

```

```

FUNCTION TFUN(T)
USE KIN1
TFUN = TEMP
RETURN
END

```

These function routines simply use the values that were initialized in SUBROUTINE GENERATE for the atmospheric density, ZM (cm^{-3}), and temperature, TEMP ($^{\circ}\text{K}$), at the altitude, ALT.

The function HTPRN(X,M) is used to generate the U.S. Standard Atmosphere values (good to $\pm 0.5\%$) as follows:

X Altitude (meters) from 0. to 1.59×10^5

M Mode (2-5)

M = 2 Temperature ($^{\circ}$ K) (TEMP = HTPRN(X,2))

M = 3 Pressure (mb)

M = 4 Atmospheric mass density (kg/m^3)

M = 5 Atmospheric number density ($\text{no.}/\text{m}^3$)
(ZM = $(1.E - 06) * \text{HTPRN}(X,5)$)

The tabular output from file HSPO appears directly below.

NG OR NPIC1 OR NPL EXCEEDS CODE LIMITS

NSP= 3 NEQN= 2 NRATE= 4 NPIC1=400 NG= 2 NPL= 50

THIS IS AN EPISODE RUN

ALTITUDE(METERS)= 3.50000E+04

FLOOR VALUES FOLLOW

1.00000000000000E-20 1.00000000000000E-20

SPECIES FROM CHEMIT

0 03 02

THE NUMBER OF INPUT INITIAL VALUES = 3

03 1.00000000000000E+12
0 1.00000000000000E+06
02 3.70000000000000E+16

GEAR INPUT

TEND= 8.00000E+08 DT= 1.00000E-19 EPS= 1.00000E-04 MF= 22

THE DIFFERENTIAL EQUATIONS ARE

$$D(0)/DT = 2 * QK(3) * 02 + QK(4) * 03 - QK(2) * 0 * 03 - QK(1) * 0 * 02$$

$$D(03)/DT = QK(1) * 0 * 02 - QK(4) * 03 - QK(2) * 0 * 03$$

GRAPH INFORMATION

NG= 2 NFINE= 2 KDEC= 7 ISDEC= -4

THE MAXIMUM NO. OF DECADES IN GRAPHS IS SET BY 1.00000E-10

03 IS GRAPH NUMBER 1

0 IS GRAPH NUMBER 2

1

QK TABLE

1	1.62678E-16
2	4.66000E-16
3	5.00000E-11
4	2.50000E-04

THE 03 SOURCE STRENGTH MAXIMUM IS 1.00000E+11

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
2.78E-08	1.02E+06	1.00E+12	3.70E+16
6.75E-08	1.06E+06	1.00E+12	3.70E+16
1.07E-07	1.10E+06	1.00E+12	3.70E+16
1.47E-07	1.13E+06	1.00E+12	3.70E+16
1.87E-07	1.17E+06	1.00E+12	3.70E+16
2.26E-07	1.20E+06	1.00E+12	3.70E+16
2.66E-07	1.24E+06	1.00E+12	3.70E+16
2.78E-07	1.25E+06	1.00E+12	3.70E+16
6.75E-07	1.60E+06	1.00E+12	3.70E+16
1.07E-06	1.94E+06	1.00E+12	3.70E+16
1.47E-06	2.29E+06	1.00E+12	3.70E+16
1.87E-06	2.63E+06	1.00E+12	3.70E+16
2.26E-06	2.96E+06	1.00E+12	3.70E+16
2.66E-06	3.30E+06	1.00E+12	3.70E+16
2.78E-06	3.40E+06	1.00E+12	3.70E+16
6.75E-06	6.58E+06	1.00E+12	3.70E+16
1.07E-05	9.51E+06	1.00E+12	3.70E+16
1.47E-05	1.22E+07	1.00E+12	3.70E+16
1.87E-05	1.47E+07	1.00E+12	3.70E+16
2.26E-05	1.70E+07	1.00E+12	3.70E+16
2.66E-05	1.90E+07	1.00E+12	3.70E+16
2.78E-05	1.96E+07	1.00E+12	3.70E+16
6.75E-05	3.25E+07	1.00E+12	3.70E+16
1.07E-04	3.78E+07	1.00E+12	3.70E+16
1.47E-04	4.01E+07	1.00E+12	3.70E+16
1.87E-04	4.14E+07	1.00E+12	3.70E+16
2.26E-04	4.23E+07	1.00E+12	3.70E+16
2.66E-04	4.33E+07	1.00E+12	3.70E+16
2.78E-04	4.36E+07	1.00E+12	3.70E+16
6.75E-04	4.59E+07	1.00E+12	3.70E+16
1.07E-03	4.52E+07	1.00E+12	3.70E+16
1.47E-03	4.48E+07	1.00E+12	3.70E+16
1.87E-03	3.85E+07	1.00E+12	3.70E+16
2.26E-03	4.14E+07	1.00E+12	3.70E+16
2.66E-03	4.21E+07	1.00E+12	3.70E+16
2.78E-03	4.21E+07	1.00E+12	3.70E+16
6.75E-03	4.22E+07	1.00E+12	3.70E+16
1.07E-02	4.22E+07	1.00E+12	3.70E+16
1.47E-02	4.22E+07	1.00E+12	3.70E+16
1.87E-02	4.23E+07	1.00E+12	3.70E+16
2.26E-02	4.23E+07	1.00E+12	3.70E+16

2.66E-02	4.23E+07	1.00E+12	3.70E+16
2.78E-02	4.23E+07	1.00E+12	3.70E+16
6.75E-02	4.26E+07	1.00E+12	3.70E+16
1.07E-01	4.28E+07	1.00E+12	3.70E+16
1.47E-01	4.31E+07	1.00E+12	3.70E+16
1.87E-01	4.33E+07	1.00E+12	3.70E+16
2.26E-01	4.36E+07	1.00E+12	3.70E+16
2.66E-01	4.38E+07	1.00E+12	3.70E+16
2.78E-01	4.39E+07	1.00E+12	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
2.78E-08	2.48E+08	-2.44E+08	0.
6.75E-08	2.47E+08	-2.44E+08	0.
1.07E-07	2.47E+08	-2.43E+08	0.
1.47E-07	2.47E+08	-2.43E+08	0.
1.87E-07	2.47E+08	-2.43E+08	0.
2.26E-07	2.46E+08	-2.43E+08	0.
2.66E-07	2.46E+08	-2.43E+08	0.
2.78E-07	2.46E+08	-2.42E+08	0.
6.75E-07	2.44E+08	-2.40E+08	0.
1.07E-06	2.42E+08	-2.38E+08	0.
1.47E-06	2.40E+08	-2.36E+08	0.
1.87E-06	2.38E+08	-2.34E+08	0.
2.26E-06	2.36E+08	-2.32E+08	0.
2.66E-06	2.34E+08	-2.30E+08	0.
2.78E-06	2.33E+08	-2.30E+08	0.
6.75E-06	2.14E+08	-2.10E+08	0.
1.07E-05	1.96E+08	-1.93E+08	0.
1.47E-05	1.80E+08	-1.77E+08	0.
1.87E-05	1.65E+08	-1.62E+08	0.
2.26E-05	1.52E+08	-1.48E+08	0.
2.66E-05	1.39E+08	-1.35E+08	0.
2.78E-05	1.36E+08	-1.32E+08	0.
6.75E-05	5.78E+07	-5.41E+07	0.
1.07E-04	2.58E+07	-2.22E+07	0.
1.47E-04	1.21E+07	-8.44E+06	0.
1.87E-04	4.56E+06	-9.03E+05	0.
2.26E-04	-9.96E+05	4.66E+06	0.
2.66E-04	-6.77E+06	1.04E+07	0.
2.78E-04	-9.07E+06	1.27E+07	0.
6.75E-04	-2.28E+07	2.65E+07	0.
1.07E-03	-1.84E+07	2.20E+07	0.
1.47E-03	-1.59E+07	1.95E+07	0.
1.87E-03	2.19E+07	-1.82E+07	0.
2.26E-03	4.80E+06	-1.14E+06	0.
2.66E-03	4.41E+05	3.22E+06	0.
2.78E-03	1.59E+04	3.64E+06	0.
6.75E-03	1.78E+03	3.66E+06	0.
1.07E-02	1.78E+03	3.66E+06	0.
1.47E-02	1.78E+03	3.66E+06	0.
1.87E-02	1.79E+03	3.66E+06	0.
2.26E-02	1.77E+03	3.66E+06	0.
2.66E-02	1.77E+03	3.66E+06	0.
2.78E-02	1.77E+03	3.66E+06	0.
6.75E-02	1.85E+03	3.66E+06	0.

1.07E-01	1.70E+03	3.66E+06	0.
1.47E-01	1.58E+03	3.66E+06	0.
1.87E-01	1.79E+03	3.66E+06	0.
2.26E-01	1.88E+03	3.66E+06	0.
2.66E-01	1.78E+03	3.66E+06	0.
2.78E-01	1.83E+03	3.66E+06	0.

TIME(HR) QQ TABLE

2.78E-08	6.17E+06	4.78E+02	1.85E+06	2.50E+08
6.75E-08	6.38E+06	4.94E+02	1.85E+06	2.50E+08
1.07E-07	6.59E+06	5.10E+02	1.85E+06	2.50E+08
1.47E-07	6.81E+06	5.27E+02	1.85E+06	2.50E+08
1.87E-07	7.02E+06	5.43E+02	1.85E+06	2.50E+08
2.26E-07	7.23E+06	5.60E+02	1.85E+06	2.50E+08
2.66E-07	7.44E+06	5.76E+02	1.85E+06	2.50E+08
2.78E-07	7.51E+06	5.81E+02	1.85E+06	2.50E+08
6.75E-07	9.61E+06	7.44E+02	1.85E+06	2.50E+08
1.07E-06	1.17E+07	9.05E+02	1.85E+06	2.50E+08
1.47E-06	1.38E+07	1.06E+03	1.85E+06	2.50E+08
1.87E-06	1.58E+07	1.22E+03	1.85E+06	2.50E+08
2.26E-06	1.78E+07	1.38E+03	1.85E+06	2.50E+08
2.66E-06	1.99E+07	1.54E+03	1.85E+06	2.50E+08
2.78E-06	2.05E+07	1.58E+03	1.85E+06	2.50E+08
6.75E-06	3.96E+07	3.07E+03	1.85E+06	2.50E+08
1.07E-05	5.72E+07	4.43E+03	1.85E+06	2.50E+08
1.47E-05	7.35E+07	5.69E+03	1.85E+06	2.50E+08
1.87E-05	8.84E+07	6.84E+03	1.85E+06	2.50E+08
2.26E-05	1.02E+08	7.90E+03	1.85E+06	2.50E+08
2.66E-05	1.15E+08	8.87E+03	1.85E+06	2.50E+08
2.78E-05	1.18E+08	9.15E+03	1.85E+06	2.50E+08
6.75E-05	1.96E+08	1.52E+04	1.85E+06	2.50E+08
1.07E-04	2.28E+08	1.76E+04	1.85E+06	2.50E+08
1.47E-04	2.42E+08	1.87E+04	1.85E+06	2.50E+08
1.87E-04	2.49E+08	1.93E+04	1.85E+06	2.50E+08
2.26E-04	2.55E+08	1.97E+04	1.85E+06	2.50E+08
2.66E-04	2.60E+08	2.02E+04	1.85E+06	2.50E+08
2.78E-04	2.63E+08	2.03E+04	1.85E+06	2.50E+08
6.75E-04	2.76E+08	2.14E+04	1.85E+06	2.50E+08
1.07E-03	2.72E+08	2.11E+04	1.85E+06	2.50E+08
1.47E-03	2.70E+08	2.09E+04	1.85E+06	2.50E+08
1.87E-03	2.32E+08	1.79E+04	1.85E+06	2.50E+08
2.26E-03	2.49E+08	1.93E+04	1.85E+06	2.50E+08
2.66E-03	2.53E+08	1.96E+04	1.85E+06	2.50E+08
2.78E-03	2.54E+08	1.96E+04	1.85E+06	2.50E+08
6.75E-03	2.54E+08	1.97E+04	1.85E+06	2.50E+08
1.07E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
1.47E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
1.87E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
2.26E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
2.66E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
2.78E-02	2.54E+08	1.97E+04	1.85E+06	2.50E+08
6.75E-02	2.54E+08	1.99E+04	1.85E+06	2.50E+08
1.07E-01	2.54E+08	2.00E+04	1.85E+06	2.50E+08
1.47E-01	2.54E+08	2.01E+04	1.85E+06	2.50E+08
1.87E-01	2.54E+08	2.02E+04	1.85E+06	2.51E+08
2.26E-01	2.54E+08	2.04E+04	1.85E+06	2.51E+08
2.66E-01	2.55E+08	2.05E+04	1.85E+06	2.51E+08

2.78E-01 2.55E+08 2.05E+04 1.85E+06 2.51E+08

TIME(HR) QK TABLE

2.78E-08	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-08	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-07	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-06	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-05	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-04	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-03	1.63E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-02	1.62E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-02	1.62E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-02	1.62E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-02	1.62E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-02	1.62E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-02	1.62E-16	4.66E-16	5.00E-11	2.50E-04
6.75E-02	1.61E-16	4.66E-16	5.00E-11	2.50E-04
1.07E-01	1.60E-16	4.66E-16	5.00E-11	2.50E-04
1.47E-01	1.59E-16	4.66E-16	5.00E-11	2.50E-04
1.87E-01	1.59E-16	4.66E-16	5.00E-11	2.50E-04
2.26E-01	1.58E-16	4.66E-16	5.00E-11	2.50E-04
2.66E-01	1.57E-16	4.66E-16	5.00E-11	2.50E-04
2.78E-01	1.57E-16	4.66E-16	5.00E-11	2.50E-04

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
6.75E-01	4.63E+07	1.01E+12	3.70E+16
1.07E+00	4.86E+07	1.01E+12	3.70E+16
1.47E+00	5.08E+07	1.02E+12	3.70E+16
1.87E+00	5.27E+07	1.02E+12	3.70E+16
2.26E+00	5.45E+07	1.03E+12	3.70E+16
2.66E+00	5.60E+07	1.03E+12	3.70E+16
2.78E+00	5.64E+07	1.04E+12	3.70E+16
6.75E+00	5.88E+07	1.09E+12	3.70E+16
1.07E+01	4.84E+07	1.14E+12	3.70E+16
1.47E+01	3.67E+07	1.19E+12	3.70E+16
1.87E+01	2.69E+07	1.25E+12	3.70E+16
2.26E+01	2.43E+07	1.30E+12	3.70E+16
2.66E+01	3.38E+07	1.35E+12	3.70E+16
2.78E+01	3.26E+07	1.37E+12	3.70E+16
6.75E+01	1.38E+05	1.89E+12	3.70E+16
1.07E+02	2.43E+04	2.42E+12	3.70E+16
1.47E+02	3.43E+05	2.95E+12	3.70E+16
1.87E+02	2.03E+06	3.48E+12	3.70E+16
2.26E+02	-7.59E+04	4.01E+12	3.70E+16
2.66E+02	-1.13E+06	4.54E+12	3.70E+16
2.78E+02	-6.28E+05	4.69E+12	3.70E+16
6.75E+02	1.47E+05	9.98E+12	3.70E+16
1.07E+03	5.13E+03	1.53E+13	3.70E+16
1.47E+03	1.47E+04	2.06E+13	3.70E+16
1.87E+03	1.74E+04	2.58E+13	3.70E+16
2.26E+03	2.28E+04	3.11E+13	3.70E+16
2.66E+03	2.33E+04	3.64E+13	3.70E+16
2.78E+03	2.42E+04	3.80E+13	3.70E+16
6.75E+03	6.45E+04	9.08E+13	3.70E+16
1.07E+04	1.02E+05	1.44E+14	3.70E+16
1.47E+04	1.39E+05	1.96E+14	3.70E+16
1.87E+04	1.76E+05	2.49E+14	3.70E+16
2.26E+04	2.13E+05	3.01E+14	3.70E+16
2.66E+04	2.50E+05	3.52E+14	3.70E+16
2.78E+04	2.61E+05	3.68E+14	3.70E+16
6.75E+04	6.10E+05	8.59E+14	3.70E+16
1.07E+05	9.06E+05	1.28E+15	3.70E+16
1.47E+05	1.14E+06	1.61E+15	3.70E+16
1.87E+05	1.31E+06	1.85E+15	3.70E+16
2.22E+05	1.43E+06	2.01E+15	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
6.75E-01	2.08E+03	3.65E+06	0.
