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ANALYTIC AND NUMERICAL CHEMISTRY ALGORITHMS FOR THE WORRY CODE. WORRY DOCUMENT NUMBER 2

David W. Goetz, et al

Air Force Weapons Laboratory
Kirtland Air Force Base, New Mexico

June 1975

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ANALYTIC AND NUMERICAL CHEMISTRY ALGORITHMS FOR THE WORRY CODE

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June 1975

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AIR FORCE WEAPONS LABORATORY
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The WORRY Chemistry Package computes the nonequilibrium chemical behavior of a parcel of air in a quiescent or disturbed environment. Such a computation requires the solution of a set of nonlinear coupled differential equations derived from the set of reactions in which the atomic and molecular species of the parcel participate. The Chemistry Package may solve this set of differential equations by either of two methods: a standard numerical integration or an analytic algorithm. The procedures used in the analytic algorithm are described in detail and comparisons with the numerical solutions are shown.

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SECTION I

INTRODUCTION

Nuclear weapon effects codes such as the Air Force Weapons Laboratory (AFWL) WORRY optical-IR systems code require the repetitive and fast computation of non-equilibrium atmospheric chemical behavior at numerous points in a disturbed environment. Such computations necessitate the solution of a set of nonlinear coupled differential equations, often stiff, which describe the kinetic behavior of the chemical species of interest. The algorithm which is chosen for solution of these differential equations must be fast in computational time, reliable, and versatile in handling various initial conditions of species, temperature, and density.

At the inception of WORRY in late 1970-early 1971 a limited but adequate set of chemical species, table I, and their reactions, table II, were chosen to describe the terrestrial atmosphere from an optical/infrared viewpoint under both ambient and disturbed conditions. Several reliable algorithms were available for numerical integration of the differential equations defined by these species and their reactions. However, none were fast enough even in the most favorable situations and under adverse conditions e.g., at altitudes below 30 km, they often become inoperative. The answer to the need for a better algorithm was found by devising an analytic solution to the set of differential equations.

An analytic solution requires the making of simplifying assumptions that decouple the differential equations to a degree which leaves the remaining equations amenable to analytic solution. These assumptions obviously limit the generality and applicability of the method. The key to choosing a useful algorithm lies in defining a working range for the solutions and balancing uncertainties - in reactions, reaction rates, and solution assumptions. The analytic algorithm for WORRY was so conceived. Since the chemical behavior to be described by the solution was limited by the structure of the WORRY code to points outside any fireballs, the two basic limiting assumptions of the analytic algorithms, (1) the molecular temperature does not exceed ~ 1200°K and (2) the fractional ionization does not exceed ~ 0.1 percent, were acceptable.

The continued development of the WORRY analytic algorithm has required a standard against which to judge its effectiveness. Therefore, a total chemistry package was developed for WORRY, containing both the analytic algorithm and a numerical algorithm to solve the same set of differential equations "exactly" and serve as a check on the "correctness" of the analytic solution. To ensure the comparability of outputs, both algorithms share the same inputs and the same subroutines which calculate initial conditions and reaction rates.

The analytic algorithm to be described in section IV is undergoing continual change. The description in section IV and the code listing (with external driver) found in section VII reflect the status of the chemistry package at the time of the writing of this document.

Table 1

WORRY SPECIES

H, Li, Be, Mg, Al, Si, Ti, Fe, Cu, U

OH, LiO, BeO, MgO, AlO, SiO, TiO, FeO, CuO, UO^+

NO^+, NO, NO_2, N_2O, CO, CO_2, O_3, H_2O, CN, e^-

N_2, $N_2(A)$, $N_2(B)$, $N(^4S)$, $N(^2D)$, $N(^2P)$, $O(^3P)$, $O(^1D)$, $O(^1S)$, O^-

N_2^+, O_2^+, N^+, O^+, $N_2^+(A)$, $N_2^+(B)$, O_2, $O_2(^1\Delta)$, $O_2(^1\Sigma)$, $O_2(^3\Sigma)$

H_2, UO, NO(A), NO(B), NO(C), NO(D), CN(A)

TABLE II

REACTIONS AND RATE CONSTANTS

$$k = a(T/300)^b \exp(-c/T)\ [M]^d$$

T = temperature (°K)