1.07E+00	6.47E+03	3.65E+06	0.
1.47E+00	2.69E+03	3.65E+06	0.
1.87E+00	2.21E+04	3.63E+06	0.
2.26E+00	2.19E+04	3.63E+06	0.
2.66E+00	4.23E+03	3.64E+06	0.
2.78E+00	-2.60E+03	3.65E+06	0.
6.75E+00	8.52E+02	3.64E+06	0.
1.07E+01	1.11E+06	2.54E+06	0.
1.47E+01	-8.69E+05	4.53E+06	0.

1.87E+01	-5.74E+06	9.41E+06	0.
2.26E+01	-1.04E+08	1.07E+08	0.
2.66E+01	-5.75E+08	5.79E+08	0.
2.78E+01	-6.64E+08	6.68E+08	0.
6.75E+01	-3.74E+07	4.11E+07	0.
1.07E+02	-1.39E+09	1.40E+09	0.
1.47E+02	-8.20E+10	8.20E+10	0.
1.87E+02	-6.50E+11	6.50E+11	0.
2.26E+02	2.71E+10	-2.71E+10	0.
2.66E+02	3.97E+11	-3.97E+11	0.
2.78E+02	2.21E+11	-2.21E+11	0.
6.75E+02	-4.92E+10	4.92E+10	0.
1.07E+03	2.01E+09	-2.01E+09	0.
1.47E+03	-2.59E+07	2.96E+07	0.
1.87E+03	3.51E+08	-3.47E+08	0.
2.26E+03	-2.34E+08	2.38E+08	0.
2.66E+03	9.05E+08	-9.01E+08	0.
2.78E+03	9.67E+08	-9.63E+08	0.
6.75E+03	2.56E-03	3.69E+06	0.
1.07E+04	-1.24E-01	3.69E+06	0.
1.47E+04	-4.93E-01	3.67E+06	0.
1.87E+04	-4.69E-01	3.66E+06	0.
2.26E+04	-2.99E+00	3.64E+06	0.
2.66E+04	9.18E-02	3.62E+06	0.
2.78E+04	4.54E-01	3.61E+06	0.
6.75E+04	7.95E+00	3.21E+06	0.
1.07E+05	4.32E+02	2.62E+06	0.
1.47E+05	-7.07E+02	1.99E+06	0.
1.87E+05	-1.17E+03	1.44E+06	0.
2.22E+05	5.02E+02	1.03E+06	0.

TIME(HR) QQ TABLE

6.75E-01	2.56E+08	2.18E+04	1.85E+06	2.52E+08
1.07E+00	2.57E+08	2.30E+04	1.85E+06	2.54E+08
1.47E+00	2.58E+08	2.41E+04	1.85E+06	2.55E+08
1.87E+00	2.60E+08	2.52E+04	1.85E+06	2.56E+08
2.26E+00	2.61E+08	2.61E+04	1.85E+06	2.57E+08
2.66E+00	2.62E+08	2.70E+04	1.85E+06	2.59E+08
2.78E+00	2.63E+08	2.72E+04	1.85E+06	2.59E+08
6.75E+00	2.76E+08	2.98E+04	1.85E+06	2.72E+08
1.07E+01	2.88E+08	2.57E+04	1.85E+06	2.85E+08
1.47E+01	3.03E+08	2.04E+04	1.85E+06	2.98E+08
1.87E+01	3.21E+08	1.56E+04	1.85E+06	3.11E+08
2.26E+01	4.32E+08	1.47E+04	1.85E+06	3.24E+08
2.66E+01	9.17E+08	2.13E+04	1.85E+06	3.38E+08
2.78E+01	1.01E+09	2.08E+04	1.85E+06	3.41E+08
6.75E+01	5.15E+08	1.22E+02	1.85E+06	4.73E+08
1.07E+02	2.00E+09	2.74E+01	1.85E+06	6.06E+08
1.47E+02	8.27E+10	4.71E+02	1.85E+06	7.38E+08
1.87E+02	6.51E+11	3.29E+03	1.85E+06	8.70E+08
2.26E+02	-2.61E+10	-1.42E+02	1.85E+06	1.00E+09
2.66E+02	-3.96E+11	-2.39E+03	1.85E+06	1.13E+09
2.78E+02	-2.20E+11	-1.37E+03	1.85E+06	1.17E+09
6.75E+02	5.17E+10	6.83E+02	1.85E+06	2.50E+09
1.07E+03	1.81E+09	3.65E+01	1.85E+06	3.82E+09
1.47E+03	5.17E+09	1.41E+02	1.85E+06	5.14E+09
1.87E+03	6.11E+09	2.09E+02	1.85E+06	6.46E+09

2.26E+03	8.02E+09	3.30E+02	1.85E+06	7.78E+09
2.66E+03	8.20E+09	3.95E+02	1.85E+06	9.10E+09
2.78E+03	8.54E+09	4.29E+02	1.85E+06	9.50E+09
6.75E+03	2.27E+10	2.73E+03	1.85E+06	2.27E+10
1.07E+04	3.59E+10	6.82E+03	1.85E+06	3.59E+10
1.47E+04	4.90E+10	1.27E+04	1.85E+06	4.90E+10
1.87E+04	6.21E+10	2.04E+04	1.85E+06	6.21E+10
2.26E+04	7.52E+10	2.99E+04	1.85E+06	7.52E+10
2.66E+04	8.81E+10	4.11E+04	1.85E+06	8.81E+10
2.78E+04	9.20E+10	4.48E+04	1.85E+06	9.20E+10
6.75E+04	2.15E+11	2.44E+05	1.85E+06	2.15E+11
1.07E+05	3.19E+11	5.39E+05	1.85E+06	3.19E+11
1.47E+05	4.01E+11	8.53E+05	1.85E+06	4.01E+11
1.87E+05	4.62E+11	1.13E+06	1.85E+06	4.62E+11
2.22E+05	5.02E+11	1.33E+06	1.85E+06	5.02E+11

TIME(HR) QK TABLE

6.75E-01	1.49E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+00	1.43E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+00	1.38E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+00	1.33E-16	4.66E-16	5.00E-11	2.50E-04
2.26E+00	1.30E-16	4.66E-16	5.00E-11	2.50E-04
2.66E+00	1.27E-16	4.66E-16	5.00E-11	2.50E-04
2.78E+00	1.26E-16	4.66E-16	5.00E-11	2.50E-04
6.75E+00	1.27E-16	4.66E-16	5.00E-11	2.50E-04
1.07E+01	1.61E-16	4.66E-16	5.00E-11	2.50E-04
1.47E+01	2.23E-16	4.66E-16	5.00E-11	2.50E-04
1.87E+01	3.22E-16	4.66E-16	5.00E-11	2.50E-04
2.26E+01	4.80E-16	4.66E-16	5.00E-11	2.50E-04
2.66E+01	7.33E-16	4.66E-16	5.00E-11	2.50E-04
2.78E+01	8.36E-16	4.66E-16	5.00E-11	2.50E-04
6.75E+01	1.00E-13	4.66E-16	5.00E-11	2.50E-04
1.07E+02	2.23E-12	4.66E-16	5.00E-11	2.50E-04
1.47E+02	6.53E-12	4.66E-16	5.00E-11	2.50E-04
1.87E+02	8.68E-12	4.66E-16	5.00E-11	2.50E-04
2.26E+02	9.31E-12	4.66E-16	5.00E-11	2.50E-04
2.66E+02	9.46E-12	4.66E-16	5.00E-11	2.50E-04
2.78E+02	9.48E-12	4.66E-16	5.00E-11	2.50E-04
6.75E+02	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.07E+03	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.47E+03	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.87E+03	9.52E-12	4.66E-16	5.00E-11	2.50E-04
2.26E+03	9.52E-12	4.66E-16	5.00E-11	2.50E-04
2.66E+03	9.52E-12	4.66E-16	5.00E-11	2.50E-04
2.78E+03	9.52E-12	4.66E-16	5.00E-11	2.50E-04
6.75E+03	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.07E+04	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.47E+04	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.87E+04	9.52E-12	4.66E-16	5.00E-11	2.50E-04
2.26E+04	9.52E-12	4.66E-16	5.00E-11	2.50E-04
2.66E+04	9.52E-12	4.66E-16	5.00E-11	2.50E-04
2.78E+04	9.52E-12	4.66E-16	5.00E-11	2.50E-04
6.75E+04	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.07E+05	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.47E+05	9.52E-12	4.66E-16	5.00E-11	2.50E-04
1.87E+05	9.52E-12	4.66E-16	5.00E-11	2.50E-04
2.22E+05	9.52E-12	4.66E-16	5.00E-11	2.50E-04

The graphical DD80 output appears below.

03

= 1 0

= 2

DD80 Output for ERUNCH Example

3. DRUNCH

The input deck INRATE contains the following information:

Card 1:	NRCHEM = 1	(Col. 4)
Card 2:	ICHEM = 0	(Col. 4)
Cards 3-10:	same as CRUNCH	
Card 11:	NCHANGE = 1	(Col. 4)
Card 12:	K = 89	(Cols. 3-4)
	RMULT = 4.66E-16	(Cols. 5-24)
	IREPLACE = 1	(Col. 28)

The output file OUTPRIN appears below.

THIS IS A DIURNAL RUN

GRAPH INFORMATION FOLLOWS

NG= 2 NFINE= 2 KDEC= 7 ISDEC= -4 YDEC= 1.00000E-10

THE NO. OF POINTS IN THE TX ARRAY IS 800

THE MAXIMUM NUMBER OF LINES IN PRINTOUT TABLES IS 125

THE NO. OF RATES TO BE READ IS 4

THE INPUT RATES FOLLOW

88 89 93 103

THE NO. OF SPECIES NOT FOLLOWED BY THE DIFFERENTIAL EQUATIONS IS 1

THE SPECIES NOT TRACKED ARE AS FOLLOWS

02

USER SHOULD VERIFY THAT UNTRACKED SPECIES APPEAR AT END OF SPECIES LIST BELOW

ALTITUDE(METERS)= 3.50000E+04 TEMPERATURE(K)= 2.36513E+02

UNORDERED RATES FOLLOW

88 89 93 103

ORDERED RATES FOLLOW

88 89 93 103

THE CHEMICAL EQUATIONS FOLLOW

0 + 02 = 03 : R88
0 + 03 = 202 : R89
02 = 0 + 0 : R93
03 = 0 + 02 : R103
END

A DESCRIPTION OF THE D. E. SUBROUTINE FOLLOWS

THE NUMBER OF EQUATIONS IS 2

SPECIES AND THEIR INDEX FOLLOWS

1 0

2 03

3 02

THE DIFFERENTIAL EQUATIONS ARE

$$D(0)/DT = 2 * QK(3) * 02 + QK(4) * 03 - QK(2) * 0 * 03 - QK(1) * 0 * 02$$

$$D(03)/DT = QK(1) * 0 * 02 - QK(4) * 03 - QK(2) * 0 * 03$$

SPECIES PER RATE FOLLOW

RATE NUMBER	1	SPECIES	1	3
RATE NUMBER	2	SPECIES	1	2
RATE NUMBER	3	SPECIES	3	
RATE NUMBER	4	SPECIES	2	

RATES PER DERIVATIVE FOLLOW

DERIVATIVE NUMBER IS	1
RATES	1 2 3 4

DERIVATIVE NUMBER IS	2
RATES	1 2 4

COEFFICIENTS OF THE RATES FOLLOW

DERIVATIVE NUMBER IS	1
COEF.	-1. -1. 2. 1.