X = Li, Be, Mg, Al, Si, Ti, Fe, or Cu

	a	b	c	d
1. $N(^4S) + O_2 \rightarrow NO + O$	6.68×10^{12}	0	3590	0
$N(^2P) + O_2 \rightarrow NO + O$				
2. $N(^2D) + O_2 \rightarrow NO + O$	6.0×10^{-12}	.5	0	0
3. $N(^4S) + NO \rightarrow N_2 + O$	5.1×10^{-11}	0	168	0
$N(^2P) + NO \rightarrow N_2 + O$				
4. $N(^2D) + NO \rightarrow N_2 + O$	6.0×10^{-11}	.5	0	0
5. $O + O_2 + M \rightarrow O_3 + M$	2.8×10^{-35}	0	-900	1
6. $O + O_3 \rightarrow O_2 + O_2$	2.0×10^{-11}	0	2400	0
7. $N_2^+ + e \rightarrow 0.99\ N(^4S) + 0{,}99\ N(^2D) + 0.02\ N(^2P)$	2.8×10^{-7}	-.2	0	0
8. $N_2^+ + O_2 \rightarrow O_2^+ + N_2$	2.0×10^{-10}	0	0	0
9. $N_2^+ + O \rightarrow NO^+ + 0.5\ N(^4S) + 0.5\ N(^2D)$	2.5×10^{-10}	0	0	0

Table II (Cont'd)

	a	b	c	d
10. $O_2^+ + e \rightarrow 0.8\ O(^3P) + 0.8\ O(^1D) + 0.4\ O(^1S)$	2.2×10^{-7}	-.7	0	0
11. $O^+ + O_2 \rightarrow O_2^+ + O(^3P)$	2.0×10^{-11}	0	0	0
12. $NO^+ + e \rightarrow 0.75\ O(^3P) + 0.75\ N(^2D) + 0.25\ O(^1D) + 0.25\ N(^4S)$	5.0×10^{-7}	-1.2	0	0
13. $O_2 + N^+ \rightarrow O_2^+ + 0.5\ N(^4S) + 0.5\ N(^2D)$	2.5×10^{-10}	0	0	0
14. $O_2 + N^+ \rightarrow NO^+ + O(^3P)$	5.0×10^{-10}	0	0	0
15. $N_2 + O^+ \rightarrow NO^+ + N(^4S)$	1.3×10^{-12}	0	0	0
16. $O^+ + NO \rightarrow NO^+ + O(^3P)$	2.4×10^{-11}	0	0	0
17. $O_2^+ + NO \rightarrow NO^+ + O_2$	8.0×10^{-10}	0	0	0
18. $N_2^+ + NO \rightarrow NO^+ + N_2$	5.0×10^{-10}	0	0	0
19. $N^+ + NO \rightarrow NO^+ + 0.5\ N(^4S) + 0.5\ N(^2D)$	8.0×10^{-10}	0	0	0

Table II (Cont'd)

	a	b	c	d
20. $O_2^+ + N \rightarrow NO^+ + O(^3P)$	1.8×10^{-10}	0	0	0
21. $H + O_3 \rightarrow OH + O_2$	2.6×10^{-11}	0	0	0
22. $OH + O \rightarrow H + O_2$	5.0×10^{-11}	0	0	0
23. $O_2(^3\Sigma) + O_2 \rightarrow O_3 + O$	1.0×10^{-12}	0	0	0
24. $O_3 + NO \rightarrow NO_2 + O_2$	9.5×10^{-13}	0	1300	0
25. $O + NO + M \rightarrow NO_2 + M$	1.3×10^{-31}	-2.5	0	1
26. $O + NO_2 \rightarrow NO + O_2$	2.8×10^{-11}	0	550	0
27. $NO_2 + N \rightarrow N_2 + O_2$	1.5×10^{-11}	0	0	0
28. $NO + N + M \rightarrow N_2O + M$	1.0×10^{-34}	0	1000	1
29. $NO_2 + N \rightarrow N_2O + O$	1.5×10^{-11}	0	0	0
30. $O_2(^1\Delta) + N_2O \rightarrow N_2 + O_3$	1.0×10^{-13}	0	0	0
31. $N(^4S) + O_3 \rightarrow NO + O_2$	3.4×10^{-11}	.5	1200	0
32. $N(^2P) \rightarrow N(^2D) + h\nu$	7.78×10^{-2}	0	0	0
33. $O(^1S) \rightarrow O(^1D) + h\nu$	6.99×10^{-1}	0	0	0
34. $O(^1D) \rightarrow O(^3P) + h\nu$	6.25×10^{-3}	0	0	0