DERIVATIVE NUMBER IS	2
COEF.	1. -1. -1.

ZM = 1.75980E+17 (CM-3)

LIBRARY RATE NO. 88 , WHICH IS QK(1), IS DEPENDENT ON ZM

THE NO. OF RATES TO BE CHANGED IS 1 THE RATES FOLLOW

K RMULT IREP

89 4.660000C000000E-16 1

GK NO. LIB. NO. QK

1	88	1.6267812916936E-16
2	89	4.6600000000000E-16
3	93	0.
4	103	0.

THE NO. OF RADIATIVE RATES IS 2

RAD NO. GK NO. LIB. NO.

1	3	93
2	4	103

JACOBIAN OUTPUT FOLLOWS

NO. OF COMPONENTS = 1

The input deck INSTIF contains the following information:

Card 1:	YFLOOR(1) = 1.E + 06	(Cols. 1-20)
	YFLOOR(2) = 1.E + 06	(Cols. 21-40)
Card 2:	Blank	
Card 3:	MYEAR = 1974	(Cols. 3-6)
	MONTH = 9	(Col. 12)
	MDAY = 23	(Col. 17-18)
	TIME = 0.	(Cols. 19-30)
	DLAT = 45.	(Cols. 31-42)
	DLONG = 0.	(Cols. 43-54)
Card 4-7:	same as CRUNCH cards 2-5	
Card 8:	DTNOW = 1.E-30	(Cols. 1-12)
	EPS = 1.E-02	(Cols. 13-24)
	MF = 22	(Cols. 27-28)
Card 9:	same as CRUNCH card 7	
Card 10:	NRDAY = 10	(Cols. 5-6)
Card 11:	DDAY = 0.5	(Cols. 1-12)
	NCOAR = 7	(Col. 16)

The tabular output from file HSP0 appears directly below. Due to the excessive length of this printout, results of the "coarse days" beyond September 25 are not shown.

NG OR NPIC1 OR NPL EXCEEDS CODE LIMITS

NSP= 3 NEQN= 2 NRATE= 4 NPIC1=400 NG= 2 NPL= 50

THIS IS AN EPISODE RUN

ALTITUDE(METERS)= 3.50000E+04

FLOOR VALUES FOLLOW

1.00000000000000E+06 1.00000000000000E+06

NO. OF RADIATIVE RATES CALCULATED BY CODE= 2

QK NO.= 3 RADIATIVE LIBRARY NO.= 15

QK NO.= 4 RADIATIVE LIBRARY NO.= 16

COLUMN DENSITIES

02= 2.59098E+22 03= 8.79959E+18 NO2=-0.

LATITUDE= 4.50000E+01 LONGITUDE=-0.

SPECIES FROM CHEMIT

0 03 02

THE NUMBER OF INPUT INITIAL VALUES = 3

03 1.00000000000000E+12
0 1.00000000000000E+06
02 3.70000000000000E+16

GEAR INPUT

DT= 1.00000E-30 EPS= 1.00000E-02 MF= 22

1

THE DIFFERENTIAL EQUATIONS ARE

$$D(\theta)/DT = 2 * QK(3) * \theta^2 + QK(4) * \theta^3 - QK(2) * \theta * \theta^3 - QK(1) * \theta * \theta^2$$

$$D(\theta^3)/DT = QK(1) * \theta * \theta^2 - QK(4) * \theta^3 - QK(2) * \theta * \theta^3$$

GRAPH INFORMATION

NG= 2 NFINE= 2 KDEC= 7 ISDEC= -4

THE MAXIMUM NO. OF DECADES IN GRAPHS IS SET BY 1.00000E-10

03 IS GRAPH NUMBER 1

0 IS GRAPH NUMBER 2

NUMBER OF DAYS TO RUN = 20

69

QK TABLE

1	1.62678E-16
2	4.66000E-16
3	0.
4	0.

SEPTEMBER 23 1974 AT 0. HOURS

TDAWN= 2.15514E+04

TGUESS= 0.

TDIFF=-2.15514E+04

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
2.78E-08	9.99E+05	1.00E+12	3.70E+16
6.75E-08	9.99E+05	1.00E+12	3.70E+16
1.07E-07	9.98E+05	1.00E+12	3.70E+16
1.47E-07	9.97E+05	1.00E+12	3.70E+16
1.87E-07	9.96E+05	1.00E+12	3.70E+16
2.26E-07	9.95E+05	1.00E+12	3.70E+16
2.66E-07	9.94E+05	1.00E+12	3.70E+16
2.78E-07	9.94E+05	1.00E+12	3.70E+16
6.75E-07	9.85E+05	1.00E+12	3.70E+16
1.07E-06	9.77E+05	1.00E+12	3.70E+16
1.47E-06	9.69E+05	1.00E+12	3.70E+16
1.87E-06	9.60E+05	1.00E+12	3.70E+16
2.26E-06	9.52E+05	1.00E+12	3.70E+16
2.66E-06	9.44E+05	1.00E+12	3.70E+16
2.78E-06	9.42E+05	1.00E+12	3.70E+16
6.75E-06	8.64E+05	1.00E+12	3.70E+16
1.07E-05	7.93E+05	1.00E+12	3.70E+16
1.47E-05	7.27E+05	1.00E+12	3.70E+16
1.87E-05	6.68E+05	1.00E+12	3.70E+16
2.26E-05	6.13E+05	1.00E+12	3.70E+16
2.66E-05	5.62E+05	1.00E+12	3.70E+16
2.78E-05	5.48E+05	1.00E+12	3.70E+16
6.75E-05	2.31E+05	1.00E+12	3.70E+16
1.07E-04	9.50E+04	1.00E+12	3.70E+16
1.47E-04	3.63E+04	1.00E+12	3.70E+16
1.87E-04	1.47E+04	1.00E+12	3.70E+16
2.26E-04	1.14E+04	1.00E+12	3.70E+16
2.66E-04	1.11E+04	1.00E+12	3.70E+16
2.78E-04	1.14E+04	1.00E+12	3.70E+16
6.75E-04	-1.38E+03	1.00E+12	3.70E+16
1.07E-03	-8.74E+02	1.00E+12	3.70E+16
1.47E-03	2.10E+02	1.00E+12	3.70E+16
1.87E-03	-9.82E+01	1.00E+12	3.70E+16
2.26E-03	-6.23E+01	1.00E+12	3.70E+16
2.66E-03	1.17E+01	1.00E+12	3.70E+16
2.78E-03	2.94E+01	1.00E+12	3.70E+16
6.75E-03	-2.22E-03	1.00E+12	3.70E+16
1.07E-02	1.50E+00	1.00E+12	3.70E+16
1.47E-02	7.19E-02	1.00E+12	3.70E+16
1.87E-02	-2.62E-02	1.00E+12	3.70E+16
2.26E-02	-1.64E-02	1.00E+12	3.70E+16

2.66E-02	-3.04E-03	1.00E+12	3.70E+16
2.78E-02	-2.61E-03	1.00E+12	3.70E+16
6.75E-02	-1.75E-08	1.00E+12	3.70E+16
1.07E-01	-1.77E-11	1.00E+12	3.70E+16
1.47E-01	-4.44E-14	1.00E+12	3.70E+16
1.87E-01	-6.68E-17	1.00E+12	3.70E+16
2.26E-01	-2.97E-17	1.00E+12	3.70E+16
2.66E-01	-4.04E-20	1.00E+12	3.70E+16
2.78E-01	-3.64E-20	1.00E+12	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
2.78E-08	-6.02E+06	6.02E+06	0.
6.75E-08	-6.01E+06	6.01E+06	0.
1.07E-07	-6.01E+06	6.00E+06	0.
1.47E-07	-6.00E+06	6.00E+06	0.
1.87E-07	-6.00E+06	5.99E+06	0.
2.26E-07	-5.99E+06	5.99E+06	0.
2.66E-07	-5.98E+06	5.98E+06	0.
2.78E-07	-5.98E+06	5.98E+06	0.
6.75E-07	-5.93E+06	5.93E+06	0.
1.07E-06	-5.88E+06	5.88E+06	0.
1.47E-06	-5.83E+06	5.83E+06	0.
1.87E-06	-5.78E+06	5.78E+06	0.
2.26E-06	-5.73E+06	5.73E+06	0.
2.66E-06	-5.68E+06	5.68E+06	0.
2.78E-06	-5.67E+06	5.67E+06	0.
6.75E-06	-5.20E+06	5.20E+06	0.
1.07E-05	-4.77E+06	4.77E+06	0.
1.47E-05	-4.38E+06	4.38E+06	0.
1.87E-05	-4.02E+06	4.02E+06	0.
2.26E-05	-3.69E+06	3.69E+06	0.
2.66E-05	-3.38E+06	3.38E+06	0.
2.78E-05	-3.30E+06	3.30E+06	0.
6.75E-05	-1.39E+06	1.39E+06	0.
1.07E-04	-5.72E+05	5.72E+05	0.
1.47E-04	-2.18E+05	2.18E+05	0.
1.87E-04	-8.87E+04	8.86E+04	0.
2.26E-04	-6.88E+04	6.88E+04	0.
2.66E-04	-6.68E+04	6.68E+04	0.
2.78E-04	-6.85E+04	6.85E+04	0.
6.75E-04	8.28E+03	-8.28E+03	0.
1.07E-03	5.26E+03	-5.26E+03	0.
1.47E-03	-1.26E+03	1.26E+03	0.
1.87E-03	5.91E+02	-5.91E+02	0.
2.26E-03	3.75E+02	-3.75E+02	0.
2.66E-03	-7.06E+01	7.06E+01	0.
2.78E-03	-1.77E+02	1.77E+02	0.
6.75E-03	1.34E-02	-1.34E-02	0.
1.07E-02	-9.03E+00	9.02E+00	0.
1.47E-02	-4.33E-01	4.33E-01	0.
1.87E-02	1.58E-01	-1.58E-01	0.
2.26E-02	9.90E-02	-9.89E-02	0.
2.66E-02	1.83E-02	-1.83E-02	0.
2.78E-02	1.57E-02	-1.57E-02	0.
6.75E-02	1.05E-07	-1.05E-07	0.

1.07E-01	1.06E-10	-1.06E-10	0.
1.47E-01	2.67E-13	-2.67E-13	0.
1.87E-01	4.02E-16	-4.02E-16	0.
2.26E-01	1.79E-16	-1.79E-16	0.
2.66E-01	2.43E-19	-2.43E-19	0.
2.78E-01	2.19E-19	-2.19E-19	0.

TIME(HR) QQ TABLE

2.78E-08	6.02E+06	4.66E+02	0.	0.
6.75E-08	6.01E+06	4.65E+02	0.	0.
1.07E-07	6.01E+06	4.65E+02	0.	0.
1.47E-07	6.00E+06	4.65E+02	0.	0.
1.87E-07	5.99E+06	4.64E+02	0.	0.
2.26E-07	5.99E+06	4.64E+02	0.	0.
2.66E-07	5.98E+06	4.63E+02	0.	0.
2.78E-07	5.98E+06	4.63E+02	0.	0.
6.75E-07	5.93E+06	4.59E+02	0.	0.
1.07E-06	5.88E+06	4.55E+02	0.	0.
1.47E-06	5.83E+06	4.51E+02	0.	0.
1.87E-06	5.78E+06	4.48E+02	0.	0.
2.26E-06	5.73E+06	4.44E+02	0.	0.
2.66E-06	5.68E+06	4.40E+02	0.	0.
2.78E-06	5.67E+06	4.39E+02	0.	0.
6.75E-06	5.20E+06	4.03E+02	0.	0.
1.07E-05	4.77E+06	3.69E+02	0.	0.
1.47E-05	4.38E+06	3.39E+02	0.	0.
1.87E-05	4.02E+06	3.11E+02	0.	0.
2.26E-05	3.69E+06	2.85E+02	0.	0.
2.66E-05	3.38E+06	2.62E+02	0.	0.
2.78E-05	3.30E+06	2.55E+02	0.	0.
6.75E-05	1.39E+06	1.08E+02	0.	0.
1.07E-04	5.72E+05	4.43E+01	0.	0.
1.47E-04	2.18E+05	1.69E+01	0.	0.
1.87E-04	8.86E+04	6.86E+00	0.	0.
2.26E-04	6.88E+04	5.33E+00	0.	0.
2.66E-04	6.68E+04	5.17E+00	0.	0.
2.78E-04	6.85E+04	5.31E+00	0.	0.
6.75E-04	-8.28E+03	-6.41E-01	0.	0.
1.07E-03	-5.26E+03	-4.07E-01	0.	0.
1.47E-03	1.26E+03	9.79E-02	0.	0.
1.87E-03	-5.91E+02	-4.58E-02	0.	0.
2.26E-03	-3.75E+02	-2.90E-02	0.	0.
2.66E-03	7.06E+01	5.46E-03	0.	0.
2.78E-03	1.77E+02	1.37E-02	0.	0.
6.75E-03	-1.34E-02	-1.03E-06	0.	0.
1.07E-02	9.03E+00	6.99E-04	0.	0.
1.47E-02	4.33E-01	3.35E-05	0.	0.
1.87E-02	-1.58E-01	-1.22E-05	0.	0.
2.26E-02	-9.90E-02	-7.66E-06	0.	0.
2.66E-02	-1.83E-02	-1.41E-06	0.	0.
2.78E-02	-1.57E-02	-1.22E-06	0.	0.
6.75E-02	-1.05E-07	-8.15E-12	0.	0.
1.07E-01	-1.06E-10	-8.23E-15	0.	0.
1.47E-01	-2.67E-13	-2.07E-17	0.	0.
1.87E-01	-4.02E-16	-3.11E-20	0.	0.
2.26E-01	-1.79E-16	-1.39E-20	0.	0.
2.66E-01	-2.43E-19	-1.88E-23	0.	0.

2.78E-01 -2.19E-19 -1.70E-23 0. 0.

TIME(HR) QK TABLE

2.78E-08	1.63E-16	4.66E-16	0.	0.
6.75E-08	1.63E-16	4.66E-16	0.	0.
1.07E-07	1.63E-16	4.66E-16	0.	0.
1.47E-07	1.63E-16	4.66E-16	0.	0.
1.87E-07	1.63E-16	4.66E-16	0.	0.
2.26E-07	1.63E-16	4.66E-16	0.	0.
2.66E-07	1.63E-16	4.66E-16	0.	0.
2.78E-07	1.63E-16	4.66E-16	0.	0.
6.75E-07	1.63E-16	4.66E-16	0.	0.
1.07E-06	1.63E-16	4.66E-16	0.	0.
1.47E-06	1.63E-16	4.66E-16	0.	0.
1.87E-06	1.63E-16	4.66E-16	0.	0.
2.26E-06	1.63E-16	4.66E-16	0.	0.
2.66E-06	1.63E-16	4.66E-16	0.	0.
2.78E-06	1.63E-16	4.66E-16	0.	0.
6.75E-06	1.63E-16	4.66E-16	0.	0.
1.07E-05	1.63E-16	4.66E-16	0.	0.
1.47E-05	1.63E-16	4.66E-16	0.	0.
1.87E-05	1.63E-16	4.66E-16	0.	0.
2.26E-05	1.63E-16	4.66E-16	0.	0.
2.66E-05	1.63E-16	4.66E-16	0.	0.
2.78E-05	1.63E-16	4.66E-16	0.	0.
6.75E-05	1.63E-16	4.66E-16	0.	0.
1.07E-04	1.63E-16	4.66E-16	0.	0.
1.47E-04	1.63E-16	4.66E-16	0.	0.
1.87E-04	1.63E-16	4.66E-16	0.	0.
2.26E-04	1.63E-16	4.66E-16	0.	0.
2.66E-04	1.63E-16	4.66E-16	0.	0.
2.78E-04	1.63E-16	4.66E-16	0.	0.
6.75E-04	1.63E-16	4.66E-16	0.	0.
1.07E-03	1.63E-16	4.66E-16	0.	0.
1.47E-03	1.63E-16	4.66E-16	0.	0.
1.87E-03	1.63E-16	4.66E-16	0.	0.
2.26E-03	1.63E-16	4.66E-16	0.	0.
2.66E-03	1.63E-16	4.66E-16	0.	0.
2.78E-03	1.63E-16	4.66E-16	0.	0.
6.75E-03	1.63E-16	4.66E-16	0.	0.
1.07E-02	1.63E-16	4.66E-16	0.	0.
1.47E-02	1.63E-16	4.66E-16	0.	0.
1.87E-02	1.63E-16	4.66E-16	0.	0.
2.26E-02	1.63E-16	4.66E-16	0.	0.
2.66E-02	1.63E-16	4.66E-16	0.	0.
2.78E-02	1.63E-16	4.66E-16	0.	0.
6.75E-02	1.63E-16	4.66E-16	0.	0.
1.07E-01	1.63E-16	4.66E-16	0.	0.
1.47E-01	1.63E-16	4.66E-16	0.	0.
1.87E-01	1.63E-16	4.66E-16	0.	0.
2.26E-01	1.63E-16	4.66E-16	0.	0.
2.66E-01	1.63E-16	4.66E-16	0.	0.
2.78E-01	1.63E-16	4.66E-16	0.	0.

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
6.75E-01	-2.48E-27	1.00E+12	3.70E+16
1.07E+00	-3.14E-31	1.00E+12	3.70E+16
1.47E+00	-4.68E-35	1.00E+12	3.70E+16
1.87E+00	-8.36E-36	1.00E+12	3.70E+16
2.26E+00	-3.05E-39	1.00E+12	3.70E+16
2.66E+00	-1.23E-39	1.00E+12	3.70E+16
2.78E+00	-6.82E-40	1.00E+12	3.70E+16
5.99E+00	-1.82E-48	1.00E+12	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
6.75E-01	1.49E-26	-1.49E-26	0.
1.07E+00	1.89E-30	-1.89E-30	0.
1.47E+00	2.82E-34	-2.82E-34	0.
1.87E+00	5.03E-35	-5.03E-35	0.
2.26E+00	1.83E-38	-1.83E-38	0.
2.66E+00	7.39E-39	-7.39E-39	0.
2.78E+00	4.10E-39	-4.10E-39	0.
5.99E+00	1.09E-47	-1.09E-47	0.

TIME(HR) QQ TABLE

6.75E-01	-1.49E-26	-1.16E-30	0.	0.
1.07E+00	-1.89E-30	-1.46E-34	0.	0.
1.47E+00	-2.82E-34	-2.18E-38	0.	0.
1.87E+00	-5.03E-35	-3.90E-39	0.	0.
2.26E+00	-1.83E-38	-1.42E-42	0.	0.
2.66E+00	-7.39E-39	-5.72E-43	0.	0.
2.78E+00	-4.10E-39	-3.18E-43	0.	0.
5.99E+00	-1.09E-47	-8.46E-52	0.	0.

TIME(HR) QK TABLE

6.75E-01	1.63E-16	4.66E-16	0.	0.
1.07E+00	1.63E-16	4.66E-16	0.	0.
1.47E+00	1.63E-16	4.66E-16	0.	0.
1.87E+00	1.63E-16	4.66E-16	0.	0.
2.26E+00	1.63E-16	4.66E-16	0.	0.
2.66E+00	1.63E-16	4.66E-16	0.	0.
2.78E+00	1.63E-16	4.66E-16	0.	0.
5.99E+00	1.63E-16	4.66E-16	0.	0.

TDAWN= 1.08073E+05

TGUESS= 1.07951E+05

TDIFF=-1.21304E+02

SEPTEMBER 24 1974 AT 6.02 HOURS

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
2.78E-08	-1.81E-48	1.00E+12	3.70E+16
6.75E-08	-1.81E-48	1.00E+12	3.70E+16
1.07E-07	-1.81E-48	1.00E+12	3.70E+16
1.47E-07	-1.81E-48	1.00E+12	3.70E+16
1.87E-07	-1.81E-48	1.00E+12	3.70E+16
2.26E-07	-1.81E-48	1.00E+12	3.70E+16
2.66E-07	-1.80E-48	1.00E+12	3.70E+16
2.78E-07	-1.80E-48	1.00E+12	3.70E+16
6.75E-07	-1.79E-48	1.00E+12	3.70E+16
1.07E-06	-1.77E-48	1.00E+12	3.70E+16
1.47E-06	-1.76E-48	1.00E+12	3.70E+16
1.87E-06	-1.74E-48	1.00E+12	3.70E+16
2.26E-06	-1.73E-48	1.00E+12	3.70E+16
2.66E-06	-1.71E-48	1.00E+12	3.70E+16
2.78E-06	-1.71E-48	1.00E+12	3.70E+16
6.75E-06	-1.57E-48	1.00E+12	3.70E+16
1.07E-05	-1.45E-48	1.00E+12	3.70E+16
1.47E-05	-1.33E-48	1.00E+12	3.70E+16
1.87E-05	-1.23E-48	1.00E+12	3.70E+16
2.26E-05	-1.14E-48	1.00E+12	3.70E+16
2.66E-05	-1.06E-48	1.00E+12	3.70E+16
2.78E-05	-1.03E-48	1.00E+12	3.70E+16
6.75E-05	-5.14E-49	1.00E+12	3.70E+16
1.07E-04	-2.75E-49	1.00E+12	3.70E+16
1.47E-04	-1.62E-49	1.00E+12	3.70E+16
1.87E-04	-9.24E-50	1.00E+12	3.70E+16
2.26E-04	-6.21E-50	1.00E+12	3.70E+16
2.66E-04	-3.44E-50	1.00E+12	3.70E+16
2.78E-04	-3.20E-50	1.00E+12	3.70E+16
6.75E-04	-1.31E-51	1.00E+12	3.70E+16
1.07E-03	-1.46E-52	1.00E+12	3.70E+16
1.47E-03	-1.80E-53	1.00E+12	3.70E+16
1.87E-03	-5.25E-54	1.00E+12	3.70E+16
2.26E-03	-1.08E-54	1.00E+12	3.70E+16
2.66E-03	-5.15E-55	1.00E+12	3.70E+16
2.78E-03	-3.46E-55	1.00E+12	3.70E+16
6.75E-03	1.38E+02	1.00E+12	3.70E+16
1.07E-02	1.06E+05	1.00E+12	3.70E+16
1.47E-02	3.08E+05	1.00E+12	3.70E+16
1.87E-02	6.12E+05	1.00E+12	3.70E+16
2.26E-02	1.00E+06	1.00E+12	3.70E+16
2.66E-02	1.45E+06	1.00E+12	3.70E+16
2.78E-02	1.60E+06	1.00E+12	3.70E+16
6.75E-02	8.16E+06	1.00E+12	3.70E+16
1.07E-01	1.54E+07	1.00E+12	3.70E+16

1.47E-01	2.14E+07	1.00E+12	3.70E+16
1.87E-01	2.62E+07	1.00E+12	3.70E+16
2.26E-01	3.00E+07	1.00E+12	3.70E+16
2.66E-01	3.31E+07	1.00E+12	3.70E+16
2.78E-01	3.40E+07	1.00E+12	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
2.78E-08	1.09E-47	-1.09E-47	0.
6.75E-08	1.09E-47	-1.09E-47	0.
1.07E-07	1.09E-47	-1.09E-47	0.
1.47E-07	1.09E-47	-1.09E-47	0.
1.87E-07	1.09E-47	-1.09E-47	0.
2.26E-07	1.09E-47	-1.09E-47	0.
2.66E-07	1.09E-47	-1.09E-47	0.
2.78E-07	1.09E-47	-1.09E-47	0.
6.75E-07	1.08E-47	-1.08E-47	0.
1.07E-06	1.07E-47	-1.07E-47	0.
1.47E-06	1.06E-47	-1.06E-47	0.
1.87E-06	1.05E-47	-1.05E-47	0.
2.26E-06	1.04E-47	-1.04E-47	0.
2.66E-06	1.03E-47	-1.03E-47	0.
2.78E-06	1.03E-47	-1.03E-47	0.
6.75E-06	9.46E-48	-9.46E-48	0.
1.07E-05	8.71E-48	-8.71E-48	0.
1.47E-05	8.03E-48	-8.03E-48	0.
1.87E-05	7.43E-48	-7.43E-48	0.
2.26E-05	6.85E-48	-6.85E-48	0.
2.66E-05	6.37E-48	-6.37E-48	0.
2.78E-05	6.23E-48	-6.23E-48	0.
6.75E-05	3.09E-48	-3.09E-48	0.
1.07E-04	1.65E-48	-1.65E-48	0.
1.47E-04	9.76E-49	-9.76E-49	0.
1.87E-04	5.56E-49	-5.56E-49	0.
2.26E-04	3.74E-49	-3.73E-49	0.
2.66E-04	2.07E-49	-2.07E-49	0.
2.78E-04	1.93E-49	-1.93E-49	0.
6.75E-04	7.87E-51	-7.87E-51	0.
1.07E-03	8.76E-52	-8.76E-52	0.
1.47E-03	1.08E-52	-1.08E-52	0.
1.87E-03	3.16E-53	-3.16E-53	0.
2.26E-03	6.50E-54	-6.50E-54	0.
2.66E-03	3.10E-54	-3.10E-54	0.
2.78E-03	2.08E-54	-2.08E-54	0.
6.75E-03	-8.31E+02	8.30E+02	0.
1.07E-02	1.04E+04	-1.05E+04	0.
1.47E-02	1.85E+04	-1.88E+04	0.
1.87E-02	2.56E+04	-2.62E+04	0.
2.26E-02	2.78E+04	-2.87E+04	0.
2.66E-02	4.15E+04	-4.29E+04	0.
2.78E-02	4.20E+04	-4.35E+04	0.
6.75E-02	4.20E+04	-4.96E+04	0.
1.07E-01	-3.38E+03	-1.10E+04	0.
1.47E-01	4.88E+04	-6.88E+04	0.
1.87E-01	-5.79E+04	3.34E+04	0.
2.26E-01	9.80E+04	-1.26E+05	0.

2.66E-01	8.27E+04	-1.14E+05	0.
2.78E-01	1.03E+05	-1.35E+05	0.

TIME(HR) QQ TABLE

2.78E-08	-1.09E-47	-8.45E-52	0.	0.
6.75E-08	-1.09E-47	-8.45E-52	0.	0.
1.07E-07	-1.09E-47	-8.44E-52	0.	0.
1.47E-07	-1.09E-47	-8.43E-52	0.	0.
1.87E-07	-1.09E-47	-8.43E-52	0.	0.
2.26E-07	-1.09E-47	-8.42E-52	0.	0.
2.66E-07	-1.09E-47	-8.41E-52	0.	0.
2.78E-07	-1.09E-47	-8.41E-52	0.	0.
6.75E-07	-1.08E-47	-8.34E-52	0.	0.
1.07E-06	-1.07E-47	-8.27E-52	0.	0.
1.47E-06	-1.06E-47	-8.20E-52	0.	0.
1.87E-06	-1.05E-47	-8.13E-52	0.	0.
2.26E-06	-1.04E-47	-8.06E-52	0.	0.
2.66E-06	-1.03E-47	-7.99E-52	0.	0.
2.78E-06	-1.03E-47	-7.97E-52	0.	0.
6.75E-06	-9.46E-48	-7.32E-52	0.	0.
1.07E-05	-8.71E-48	-6.75E-52	0.	0.
1.47E-05	-8.03E-48	-6.22E-52	0.	0.
1.87E-05	-7.43E-48	-5.75E-52	0.	0.
2.26E-05	-6.85E-48	-5.30E-52	0.	0.
2.66E-05	-6.37E-48	-4.93E-52	0.	0.
2.78E-05	-6.23E-48	-4.82E-52	0.	0.
6.75E-05	-3.09E-48	-2.39E-52	0.	0.
1.07E-04	-1.65E-48	-1.28E-52	0.	0.
1.47E-04	-9.76E-49	-7.56E-53	0.	0.
1.87E-04	-5.56E-49	-4.31E-53	0.	0.