Table II (Cont'd)

		a	b	c	d
35.	$N^+ + O \rightarrow O^+ + N(^4S)$	1.0×10^{-12}	0	0	0
36 - 49	for future expansion				
50 - 83	for metals reactions				
	$X + O_2 \rightarrow XO + O$				
	$X + O + M \rightarrow XO + M$				
	$X + O_3 \rightarrow XO + O_2$				
	$XO + O \rightarrow X + O_2$				
	$XO + O_3 \rightarrow X + O_2 + O_2$				
84 - 89	for future expansion				
90	$O_3 + h\nu \rightarrow O_2 + O(^3P)$				

SECTION II

CHEMISTRY PACKAGE STRUCTURE

The WORRY Chemistry Package is structured as shown in the flow chart of figure 1. A requesting program calls DECAYR which either executes the analytic algorithm or transfers control to the numerical algorithm executive, DECAR, which employs subroutines FUNG and EVIL. The three routines and one entry point shared by both analytic and numerical solutions are ENTDEP, ENQDEP, RATE, and RRCRT. ENTDEP calculates the initial distribution of ions and neutrals produced by prompt energy deposition (ergs/cc), while the entry point ENQDEP partitions the continuous energy deposition (ion pairs/cc/sec) among the same set of ions and neutrals. For a given temperature and total density, the RATE subroutine fills the R array with the first-order, second-order, and pseudo-second-order reaction rate constants of the set of reactions in table II. RRCRT stores the species destruction rates and transforms the species formation rates as calculated by either algorithm into vibrational level formation rates to be used in the WORRY calculation of chemiluminescence. The remaining entries in figure 1 are functions used by DECAYR in its analytic solutions and will be elaborated in sections IV and V.

The chemistry package requires the following inputs for a problem:

1. The time, t_c, after instantaneous energy deposition for which the calculation is to be performed.
2. The initial, predeposition temperature (°K).
3. The instantaneous energy deposition (ergs/cm^3) at $t = 0$.
4. The continuous energy deposition (ion pairs/cm^2/sec) at t_c.
5. The time of calculation, as day or night.
6. Concentrations for any metals present.

7. An initial set of species concentrations at t = 0 for ambient or previously insulted conditions. Ambient initialization may be accomplished by a prior call to the chemistry package with ambient inputs for 2, 3, and 4, a large value for t_c, and values for the concentrations of N_2, O_2, O, O_3, NO, CO_2, H, and OH.

The inputs as well as chemistry package outputs are accomplished through either the DECAYR calling arguments or COMMON blocks. The energy depositions (inputs), temperature (input/output), and time of calculation (input), are found in the DECAYR calling arguments. The variable DAY (input) is found in COMMON BURST and the DYMETL array (input) holds the metals concentrations (to be added to any preexisting concentrations). The CMD array (input/output) in COMMON XUX holds the concentrations of all species while the outputs of subroutine RRCRT are found in commoned arrays RR and RCRT.