2.26E-04	-3.74E-49	-2.89E-53	0.	0.
2.66E-04	-2.07E-49	-1.60E-53	0.	0.
2.78E-04	-1.93E-49	-1.49E-53	0.	0.
6.75E-04	-7.87E-51	-6.10E-55	0.	0.
1.07E-03	-8.76E-52	-6.78E-56	0.	0.
1.47E-03	-1.08E-52	-8.37E-57	0.	0.
1.87E-03	-3.16E-53	-2.45E-57	0.	0.
2.26E-03	-6.50E-54	-5.03E-58	0.	0.
2.66E-03	-3.10E-54	-2.40E-58	0.	0.
2.78E-03	-2.08E-54	-1.61E-58	0.	0.
6.75E-03	8.30E+02	6.43E-02	0.	1.67E-27
1.07E-02	6.41E+05	4.96E+01	0.	6.51E+05
1.47E-02	1.85E+06	1.44E+02	0.	1.87E+06
1.87E-02	3.68E+06	2.85E+02	0.	3.71E+06
2.26E-02	6.03E+06	4.67E+02	0.	6.05E+06
2.66E-02	8.74E+06	6.77E+02	0.	8.78E+06
2.78E-02	9.62E+06	7.45E+02	0.	9.66E+06
6.75E-02	4.91E+07	3.80E+03	3.69-129	4.92E+07
1.07E-01	9.26E+07	7.17E+03	3.72E-76	9.26E+07
1.47E-01	1.29E+08	9.98E+03	3.52E-53	1.29E+08
1.87E-01	1.58E+08	1.22E+04	2.38E-40	1.58E+08
2.26E-01	1.81E+08	1.40E+04	3.69E-32	1.81E+08
2.66E-01	1.99E+08	1.54E+04	1.06E-23	2.00E+08
2.78E-01	2.04E+08	1.58E+04	2.03E-22	2.04E+08

TIME(HR) QK TABLE

2.78E-08	1.63E-16	4.66E-16	0.	0.
6.75E-08	1.63E-16	4.66E-16	0.	0.
1.07E-07	1.63E-16	4.66E-16	0.	0.
1.47E-07	1.63E-16	4.66E-16	0.	0.
1.87E-07	1.63E-16	4.66E-16	0.	0.
2.26E-07	1.63E-16	4.66E-16	0.	0.
2.66E-07	1.63E-16	4.66E-16	0.	0.
2.78E-07	1.63E-16	4.66E-16	0.	0.
6.75E-07	1.63E-16	4.66E-16	0.	0.
1.07E-06	1.63E-16	4.66E-16	0.	0.
1.47E-06	1.63E-16	4.66E-16	0.	0.
1.87E-06	1.63E-16	4.66E-16	0.	0.
2.26E-06	1.63E-16	4.66E-16	0.	0.
2.66E-06	1.63E-16	4.66E-16	0.	0.
2.78E-06	1.63E-16	4.66E-16	0.	0.
6.75E-06	1.63E-16	4.66E-16	0.	0.
1.07E-05	1.63E-16	4.66E-16	0.	0.
1.47E-05	1.63E-16	4.66E-16	0.	0.
1.87E-05	1.63E-16	4.66E-16	0.	0.
2.26E-05	1.63E-16	4.66E-16	0.	0.
2.66E-05	1.63E-16	4.66E-16	0.	0.
2.78E-05	1.63E-16	4.66E-16	0.	0.
6.75E-05	1.63E-16	4.66E-16	0.	0.
1.07E-04	1.63E-16	4.66E-16	0.	0.
1.47E-04	1.63E-16	4.66E-16	0.	0.
1.87E-04	1.63E-16	4.66E-16	0.	0.
2.26E-04	1.63E-16	4.66E-16	0.	0.
2.66E-04	1.63E-16	4.66E-16	0.	0.
2.78E-04	1.63E-16	4.66E-16	0.	0.
6.75E-04	1.63E-16	4.66E-16	0.	0.
1.07E-03	1.63E-16	4.66E-16	0.	0.
1.47E-03	1.63E-16	4.66E-16	0.	0.
1.87E-03	1.63E-16	4.66E-16	0.	0.
2.26E-03	1.63E-16	4.66E-16	0.	0.
2.66E-03	1.63E-16	4.66E-16	0.	0.
2.78E-03	1.63E-16	4.66E-16	0.	0.
6.75E-03	1.63E-16	4.66E-16	0.	1.67E-39
1.07E-02	1.63E-16	4.66E-16	0.	6.51E-07
1.47E-02	1.63E-16	4.66E-16	0.	1.87E-06
1.87E-02	1.63E-16	4.66E-16	0.	3.71E-06
2.26E-02	1.63E-16	4.66E-16	0.	6.05E-06
2.66E-02	1.63E-16	4.66E-16	0.	8.78E-06
2.78E-02	1.63E-16	4.66E-16	0.	9.66E-06
6.75E-02	1.63E-16	4.66E-16	9.97-146	4.92E-05
1.07E-01	1.63E-16	4.66E-16	1.01E-92	9.26E-05
1.47E-01	1.63E-16	4.66E-16	9.51E-70	1.29E-04
1.87E-01	1.63E-16	4.66E-16	6.44E-57	1.58E-04
2.26E-01	1.63E-16	4.66E-16	9.97E-49	1.81E-04
2.66E-01	1.63E-16	4.66E-16	2.86E-40	2.00E-04
2.78E-01	1.63E-16	4.66E-16	5.49E-39	2.04E-04

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
6.75E-01	4.77E+07	1.00E+12	3.70E+16

1.07E+00	5.30E+07	1.00E+12	3.70E+16
1.47E+00	5.62E+07	1.00E+12	3.70E+16
1.87E+00	5.84E+07	1.00E+12	3.70E+16
2.26E+00	6.01E+07	1.00E+12	3.70E+16
2.66E+00	6.15E+07	9.99E+11	3.70E+16
2.78E+00	6.19E+07	9.99E+11	3.70E+16
6.75E+00	6.59E+07	1.00E+12	3.70E+16
1.07E+01	5.51E+07	9.99E+11	3.70E+16
1.47E+01	2.53E-22	9.99E+11	3.70E+16
1.87E+01	1.67E-31	9.99E+11	3.70E+16
2.26E+01	1.42E-32	9.99E+11	3.70E+16
2.40E+01	1.55E-32	9.99E+11	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
6.75E-01	4.39E+04	-8.84E+04	0.
1.07E+00	1.33E+05	-1.82E+05	0.
1.47E+00	1.63E+05	-2.15E+05	0.
1.87E+00	1.02E+05	-1.56E+05	0.
2.26E+00	-1.83E+04	-3.59E+04	0.
2.66E+00	-2.56E+04	-2.58E+04	0.
2.78E+00	-5.71E+04	7.33E+03	0.
6.75E+00	1.04E+05	-7.18E+04	0.
1.07E+01	5.07E+04	-1.02E+05	0.
1.47E+01	-1.52E-21	1.52E-21	0.
1.87E+01	-1.01E-30	1.01E-30	0.
2.26E+01	-8.53E-32	8.53E-32	0.
2.40E+01	-9.32E-32	9.32E-32	0.

TIME(HR) QQ TABLE

6.75E-01	2.87E+08	2.22E+04	8.63E-06	2.87E+08
1.07E+00	3.19E+08	2.47E+04	1.56E-01	3.19E+08
1.47E+00	3.38E+08	2.62E+04	1.38E+01	3.38E+08
1.87E+00	3.52E+08	2.72E+04	1.81E+02	3.52E+08
2.26E+00	3.62E+08	2.80E+04	9.47E+02	3.62E+08
2.66E+00	3.70E+08	2.87E+04	2.98E+03	3.70E+08
2.78E+00	3.72E+08	2.88E+04	3.93E+03	3.72E+08
6.75E+00	3.96E+08	3.07E+04	4.67E+04	3.97E+08
1.07E+01	3.32E+08	2.57E+04	3.29E+00	3.32E+08
1.47E+01	1.52E-21	1.18E-25	0.	0.
1.87E+01	1.01E-30	7.79E-35	0.	0.
2.26E+01	8.53E-32	6.60E-36	0.	0.
2.40E+01	9.32E-32	7.21E-36	0.	0.

TIME(HR) QK TABLE

6.75E-01	1.63E-16	4.66E-16	2.33E-22	2.87E-04
1.07E+00	1.63E-16	4.66E-16	4.21E-18	3.20E-04
1.47E+00	1.63E-16	4.66E-16	3.72E-16	3.38E-04
1.87E+00	1.63E-16	4.66E-16	4.89E-15	3.52E-04
2.26E+00	1.63E-16	4.66E-16	2.56E-14	3.62E-04

2.66E+00	1.63E-16	4.66E-16	8.05E-14	3.70E-04
2.78E+00	1.63E-16	4.66E-16	1.06E-13	3.73E-04
6.75E+00	1.63E-16	4.66E-16	1.26E-12	3.97E-04
1.07E+01	1.63E-16	4.66E-16	8.89E-17	3.32E-04
1.47E+01	1.63E-16	4.66E-16	0.	0.
1.87E+01	1.63E-16	4.66E-16	0.	0.
2.26E+01	1.63E-16	4.66E-16	0.	0.
2.40E+01	1.63E-16	4.66E-16	0.	0.

DEL TIME IN HOURS FOR COARSE GRAPHS = 5.00000E-01

THE NUMBER OF DAYS PER COARSE GRAPH IS 7

TDawn= 1.94570E+05

TGuess= 1.94473E+05

TDIFF=-9.72125E+01

SEPTEMBER 25 1974 AT 6.05 HOURS

SPECIE CONCENTRATIONS(CM-3)

TIME(HR)	0	03	02
5.00E-01	4.38E+07	9.99E+11	3.70E+16
1.00E+00	5.24E+07	9.99E+11	3.70E+16
1.50E+00	5.64E+07	9.99E+11	3.70E+16
2.00E+00	5.90E+07	9.99E+11	3.70E+16
2.50E+00	6.09E+07	9.99E+11	3.70E+16
3.00E+00	6.24E+07	9.99E+11	3.70E+16
3.50E+00	6.36E+07	9.98E+11	3.70E+16
4.00E+00	6.45E+07	9.98E+11	3.70E+16
4.50E+00	6.51E+07	9.98E+11	3.70E+16
5.00E+00	6.56E+07	9.98E+11	3.70E+16
5.50E+00	6.59E+07	9.98E+11	3.70E+16
6.00E+00	6.59E+07	9.99E+11	3.70E+16
6.50E+00	6.58E+07	9.99E+11	3.70E+16
7.00E+00	6.56E+07	9.99E+11	3.70E+16
7.50E+00	6.51E+07	9.99E+11	3.70E+16
8.00E+00	6.43E+07	9.99E+11	3.70E+16
8.50E+00	6.34E+07	9.98E+11	3.70E+16
9.00E+00	6.22E+07	9.98E+11	3.70E+16
9.50E+00	6.04E+07	9.98E+11	3.70E+16
1.00E+01	5.81E+07	9.98E+11	3.70E+16
1.05E+01	5.55E+07	9.98E+11	3.70E+16
1.10E+01	5.19E+07	9.98E+11	3.70E+16
1.15E+01	4.25E+07	9.98E+11	3.70E+16
1.20E+01	3.64E+06	9.98E+11	3.70E+16
1.25E+01	-8.67E-28	9.98E+11	3.70E+16
1.30E+01	-2.22E-32	9.98E+11	3.70E+16
1.35E+01	-2.36E-36	9.98E+11	3.70E+16
1.40E+01	-9.94E-40	9.98E+11	3.70E+16
1.45E+01	-1.25E-43	9.98E+11	3.70E+16
1.50E+01	-5.88E-44	9.98E+11	3.70E+16
1.55E+01	-5.93E-48	9.98E+11	3.70E+16
1.60E+01	-4.13E-48	9.98E+11	3.70E+16
1.65E+01	-2.34E-48	9.98E+11	3.70E+16
1.70E+01	-5.40E-49	9.98E+11	3.70E+16
1.75E+01	-1.43E-52	9.98E+11	3.70E+16
1.80E+01	-1.11E-52	9.98E+11	3.70E+16
1.85E+01	-7.84E-53	9.98E+11	3.70E+16
1.90E+01	-4.61E-53	9.98E+11	3.70E+16
1.95E+01	-1.38E-53	9.98E+11	3.70E+16
2.00E+01	-3.17E-54	9.98E+11	3.70E+16
2.05E+01	-8.69E-54	9.98E+11	3.70E+16
2.10E+01	-1.42E-53	9.98E+11	3.70E+16
2.15E+01	-1.97E-53	9.98E+11	3.70E+16
2.20E+01	-2.52E-53	9.98E+11	3.70E+16
2.25E+01	-3.08E-53	9.98E+11	3.70E+16

2.30E+01	-2.89E-53	9.98E+11	3.70E+16
2.35E+01	-2.15E-53	9.98E+11	3.70E+16
2.40E+01	-1.41E-53	9.98E+11	3.70E+16
2.40E+01	-1.37E-53	9.98E+11	3.70E+16

SPECIE DERIVATIVES(CM-3 S-1)

TIME(HR)	0	03	02
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5.00E-01	3.99E+05	-4.40E+05	0.
1.00E+00	-9.72E+04	4.85E+04	0.
1.50E+00	-2.62E+05	2.09E+05	0.
2.00E+00	1.22E+05	-1.76E+05	0.
2.50E+00	-4.38E+04	-8.97E+03	0.
3.00E+00	1.15E+05	-1.61E+05	0.
3.50E+00	1.41E+03	-3.42E+04	0.
4.00E+00	-2.02E+04	5.30E+03	0.
4.50E+00	-2.38E+04	2.84E+04	0.
5.00E+00	-6.93E+04	9.13E+04	0.
5.50E+00	-4.18E+03	3.80E+04	0.
6.00E+00	-1.71E+04	5.49E+04	0.
6.50E+00	-1.21E+04	4.53E+04	0.
7.00E+00	-2.15E+02	2.10E+04	0.
7.50E+00	2.06E+05	-2.03E+05	0.
8.00E+00	4.44E+05	-4.61E+05	0.