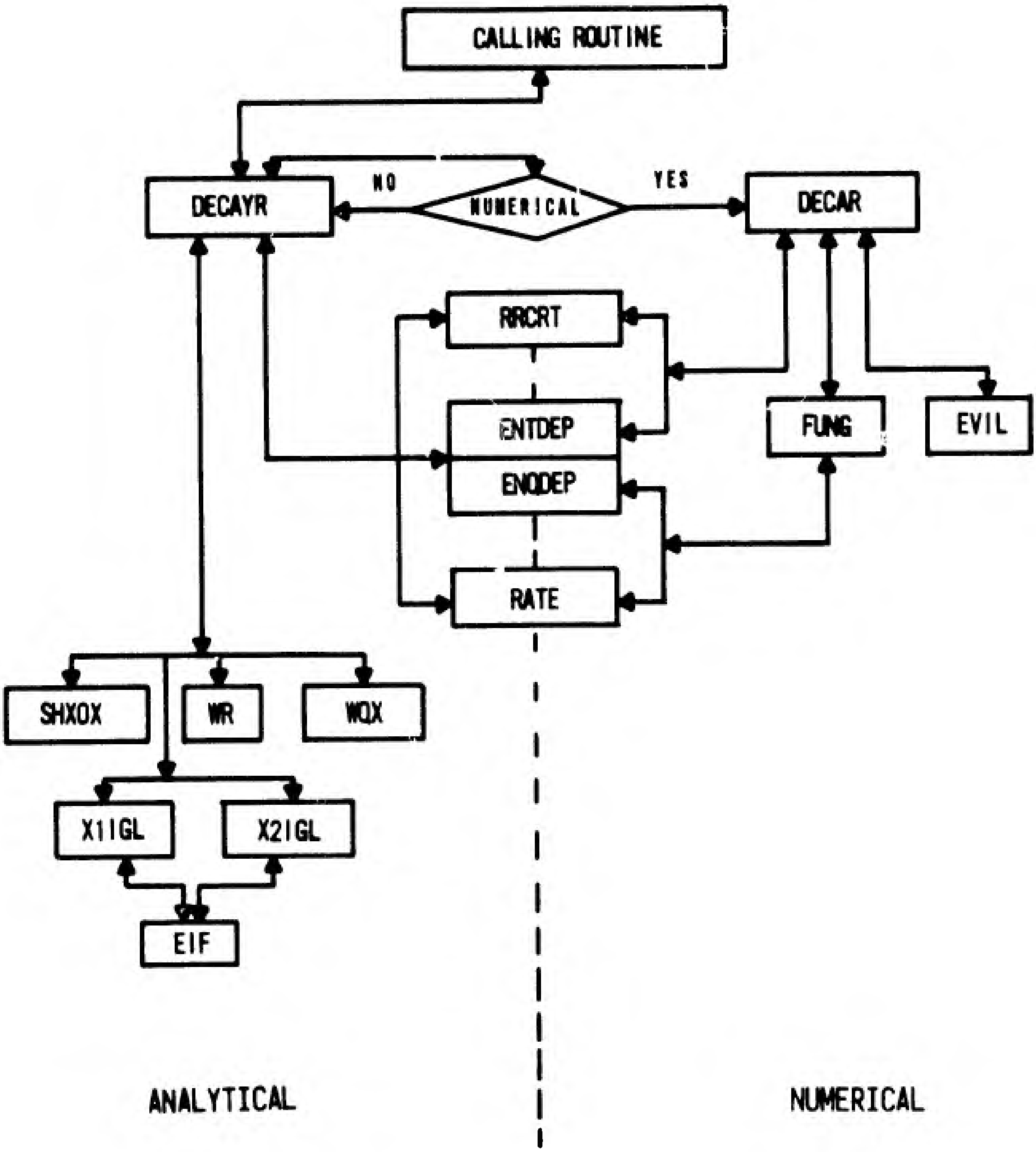

Figure 1. Flow Chart of Routines in WORRY Chemistry Package.

SECTION III

NUMERICAL CHEMISTRY

In DECAR, the numerical chemistry algorithm begins by calling ENTDEP to initialize the species concentrations and choosing an initial time step, DT, of 10^5/CON, where CON is the total number density. The numerical integration is performed by a modified Kenneshea technique. The differential equation for each species is assued to have the form $d[x]/dt = P - R\,[x]$, where $[x]$ is the species concentration, P is the production rate in $cc^{-1}\ sec^{-1}$, and R is the removal rate in sec^{-1}. P and R are assumed to be independent of [x]; and if they are assumed to be constant over the time interval DT, the solution may be written.

$$[x(T+DT)] = ([x(T)] - P/R)E^{-RT} + P/R \qquad (1)$$

P and R are evaluated at time T; [x] is then evaluated at (T+DT) and used to evaluate P and R at (T+DT). These values of P and R are then used with [x(T)] to re-evaluate [x] at (T+DT). It is required that $|[x(T+DT)] - [x(T)]|/[x(T)]$ be less than ε for each species, where $\varepsilon = 10^{-4}$ at the present time. The above process of requiring convergence is repeated three times, and if the requirement is not met, DT is halved. If the requirement is met, DT is doubled for the next step. This process is continued until the desired calculational time, END, is reached. When END is reached, RRCRT is called and the algorithm is complete.

The subroutine FUNG is used to evaluate P and R, and the subroutine EVIL is used to calculate [x(T+DT)] from [x(T)], P, and R. In addition to the species concentrations, the internal kinetic energy of the gas is carried as a variable in the CMD array. The release and absorption of energy for each reaction is calculated in FUNG, and the energy is updated along with the other species. The updated energy is used to calculate a new temperature for each time step and a call to RATE is made to recalculate the reaction rate constants if necessary.

SECTION IV

ANALYTIC CHEMISTRY

As in the numerical chemistry, the analytic algorithm found in subroutine DECAYR begins by calling ENTDEP to update the CMD species array for the prompt energy deposition production of ions and neutrals at $t = 0$. The resultant updated temperature from ENTDEP is then used in a call to the RATE routine which fills the R array with all necessary rates constants for the reactions of table 2. As a final initialization step, the algorithm calculates the total energy of the sample volume using a table of heats of formation, the CMD array of species concentrations, and the total internal kinetic energy of the volume as calculated in ENTDEP.

The first assumption in the analytic algorithm is the separation of the fast-charged species from the slower neutral species chemistry. This separation and the following treatment are acceptable under (and lead to) the two basic assumptions of the analytic algorithm listed in section I. The faster charged species reactions are treated first and the resultant heating is calculated before the neutral species chemistry is begun. The charged species--N^+, O^+, N_2^+, O_2^+, and NO^+ --react primarily through charge exchange and recombination reactions as found in reactions 7-20 and 35. The following description tracks the computer coding closely through the charged species and neutral species chemistries.

1. NITROGEN ION (N^+)

N^+ is at the top of the charge exchange chain and has no production from other species reactions. Assuming, as will be done successfully in many cases throughout the analytic treatment, that the concentrations of the species with which N^+ reacts are constant, the N^+ loss mechanisms of reactions 13, 14, 19 and 35 result in the homogeneous differential equation for $[N^+]$.

$$d[N^+]/dt = - \left\{k_{13}[O_2] + k_{14}[O_2] + k_{19}[NO] + k_{35}[O]\right\} [N^+] \qquad (2)$$

The sum of constant quantities multiplying $[N^+]$ is defined as β_N and the equation is rewritten as

$$d[N^+]/dt = - \beta_N[N^+] \qquad (3)$$

to which the solution is a simple exponential decay.

$$[N^+] = [N^+]_o e^{-\beta_N t} \qquad (4)$$

The full differential equation for $[N^+]$ including the continuous source is

$$d[N^+]/dt = Q_N{+} - \beta_N[N^+] \qquad (5)$$

where $Q_N{+}$ is the production rate of $[N^+]$ from the continuous energy deposition. The particular solution to this inhomogeneous equation form is calculated in the Chemistry Package by FUNCTION WQX, which is described in Section V.

The final concentration of N^+ at the calculational time is taken as the sum of the solution, $[N^+]_t$, of Eq (4) and the particular solution for Eq (5) where $[N^+]_o$ in the later case is assumed to be zero. This procedure is general throughout the analytic treatment. Each species is treated twice - once without and once with the continuous energy deposition considered- and the results are either added or the maximum is taken depending upon the species and the specific mathematical treatment and boundary conditions assumed.

2. OXYGEN ION (O^+)

O^+ is handled in a manner similar to N^+ except that the differential equation for $[O^+]$ includes a production term from the charge exchange of N^+ with O. Consideration of Reactions 11, 15, 16, and 35 leads to the inhomogeneous equation for the instantaneous solution.

$$d[O^+]/dt = -\left\{k_{11}[O_2] + k_{15}[N_2] + k_{16}[NO]\right\}[O^+] + k_{35}[N^+][O] \qquad (6)$$

The equation is rewritten by defining the constants β_O and γ.

$$d[O^+]/dt = -\beta_O[O^+] + \gamma[N^+] \qquad (7)$$

Substituting Eq (4) for $[N^+]$ gives

$$d[O^+]/dt = -\beta_O[O^+] + \gamma[N^+]_o e^{-\beta_N t} \qquad (8)$$

to which the general solution is of the form

$$[O^+] = \alpha e^{-\beta_O t} + [\gamma[N^+]_o/(\beta_O-\beta_N)]e^{-\beta_N t} \qquad (9)$$

The value of α is determined from initial conditions and the solution takes the form

$$[O^+] = \left\{[O^+]_o - \gamma[N^+]_o/(\beta_O-\beta_N)\right\} e^{-\beta_O t} + \left\{\gamma[N^+]_o/(\beta_O-\beta_N)\right\} e^{-\beta_N t} \qquad (10)$$

If $y = \gamma[N^+]_o/(\beta_O-\beta_N)$ the final form of the instantaneous solution is

$$[O^+] = ([O^+]_o - y)e^{-\beta_O t} + ye^{-\beta_N t} \qquad (11)$$

The solution for $[O^+]$ including the continuous source is found as for $[N^+]$ from the equation

$$d[O^+]/dt = Q - \beta_0[O^+] \tag{12}$$

where $Q = Q_{O^+} + \gamma[N^+]_t$ and $[O^+]_o$ is assumed to be zero.