8.50E+00	5.49E+05	-5.83E+05	0.
9.00E+00	5.21E+05	-5.67E+05	0.
9.50E+00	2.49E+06	-2.54E+06	0.
1.00E+01	4.16E+06	-4.21E+06	0.
1.05E+01	3.85E+06	-3.90E+06	0.
1.10E+01	-1.07E+02	-4.81E+04	0.
1.15E+01	4.10E+05	-4.50E+05	0.
1.20E+01	-2.19E+07	2.19E+07	0.
1.25E+01	5.22E-27	-5.22E-27	0.
1.30E+01	1.34E-31	-1.34E-31	0.
1.35E+01	1.42E-35	-1.42E-35	0.
1.40E+01	5.98E-39	-5.98E-39	0.
1.45E+01	7.54E-43	-7.54E-43	0.
1.50E+01	3.54E-43	-3.54E-43	0.
1.55E+01	3.57E-47	-3.57E-47	0.
1.60E+01	2.49E-47	-2.49E-47	0.
1.65E+01	1.41E-47	-1.41E-47	0.
1.70E+01	3.25E-48	-3.25E-48	0.
1.75E+01	8.61E-52	-8.61E-52	0.
1.80E+01	6.67E-52	-6.67E-52	0.
1.85E+01	4.72E-52	-4.72E-52	0.
1.90E+01	2.78E-52	-2.77E-52	0.
1.95E+01	8.29E-53	-8.29E-53	0.
2.00E+01	1.91E-53	-1.91E-53	0.
2.05E+01	5.23E-53	-5.23E-53	0.
2.10E+01	8.55E-53	-8.55E-53	0.
2.15E+01	1.19E-52	-1.19E-52	0.
2.20E+01	1.52E-52	-1.52E-52	0.
2.25E+01	1.85E-52	-1.85E-52	0.
2.30E+01	1.74E-52	-1.74E-52	0.
2.35E+01	1.29E-52	-1.29E-52	0.
2.40E+01	8.46E-53	-8.46E-53	0.
2.40E+01	8.22E-53	-8.22E-53	0.

TIME(HR) QQ TABLE

5.00E-01	2.63E+08	2.04E+04	1.28E-09	2.64E+08
1.00E+00	3.15E+08	2.44E+04	5.26E-02	3.15E+08
1.50E+00	3.40E+08	2.63E+04	1.84E+01	3.39E+08
2.00E+00	3.55E+08	2.75E+04	3.46E+02	3.55E+08
2.50E+00	3.67E+08	2.84E+04	1.97E+03	3.67E+08
3.00E+00	3.76E+08	2.90E+04	6.11E+03	3.76E+08
3.50E+00	3.83E+08	2.96E+04	1.32E+04	3.83E+08
4.00E+00	3.88E+08	3.00E+04	2.25E+04	3.88E+08
4.50E+00	3.92E+08	3.03E+04	3.26E+04	3.92E+08
5.00E+00	3.95E+08	3.05E+04	4.15E+04	3.95E+08
5.50E+00	3.96E+08	3.06E+04	4.76E+04	3.96E+08
6.00E+00	3.97E+08	3.07E+04	4.96E+04	3.97E+08
6.50E+00	3.96E+08	3.06E+04	4.72E+04	3.96E+08
7.00E+00	3.95E+08	3.05E+04	4.09E+04	3.95E+08
7.50E+00	3.92E+08	3.03E+04	3.18E+04	3.92E+08
8.00E+00	3.87E+08	2.99E+04	2.17E+04	3.88E+08
8.50E+00	3.82E+08	2.95E+04	1.25E+04	3.82E+08
9.00E+00	3.74E+08	2.89E+04	5.66E+03	3.75E+08
9.50E+00	3.63E+08	2.81E+04	1.76E+03	3.66E+08
1.00E+01	3.50E+08	2.70E+04	2.89E+02	3.54E+08
1.05E+01	3.34E+08	2.58E+04	1.33E+01	3.38E+08
1.10E+01	3.12E+08	2.41E+04	2.51E-02	3.12E+08
1.15E+01	2.56E+08	1.98E+04	5.88E-11	2.56E+08
1.20E+01	2.19E+07	1.69E+03	0.	0.
1.25E+01	-5.22E-27	-4.03E-31	0.	0.
1.30E+01	-1.34E-31	-1.03E-35	0.	0.
1.35E+01	-1.42E-35	-1.10E-39	0.	0.
1.40E+01	-5.98E-39	-4.62E-43	0.	0.
1.45E+01	-7.54E-43	-5.82E-47	0.	0.
1.50E+01	-3.54E-43	-2.73E-47	0.	0.
1.55E+01	-3.57E-47	-2.76E-51	0.	0.
1.60E+01	-2.49E-47	-1.92E-51	0.	0.
1.65E+01	-1.41E-47	-1.09E-51	0.	0.
1.70E+01	-3.25E-48	-2.51E-52	0.	0.
1.75E+01	-8.61E-52	-6.66E-56	0.	0.
1.80E+01	-6.67E-52	-5.15E-56	0.	0.
1.85E+01	-4.72E-52	-3.65E-56	0.	0.
1.90E+01	-2.78E-52	-2.14E-56	0.	0.
1.95E+01	-8.29E-53	-6.41E-57	0.	0.
2.00E+01	-1.91E-53	-1.48E-57	0.	0.
2.05E+01	-5.23E-53	-4.04E-57	0.	0.
2.10E+01	-8.55E-53	-6.61E-57	0.	0.
2.15E+01	-1.19E-52	-9.17E-57	0.	0.
2.20E+01	-1.52E-52	-1.17E-56	0.	0.
2.25E+01	-1.85E-52	-1.43E-56	0.	0.
2.30E+01	-1.74E-52	-1.34E-56	0.	0.
2.35E+01	-1.29E-52	-9.98E-57	0.	0.
2.40E+01	-8.46E-53	-6.54E-57	0.	0.
2.40E+01	-8.22E-53	-6.35E-57	0.	0.

TIME(HR) QK TABLE

5.00E-01	1.63E-16	4.66E-16	3.45E-26	2.64E-04
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1.00E+00	1.63E-16	4.66E-16	1.42E-18	3.15E-04
1.50E+00	1.63E-16	4.66E-16	4.99E-16	3.40E-04
2.00E+00	1.63E-16	4.66E-16	9.36E-15	3.56E-04
2.50E+00	1.63E-16	4.66E-16	5.33E-14	3.67E-04
3.00E+00	1.63E-16	4.66E-16	1.65E-13	3.76E-04
3.50E+00	1.63E-16	4.66E-16	3.57E-13	3.83E-04
4.00E+00	1.63E-16	4.66E-16	6.09E-13	3.89E-04
4.50E+00	1.63E-16	4.66E-16	8.81E-13	3.93E-04
5.00E+00	1.63E-16	4.66E-16	1.12E-12	3.95E-04
5.50E+00	1.63E-16	4.66E-16	1.29E-12	3.97E-04
6.00E+00	1.63E-16	4.66E-16	1.34E-12	3.97E-04
6.50E+00	1.63E-16	4.66E-16	1.28E-12	3.97E-04
7.00E+00	1.63E-16	4.66E-16	1.10E-12	3.95E-04
7.50E+00	1.63E-16	4.66E-16	8.59E-13	3.92E-04
8.00E+00	1.63E-16	4.66E-16	5.87E-13	3.88E-04
8.50E+00	1.63E-16	4.66E-16	3.38E-13	3.83E-04
9.00E+00	1.63E-16	4.66E-16	1.53E-13	3.76E-04
9.50E+00	1.63E-16	4.66E-16	4.76E-14	3.67E-04
1.00E+01	1.63E-16	4.66E-16	7.81E-15	3.55E-04
1.05E+01	1.63E-16	4.66E-16	3.60E-16	3.38E-04
1.10E+01	1.63E-16	4.66E-16	6.78E-19	3.13E-04
1.15E+01	1.63E-16	4.66E-16	1.59E-27	2.57E-04
1.20E+01	1.63E-16	4.66E-16	0.	0.
1.25E+01	1.63E-16	4.66E-16	0.	0.
1.30E+01	1.63E-16	4.66E-16	0.	0.
1.35E+01	1.63E-16	4.66E-16	0.	0.
1.40E+01	1.63E-16	4.66E-16	0.	0.
1.45E+01	1.63E-16	4.66E-16	0.	0.
1.50E+01	1.63E-16	4.66E-16	0.	0.
1.55E+01	1.63E-16	4.66E-16	0.	0.
1.60E+01	1.63E-16	4.66E-16	0.	0.
1.65E+01	1.63E-16	4.66E-16	0.	0.
1.70E+01	1.63E-16	4.66E-16	0.	0.
1.75E+01	1.63E-16	4.66E-16	0.	0.
1.80E+01	1.63E-16	4.66E-16	0.	0.
1.85E+01	1.63E-16	4.66E-16	0.	0.
1.90E+01	1.63E-16	4.66E-16	0.	0.
1.95E+01	1.63E-16	4.66E-16	0.	0.
2.00E+01	1.63E-16	4.66E-16	0.	0.
2.05E+01	1.63E-16	4.66E-16	0.	0.
2.10E+01	1.63E-16	4.66E-16	0.	0.
2.15E+01	1.63E-16	4.66E-16	0.	0.
2.20E+01	1.63E-16	4.66E-16	0.	0.
2.25E+01	1.63E-16	4.66E-16	0.	0.
2.30E+01	1.63E-16	4.66E-16	0.	0.
2.35E+01	1.63E-16	4.66E-16	0.	0.
2.40E+01	1.63E-16	4.66E-16	0.	0.
2.40E+01	1.63E-16	4.66E-16	0.	0.

TDawn= 2.81067E+05

TGUESS= 2.80970E+05

TDIFF=-9.71604E+01

The DD80 graphical output appears below. Other examples of DRUNCH applications appear in reference 16.

03

= 1 0

= 2

DD80 Output for DRUNCH Example

SPECIE CONCENTRATION(CM.-3)

OCTOBER 1 1974 TIME (HOURS)

03 * 1 0 * 2

SPECIE CONCENTRATION(CM.-3)

03

= 1 0

= 2

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Appendix A

SOLAR ZENITH ANGLE FORMULAE

The solar zenith angle, θ_z , is shown schematically in Figure A-1. Since atmospheric altitudes of interest are much less than one A.U., the following formula is valid to a good approximation at arbitrary altitudes

$$\begin{aligned} \cos(\theta_z) = & \cos\left[(\text{DLAT})\left(\frac{\pi}{180}\right)\right] \cos(\delta) \cos(\text{LHA}) \\ & + \sin\left[(\text{DLAT})\left(\frac{\pi}{180}\right)\right] \sin(\delta) \end{aligned} \quad , \quad (\text{A-1})$$

where

DLAT $\equiv$ degrees north latitude

$\delta \equiv$ declination angle

LHA $\equiv$ local hour angle

The sine of declination angle, δ , is defined by

$$\sin(\delta) = \sin\left[-23.5 \left(\frac{\pi}{180}\right) \cdot \sin(2\pi \cdot \text{TIMVAR})\right] \quad , \quad (\text{A-2})$$

where

TIMVAR $\equiv$ (hours since autumn equinox)/8760. (there are 8760 hrs/
365 day year)

$$\cos(\delta) = (1 - \sin^2(\delta))^{\frac{1}{2}} \quad (\text{A-3})$$

and

$$\text{LHA} = (\text{hours from local noon}) \cdot \left(\frac{\pi}{12}\right) \quad (\text{A-4})$$

or

$$\text{LHA} = (\text{hours from local midnight} - 12) \cdot \left(\frac{\pi}{12}\right) \quad (\text{A-5})$$

Account has not been taken in these formulae for center of mass aperiodicity of the sun.

Strictly speaking the codes are set up to use TIME in Greenwich time which is simply equal to local time + $\frac{12 \text{ DLONG}}{180}$. DLONG runs from 0 to $\pm 180^\circ$. West longitude is positive, and east is negative. For practical purposes one can input the local time by setting DLONG = 0.

Figure A-1

Appendix B

Radiative Reaction Code #	LLL Library #	Photodissociation Process
1	6	$\text{CH}_2\text{O} \xrightarrow{h\nu} \text{CHO} + \text{H}$
2	7	$\text{CH}_2\text{O} \xrightarrow{h\nu} \text{CO} + \text{H}_2$
3	29	$\text{H}_2\text{O} \xrightarrow{h\nu} \text{HO} + \text{H}$
4	33	$\text{H}_2\text{O}_2 \xrightarrow{h\nu} \text{HO} + \text{HO}$
5	36	$\text{HNO}_2 \xrightarrow{h\nu} \text{HO} + \text{NO}$
6	37	$\text{HNO}_2 \xrightarrow{h\nu} \text{H} + \text{NO}_2$
7	41	$\text{HNO}_3 \xrightarrow{h\nu} \text{HO} + \text{NO}_2$
8	492	$\text{CH}_3\text{CO}_2\text{NO}_2 \xrightarrow{h\nu} \text{CH}_3\text{CO}_3 + \text{NO}_2$
9	61	$\text{N}_2\text{O} \rightarrow \text{N}_2 + \text{O}(\text{D})$
10	64	$\text{N}_2\text{O}_5 \xrightarrow{h\nu} \text{NO}_2 + \text{NO}_2 + \text{O}$
11	65	$\text{N}_2\text{O}_5 \xrightarrow{h\nu} \text{NO}_2 + \text{NO}_3$
12	86	$\text{NO}_2 \xrightarrow{h\nu} \text{NO} + \text{O}(\text{D})$
13	83	$\text{NO}_2 \xrightarrow{h\nu} \text{NO} + \text{O}$
14	85	$\text{NO}_3 \xrightarrow{h\nu} \text{NO}_2 + \text{O}$
15	93	$\text{O}_2 \xrightarrow{h\nu} \text{O} + \text{O}$
16	103	$\text{O}_3 \xrightarrow{h\nu} \text{O} + \text{O}_2$
17	567	$\text{CH}_3\text{ONO}_2 \rightarrow \text{CH}_3\text{O} + \text{NO}_2$

Appendix B

Radiative Reaction Code #	LLL Library #	Photodissociation Process
18	105	$O_3 \rightarrow O_1D + O_2$
19	108	$HN_3 \xrightarrow{h\nu} H + N_3$
20	493	$CH_3CO_2NO_2 \xrightarrow{h\nu} CH_3CO + NO_2 + O_2$
21		
22		
23	114	$N_2O \rightarrow N + NO$
24	116	$NO_3 \xrightarrow{h\nu} NO + O_2$
25	125	$CO_2 \rightarrow CO + O$
26	126	$NH_3 \rightarrow NH_2 + H$
27	570	$CH_3ONO \xrightarrow{h\nu} CH_3O + NO$

LISTINGS OF RADIATIVE LIBRARY DATA

Radiative Bin Limits (nm) and SFLXIN = $I_{\Delta}(\infty)$ (photons/cm² sec)

WLU = Upper

WLC= Center

WLL = Lower

I=	1	WLU= 7.35000E+02	WLC= 7.29966E+02	WLL= 7.25000E+02	SFLXIN= 4.90000E+15
I=	2	WLU= 7.25000E+02	WLC= 7.19966E+02	WLL= 7.15001E+02	SFLXIN= 4.94000E+15
I=	3	WLU= 7.15001E+02	WLC= 7.09966E+02	WLL= 7.05000E+02	SFLXIN= 4.99000E+15
I=	4	WLU= 7.05000E+02	WLC= 6.99964E+02	WLL= 6.94999E+02	SFLXIN= 5.04000E+15
I=	5	WLU= 6.94999E+02	WLC= 6.89964E+02	WLL= 6.85000E+02	SFLXIN= 5.09000E+15
I=	6	WLU= 6.85000E+02	WLC= 6.79964E+02	WLL= 6.75001E+02	SFLXIN= 5.14000E+15
I=	7	WLU= 6.75001E+02	WLC= 6.69963E+02	WLL= 6.65000E+02	SFLXIN= 5.18000E+15
I=	8	WLU= 6.65000E+02	WLC= 6.59962E+02	WLL= 6.55000E+02	SFLXIN= 5.22000E+15
I=	9	WLU= 6.55000E+02	WLC= 6.49962E+02	WLL= 6.45000E+02	SFLXIN= 3.95000E+15
I=	10	WLU= 6.47501E+02	WLC= 6.44991E+02	WLL= 6.42500E+02	SFLXIN= 2.65000E+15
I=	11	WLU= 6.42500E+02	WLC= 6.39990E+02	WLL= 6.37500E+02	SFLXIN= 2.65000E+15
I=	12	WLU= 6.37500E+02	WLC= 6.34991E+02	WLL= 6.32500E+02	SFLXIN= 2.67000E+15
I=	13	WLU= 6.32500E+02	WLC= 6.29990E+02	WLL= 6.27500E+02	SFLXIN= 2.68000E+15
I=	14	WLU= 6.27500E+02	WLC= 6.24990E+02	WLL= 6.22500E+02	SFLXIN= 2.69000E+15
I=	15	WLU= 6.22500E+02	WLC= 6.19990E+02	WLL= 6.17500E+02	SFLXIN= 2.70000E+15
I=	16	WLU= 6.17500E+02	WLC= 6.14990E+02	WLL= 6.12500E+02	SFLXIN= 2.70000E+15
I=	17	WLU= 6.12500E+02	WLC= 6.09990E+02	WLL= 6.07500E+02	SFLXIN= 2.70000E+15
I=	18	WLU= 6.07500E+02	WLC= 6.04990E+02	WLL= 6.02503E+02	SFLXIN= 2.71000E+15
I=	19	WLU= 6.02503E+02	WLC= 5.99990E+02	WLL= 5.97500E+02	SFLXIN= 2.72000E+15
I=	20	WLU= 5.97500E+02	WLC= 5.94990E+02	WLL= 5.92500E+02	SFLXIN= 2.73000E+15
I=	21	WLU= 5.92500E+02	WLC= 5.89990E+02	WLL= 5.87500E+02	SFLXIN= 2.74000E+15
I=	22	WLU= 5.87500E+02	WLC= 5.84990E+02	WLL= 5.82501E+02	SFLXIN= 2.74000E+15

I= 23	WLU= 5.82501E+02	WLC= 5.75989E+02	WLL= 5.77499E+02	SFLXIN= 2.71000E+15
I= 24	WLU= 5.77499E+02	WLC= 5.74989E+02	WLL= 5.72501E+02	SFLXIN= 2.69000E+15
I= 25	WLU= 5.72501E+02	WLC= 5.69989E+02	WLL= 5.67500E+02	SFLXIN= 2.67000E+15
I= 26	WLU= 5.67500E+02	WLC= 5.64989E+02	WLL= 5.62500E+02	SFLXIN= 2.67000E+15
I= 27	WLU= 5.62500E+02	WLC= 5.59989E+02	WLL= 5.57500E+02	SFLXIN= 2.65000E+15
I= 28	WLU= 5.57500E+02	WLC= 5.54989E+02	WLL= 5.52500E+02	SFLXIN= 2.66000E+15
I= 29	WLU= 5.52500E+02	WLC= 5.49989E+02	WLL= 5.47500E+02	SFLXIN= 2.68000E+15
I= 30	WLU= 5.47500E+02	WLC= 5.44989E+02	WLL= 5.42500E+02	SFLXIN= 2.70000E+15
I= 31	WLU= 5.42500E+02	WLC= 5.39989E+02	WLL= 5.37500E+02	SFLXIN= 2.67000E+15
I= 32	WLU= 5.37500E+02	WLC= 5.34989E+02	WLL= 5.32500E+02	SFLXIN= 2.64000E+15
I= 33	WLU= 5.32500E+02	WLC= 5.29989E+02	WLL= 5.27500E+02	SFLXIN= 2.58000E+15
I= 34	WLU= 5.27500E+02	WLC= 5.24989E+02	WLL= 5.22500E+02	SFLXIN= 2.52000E+15
I= 35	WLU= 5.22500E+02	WLC= 5.19989E+02	WLL= 5.17500E+02	SFLXIN= 2.43000E+15
I= 36	WLU= 5.17500E+02	WLC= 5.14989E+02	WLL= 5.12500E+02	SFLXIN= 2.43000E+15
I= 37	WLU= 5.12500E+02	WLC= 5.09989E+02	WLL= 5.07500E+02	SFLXIN= 2.50000E+15
I= 38	WLU= 5.07500E+02	WLC= 5.04989E+02	WLL= 5.02500E+02	SFLXIN= 2.49000E+15
I= 39	WLU= 5.02500E+02	WLC= 4.99989E+02	WLL= 4.97500E+02	SFLXIN= 2.48000E+15
I= 40	WLU= 4.97500E+02	WLC= 4.94987E+02	WLL= 4.92500E+02	SFLXIN= 2.53000E+15
I= 41	WLU= 4.92500E+02	WLC= 4.89987E+02	WLL= 4.87500E+02	SFLXIN= 2.44000E+15
I= 42	WLU= 4.87500E+02	WLC= 4.84987E+02	WLL= 4.82500E+02	SFLXIN= 2.46000E+15
I= 43	WLU= 4.82500E+02	WLC= 4.79987E+02	WLL= 4.77500E+02	SFLXIN= 2.54000E+15
I= 44	WLU= 4.77500E+02	WLC= 4.74987E+02	WLL= 4.72500E+02	SFLXIN= 2.61000E+15
I= 45	WLU= 4.72500E+02	WLC= 4.69987E+02	WLL= 4.67500E+02	SFLXIN= 2.55000E+15
I= 46	WLU= 4.67500E+02	WLC= 4.64987E+02	WLL= 4.62500E+02	SFLXIN= 2.50000E+15
I= 47	WLU= 4.62500E+02	WLC= 4.59986E+02	WLL= 4.57500E+02	SFLXIN= 2.48000E+15
I= 48	WLU= 4.57500E+02	WLC= 4.54986E+02	WLL= 4.52500E+02	SFLXIN= 2.49000E+15
I= 49	WLU= 4.52500E+02	WLC= 4.49986E+02	WLL= 4.47500E+02	SFLXIN= 2.40000E+15
I= 50	WLU= 4.47500E+02	WLC= 4.44986E+02	WLL= 4.42500E+02	SFLXIN= 2.33000E+15
I= 51	WLU= 4.42500E+02	WLC= 4.39986E+02	WLL= 4.37500E+02	SFLXIN= 2.25000E+15
I= 52	WLU= 4.37500E+02	WLC= 4.34986E+02	WLL= 4.32500E+02	SFLXIN= 1.99000E+15

I= 53	WLU= 4.32500E+02	WLC= 4.29985E+02	WLL= 4.27500E+02	SFLXIN= 1.94000E+15
I= 54	WLU= 4.27500E+02	WLC= 4.24985E+02	WLL= 4.22500E+02	SFLXIN= 2.01000E+15
I= 55	WLU= 4.22500E+02	WLC= 4.19985E+02	WLL= 4.17500E+02	SFLXIN= 2.02000E+15
I= 56	WLU= 4.17500E+02	WLC= 4.14985E+02	WLL= 4.12500E+02	SFLXIN= 1.99000E+15
I= 57	WLU= 4.12500E+02	WLC= 4.09985E+02	WLL= 4.07500E+02	SFLXIN= 1.99000E+15
I= 58	WLU= 4.07500E+02	WLC= 4.04985E+02	WLL= 4.02500E+02	SFLXIN= 1.90000E+15
I= 59	WLU= 4.02500E+02	WLC= 3.99984E+02	WLL= 3.97500E+02	SFLXIN= 1.54000E+15
I= 60	WLU= 3.97500E+02	WLC= 3.94984E+02	WLL= 3.92500E+02	SFLXIN= 1.19000E+15
I= 61	WLU= 3.92500E+02	WLC= 3.89984E+02	WLL= 3.87500E+02	SFLXIN= 1.09000E+15
I= 62	WLU= 3.87500E+02	WLC= 3.84984E+02	WLL= 3.82500E+02	SFLXIN= 1.11000E+15
I= 63	WLU= 3.82500E+02	WLC= 3.79983E+02	WLL= 3.77500E+02	SFLXIN= 1.17000E+15
I= 64	WLU= 3.77500E+02	WLC= 3.74983E+02	WLL= 3.72500E+02	SFLXIN= 1.24000E+15
I= 65	WLU= 3.72500E+02	WLC= 3.69983E+02	WLL= 3.67500E+02	SFLXIN= 1.23000E+15
I= 66	WLU= 3.67500E+02	WLC= 3.64983E+02	WLL= 3.62500E+02	SFLXIN= 1.18000E+15
I= 67	WLU= 3.62500E+02	WLC= 3.59983E+02	WLL= 3.57500E+02	SFLXIN= 1.04000E+15
I= 68	WLU= 3.57500E+02	WLC= 3.54982E+02	WLL= 3.52500E+02	SFLXIN= 1.03000E+15
I= 69	WLU= 3.52500E+02	WLC= 3.49982E+02	WLL= 3.47500E+02	SFLXIN= 1.03000E+15
I= 70	WLU= 3.47500E+02	WLC= 3.44982E+02	WLL= 3.42500E+02	SFLXIN= 1.01000E+15
I= 71	WLU= 3.42500E+02	WLC= 3.39982E+02	WLL= 3.37500E+02	SFLXIN= 9.44000E+14
I= 72	WLU= 3.37500E+02	WLC= 3.34981E+02	WLL= 3.32500E+02	SFLXIN= 8.97000E+14
I= 73	WLU= 3.32500E+02	WLC= 3.29981E+02	WLL= 3.27500E+02	SFLXIN= 9.71000E+14
I= 74	WLU= 3.27500E+02	WLC= 3.24981E+02	WLL= 3.22500E+02	SFLXIN= 8.12000E+14
I= 75	WLU= 3.22500E+02	WLC= 3.19980E+02	WLL= 3.17500E+02	SFLXIN= 6.94000E+14
I= 76	WLU= 3.17500E+02	WLC= 3.14980E+02	WLL= 3.12500E+02	SFLXIN= 6.85000E+14
I= 77	WLU= 3.12500E+02	WLC= 3.09980E+02	WLL= 3.07500E+02	SFLXIN= 5.92000E+14
I= 78	WLU= 3.07500E+02	WLC= 3.05332E+02	WLL= 3.03900E+02	SFLXIN= 5.00000E+14
I= 79	WLU= 3.03900E+02	WLC= 3.00732E+02	WLL= 2.99450E+02	SFLXIN= 3.86000E+14
I= 80	WLU= 2.99450E+02	WLC= 2.96203E+02	WLL= 2.94100E+02	SFLXIN= 3.39000E+14
I= 81	WLU= 2.94100E+02	WLC= 2.91985E+02	WLL= 2.90300E+02	SFLXIN= 3.56000E+14
I= 82	WLU= 2.89900E+02	WLC= 2.87785E+02	WLL= 2.85700E+02	SFLXIN= 2.46000E+14

I= 83	WLU= 2.85701E+02	WLC= 2.83687E+02	WLL= 2.81701E+02	SFLXIN= 1.70000E+14
I= 84	WLU= 2.81701E+02	WLC= 2.79737E+02	WLL= 2.77901E+02	SFLXIN= 1.38000E+14
I= 85	WLU= 2.77801E+02	WLC= 2.75887E+02	WLL= 2.74000E+02	SFLXIN= 1.19000E+14
I= 86	WLU= 2.74000E+02	WLC= 2.72137E+02	WLL= 2.70299E+02	SFLXIN= 1.10000E+14
I= 87	WLU= 2.70299E+02	WLC= 2.68438E+02	WLL= 2.66700E+02	SFLXIN= 1.25000E+14
I= 88	WLU= 2.66700E+02	WLC= 2.64938E+02	WLL= 2.63199E+02	SFLXIN= 1.12000E+14
I= 89	WLU= 2.63199E+02	WLC= 2.61439E+02	WLL= 2.59700E+02	SFLXIN= 4.37000E+13
I= 90	WLU= 2.59700E+02	WLC= 2.58039E+02	WLL= 2.56399E+02	SFLXIN= 7.13000E+13
I= 91	WLU= 2.56399E+02	WLC= 2.54790E+02	WLL= 2.53201E+02	SFLXIN= 3.97000E+13
I= 92	WLU= 2.53201E+02	WLC= 2.51590E+02	WLL= 2.50000E+02	SFLXIN= 3.02000E+13
I= 93	WLU= 2.50000E+02	WLC= 2.48440E+02	WLL= 2.46899E+02	SFLXIN= 2.88000E+13
I= 94	WLU= 2.46899E+02	WLC= 2.45391E+02	WLL= 2.43900E+02	SFLXIN= 2.73000E+13
I= 95	WLU= 2.43900E+02	WLC= 2.42442E+02	WLL= 2.41001E+02	SFLXIN= 2.50000E+13
I= 96	WLU= 2.41001E+02	WLC= 2.39542E+02	WLL= 2.38101E+02	SFLXIN= 2.32000E+13
I= 97	WLU= 2.38101E+02	WLC= 2.36692E+02	WLL= 2.35300E+02	SFLXIN= 2.21000E+13
I= 98	WLU= 2.35300E+02	WLC= 2.33942E+02	WLL= 2.32600E+02	SFLXIN= 2.25000E+13
I= 99	WLU= 2.32600E+02	WLC= 2.31241E+02	WLL= 2.29899E+02	SFLXIN= 2.40000E+13
I= 100	WLU= 2.29899E+02	WLC= 2.28592E+02	WLL= 2.27300E+02	SFLXIN= 2.26000E+13
I= 101	WLU= 2.27300E+02	WLC= 2.25933E+02	WLL= 2.24701E+02	SFLXIN= 1.82000E+13
I= 102	WLU= 2.24701E+02	WLC= 2.23443E+02	WLL= 2.22199E+02	SFLXIN= 1.80000E+13
I= 103	WLU= 2.22199E+02	WLC= 2.20993E+02	WLL= 2.19800E+02	SFLXIN= 1.73000E+13
I= 104	WLU= 2.19800E+02	WLC= 2.18594E+02	WLL= 2.17401E+02	SFLXIN= 1.32000E+13
I= 105	WLU= 2.17401E+02	WLC= 2.16104E+02	WLL= 2.15000E+02	SFLXIN= 1.34000E+13
I= 106	WLU= 2.15000E+02	WLC= 2.13895E+02	WLL= 2.12801E+02	SFLXIN= 1.06000E+13
I= 107	WLU= 2.12801E+02	WLC= 2.11646E+02	WLL= 2.10500E+02	SFLXIN= 9.42000E+12
I= 108	WLU= 2.10500E+02	WLC= 2.09394E+02	WLL= 2.08300E+02	SFLXIN= 7.30000E+12
I= 109	WLU= 2.08300E+02	WLC= 2.07245E+02	WLL= 2.06200E+02	SFLXIN= 4.20000E+12
I= 110	WLU= 2.06200E+02	WLC= 2.05600E+02	WLL= 2.05000E+02	SFLXIN= 1.31968E+12
I= 111	WLU= 2.05000E+02	WLC= 2.03750E+02	WLL= 2.02500E+02	SFLXIN= 2.31585E+12
I= 112	WLU= 2.02500E+02	WLC= 2.01250E+02	WLL= 2.00000E+02	SFLXIN= 2.31448E+12

I= 113	WLU= 2.00000E+02	WLC= 1.96250E+02	WLL= 1.98320E+02	SFLXIN= 1.14761E+12
I= 114	WLU= 1.98532E+02	WLC= 1.97840E+02	WLL= 1.97182E+02	SFLXIN= 9.82433E+11
I= 115	WLU= 1.97130E+02	WLC= 1.95940E+02	WLL= 1.94700E+02	SFLXIN= 1.72573E+12
I= 116	WLU= 1.94700E+02	WLC= 1.93550E+02	WLL= 1.92400E+02	SFLXIN= 1.26752E+12
I= 117	WLU= 1.92400E+02	WLC= 1.91320E+02	WLL= 1.90240E+02	SFLXIN= 8.72977E+11
I= 118	WLU= 1.90240E+02	WLC= 1.89230E+02	WLL= 1.88220E+02	SFLXIN= 7.21946E+11
I= 119	WLU= 1.88220E+02	WLC= 1.87280E+02	WLL= 1.85340E+02	SFLXIN= 5.98759E+11
I= 120	WLU= 1.86340E+02	WLC= 1.85480E+02	WLL= 1.84520E+02	SFLXIN= 4.83141E+11
I= 121	WLU= 1.84620E+02	WLC= 1.83840E+02	WLL= 1.83060E+02	SFLXIN= 3.90408E+11
I= 122	WLU= 1.83060E+02	WLC= 1.82350E+02	WLL= 1.81640E+02	SFLXIN= 3.13765E+11
I= 123	WLU= 1.81640E+02	WLC= 1.81000E+02	WLL= 1.80360E+02	SFLXIN= 2.51233E+11
I= 124	WLU= 1.80360E+02	WLC= 1.79810E+02	WLL= 1.79260E+02	SFLXIN= 2.00659E+11
I= 125	WLU= 1.79260E+02	WLC= 1.78760E+02	WLL= 1.78260E+02	SFLXIN= 1.74486E+11
I= 126	WLU= 1.78260E+02	WLC= 1.76930E+02	WLL= 1.75400E+02	SFLXIN= 4.40325E+11
I= 127	WLU= 1.75400E+02	WLC= 1.74647E+02	WLL= 1.73960E+02	SFLXIN= 1.83900E+11
I= 128	WLU= 1.73960E+02	WLC= 1.73147E+02	WLL= 1.72400E+02	SFLXIN= 1.44000E+11
I= 129	WLU= 1.72400E+02	WLC= 1.70938E+02	WLL= 1.69500E+02	SFLXIN= 2.32000E+11
I= 130	WLU= 1.69500E+02	WLC= 1.68000E+02	WLL= 1.66700E+02	SFLXIN= 1.76000E+11
I= 131	WLU= 1.66700E+02	WLC= 1.65288E+02	WLL= 1.63900E+02	SFLXIN= 1.19000E+11
I= 132	WLU= 1.63900E+02	WLC= 1.62590E+02	WLL= 1.61300E+02	SFLXIN= 5.49000E+10
I= 133	WLU= 1.61300E+02	WLC= 1.59989E+02	WLL= 1.58700E+02	SFLXIN= 6.40000E+10
I= 134	WLU= 1.58700E+02	WLC= 1.57440E+02	WLL= 1.56200E+02	SFLXIN= 4.75000E+10
I= 135	WLU= 1.56200E+02	WLC= 1.54991E+02	WLL= 1.53800E+02	SFLXIN= 3.60000E+10
I= 136	WLU= 1.53800E+02	WLC= 1.52641E+02	WLL= 1.51500E+02	SFLXIN= 2.90000E+10
I= 137	WLU= 1.51500E+02	WLC= 1.50341E+02	WLL= 1.49200E+02	SFLXIN= 2.66000E+10
I= 138	WLU= 1.49200E+02	WLC= 1.48092E+02	WLL= 1.47000E+02	SFLXIN= 2.33000E+10
I= 139	WLU= 1.47000E+02	WLC= 1.45942E+02	WLL= 1.44900E+02	SFLXIN= 1.92000E+10
I= 140	WLU= 1.44900E+02	WLC= 1.43842E+02	WLL= 1.42800E+02	SFLXIN= 1.30000E+10
I= 141	WLU= 1.42800E+02	WLC= 1.41793E+02	WLL= 1.40800E+02	SFLXIN= 1.01000E+10
I= 142	WLU= 1.40800E+02	WLC= 1.39844E+02	WLL= 1.38900E+02	SFLXIN= 7.60000E+09

I= 143 WLU= 1.38593E+02 WLC= 1.38393E+02 WLL= 1.37900E+02 SFLXIN= 3.10000E+09
I= 144 WLU= 1.37900E+02 WLC= 1.37445E+02 WLL= 1.37003E+02 SFLXIN= 2.74000E+09
I= 145 WLU= 1.37000E+02 WLC= 1.36498E+02 WLL= 1.36000E+02 SFLXIN= 2.57000E+09
I= 146 WLU= 1.36000E+02 WLC= 1.35549E+02 WLL= 1.35103E+02 SFLXIN= 2.09000E+09
I= 147 WLU= 1.35100E+02 WLC= 1.34643E+02 WLL= 1.34200E+02 SFLXIN= 1.99000E+09
I= 148 WLU= 1.34200E+02 WLC= 1.33749E+02 WLL= 1.33300E+02 SFLXIN= 1.24000E+10

2.700000E	2.235360E+02	1.278711E+17	8.454574E+22	4.142500E+12	3.971753E+18
2.800000E+04	2.245270E+02	1.094440E+17	7.270747E+22	3.955800E+12	3.566838E+18
2.900000E+04	2.255180E+02	9.374134E+16	6.257151E+22	3.756400E+12	3.181228E+18
3.000000E+04	2.265090E+02	8.034972E+16	5.388673E+22	3.546000E+12	2.816108E+18
3.100000E+04	2.275000E+02	6.892066E+16	4.644147E+22	3.339800E+12	2.471818E+18
3.200000E+04	2.284900E+02	5.916031E+16	4.004698E+22	3.153200E+12	2.147168E+18
3.300000E+04	2.309730E+02	5.051034E+16	3.457628E+22	2.888200E+12	1.845098E+18
3.400000E+04	2.337430E+02	4.315334E+16	2.990468E+22	2.612300E+12	1.570073E+18
3.500000E+04	2.365130E+02	3.693820E+16	2.590976E+22	2.340900E+12	1.322413E+18
3.750000E+04	2.434344E+02	2.524260E+16	1.823906E+22	1.733500E+12	8.131127E+17
4.000000E+04	2.503500E+02	1.743891E+16	1.296978E+22	1.171900E+12	4.499377E+17
4.250000E+04	2.572596E+02	1.217394E+16	9.311407E+21	6.467200E+11	2.226102E+17
4.500000E+04	2.641640E+02	8.581761E+15	5.745680E+21	2.969900E+11	1.045465E+17
4.750000E+04	2.703481E+02	6.122744E+15	4.928872E+21	1.374500E+11	5.034150E+16
5.000000E+04	2.706503E+02	4.481785E+15	3.614877E+21	7.629800E+10	2.362300E+16
5.250000E+04	2.702463E+02	3.290576E+15	2.651867E+21	4.305400E+10	8.704000E+15

ALTITUDES ABOVE 55 KM ARE ASSIGNED COLO3=0.

5.500000E+04	2.655940E+02	2.447434E+15	1.939938E+21	2.657800E+10	0.
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Appendix C

W. UPDATED CO3

STANDARD ATMOSPHERE USED IN LLL KINETICS CODES

ALTITUDE (M)	TEMP(DEG. K)	O2 (NO./CM+3)	COLO2	O3 (NO./CM+3)	COLO3
1.000000E+03	2.816510E+02	4.851830E+18	4.010180E+24	1.118500E+12	8.613049E+18
2.000000E+03	2.751540E+02	4.392997E+18	3.548267E+24	1.001500E+12	8.507049E+18
3.000000E+03	2.686590E+02	3.968369E+18	3.130511E+24	8.974000E+11	8.412104E+18
4.000000E+03	2.621660E+02	3.576066E+18	2.753582E+24	8.047300E+11	8.326997E+18
5.000000E+03	2.556760E+02	3.214199E+18	2.414347E+24	7.224600E+11	8.250638E+18
6.000000E+03	2.491870E+02	2.881087E+18	2.109842E+24	6.498900E+11	8.182020E+18
7.000000E+03	2.427000E+02	2.575053E+18	1.837286E+24	5.867300E+11	8.120189E+18
8.000000E+03	2.362150E+02	2.294837E+18	1.594021E+24	5.335700E+11	8.064174E+18
9.000000E+03	2.297330E+02	2.038465E+18	1.377575E+24	4.936300E+11	8.012814E+18
1.000000E+04	2.232520E+02	1.804741E+18	1.185797E+24	4.853800E+11	7.963864E+18
1.100000E+04	2.167740E+02	1.592154E+18	1.015543E+24	5.767200E+11	7.910759E+18
1.200000E+04	2.166500E+02	1.361432E+18	8.681907E+23	6.764500E+11	7.848100E+18
1.300000E+04	2.166500E+02	1.163539E+18	7.422321E+23	8.047500E+11	7.774039E+18
1.400000E+04	2.166500E+02	9.944642E+17	6.345793E+23	9.643400E+11	7.685585E+18
1.500000E+04	2.166500E+02	8.499900E+17	5.425682E+23	1.158800E+12	7.579428E+18
1.600000E+04	2.166500E+02	7.265479E+17	4.639221E+23	1.391300E+12	7.451923E+18
1.700000E+04	2.166500E+02	6.210731E+17	3.966950E+23	1.666000E+12	7.299058E+18
1.800000E+04	2.166500E+02	5.309211E+17	3.392274E+23	1.98E100E+12	7.116453E+18
1.900000E+04	2.166500E+02	4.538878E+17	2.901056E+23	2.350700E+12	6.899613E+18
2.000000E+04	2.166500E+02	3.880421E+17	2.480843E+23	2.751900E+12	6.644483E+18
2.100000E+04	2.175810E+02	3.304456E+17	2.122477E+23	3.157800E+12	6.348998E+18
2.200000E+04	2.185740E+02	2.815599E+17	1.817219E+23	3.551500E+12	6.013538E+18
2.300000E+04	2.195670E+02	2.400626E+17	1.557044E+23	3.892900E+12	5.641313E+18
2.400000E+04	2.205600E+02	2.048582E+17	1.335118E+23	4.145500E+12	5.239393E+18
2.500000E+04	2.215520E+02	1.749433E+17	1.145670E+23	4.270400E+12	4.818598E+18
2.600000E+04	2.225440E+02	1.495118E+17	9.838247E+22	4.262000E+12	4.391978E+18

Figure C-1

Distribution

Internal

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A. Holzer	
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