The final concentration of O^+ at the calculational time is the sum of the instantaneous and continuous energy deposition solutions.

3. ELECTRON CONCENTRATION

Before proceeding with the positive molecular ions, an intermediate update is made to the electron concentration. The same calculational scheme is repeated after the positive molecular ions have been treated to give the final electron concentration. (At present, n_e is considered as the total negative charge concentration in an equal α approximation.)

Consideration of the continuous source production rate is posponed as usual, and Reactions 7, 10, and 12 define the electron concentration behavior

$$dn_e/dt = - \left\{k_7[N_2^+] + k_{10}[O_2^+] + k_{12}[NO^+]\right\} n_e \tag{13}$$

where the approximation has been made that atomic ions do not recombine-a valid approximation due to their very slow recombination rates compared to the molecular ions. An average recombination rate, α_r, is defined

$$\alpha_r = \frac{k_7[N_2^+] + k_{10}[O_2^+] + k_{12}[NO^+]}{[N_2^+] + [O_2^+] + [NO^+] + [O^+] + [N^+]}$$

and Eq (13) is replaced by

$$dn_e/dt = - \alpha_r n_e P \tag{14}$$

where P is the number of molecular positive ions, $P = n_e-([O^+] + [N^+])$. Defining $[A^+] = [O^+] + [N^+]$, Eq (14) is rewritten as

$$dn_e/dt = -\alpha_r n_e(n_e - [A^+]) \tag{15}$$

and if $[A^+]$ is treated as a constant the solution for n_e is

$$n_e = [A^+] + (n_o - [A^+])/(1 + \alpha_r' n_o t) \tag{16}$$

where $\alpha_r' = \alpha_r[\exp(\alpha_r[A^+]t)-1)]/(\alpha_r[A^+]t)$ and n_o is the initial electron concentration at t = 0. This expression for n_e is exact in the limits of $[A^+]$ equal to zero and infinity, and from comparisons with numerical solutions, Eq (16) appears to be valid over a wide range of $[A^+]$ values.

The continuous source production of negative charge is handled simply by the solution of the equation

$$dn_e/dt = Q - \alpha_r n_e^2 \tag{17}$$

where the ion-pair production rate, Q, has been added to Eq (14) and the approximation, $P = n_e$, has been made.

The solution to Eq (17) is

$$n_e = \sqrt{\frac{Q}{\alpha_r}}\,(1 + ae^{-2\sqrt{\alpha_r Qt}})/(1 - ae^{-2\sqrt{\alpha_r Qt}}) \tag{18}$$

where $a = (n_o - \sqrt{\frac{Q}{\alpha_r}})/(n_o + \sqrt{\frac{Q}{\alpha_r}})$. This solution is contained in the Chemistry Package as FUNCTION WR.

The final electron concentration n_e at the calculational time is the maximum of the instantaneous and continuous source solutions.

4. MOLECULAR NITROGEN ION (N_2^+)

N_2^+ is considered next in the charge exchange chain of positive ions. The differential equation for $[N_2^+]$ is derived from Reactions 7, 8, 9, and 18

$$d[N_2^+]/dt = -k_7 n_e [N_2^+] - \left\{ k_8[O_2] + k_9[O] + k_{18}[NO] \right\} [N_2^+] \qquad (19)$$

Equation (19) may be rewritten by defining $\beta_{N_2} = k_8[O_2] + k_9[O] + k_{18}[NO]$ and substituting Eq (16) for n_e

$$d[N_2^+]/dt = -\left\{ k_7[A^+] + k_7(n_o - [A^+])/(1 + \alpha_r' n_o t) + \beta_{N_2} \right\} [N_2^+] \qquad (20)$$

If α_r' and β_{N_2} are treated as constants and Eq (4) and Eq (11) define $[A^+] = [O^+] + [N^+]$, the instantaneous solution for N_2^+ is

$$[N_2^+] = [N_2^+]_o \exp\left\{ -\beta_{N_2} t - k_7(([O^+]_o - y)/\beta_0)(1 - e^{-\beta_0 t}) \right.$$

$$- k_7(([N^+]_o + y)/\beta_N)(1 - e^{-\beta_N t}) + (k_7/(\alpha_r' n_o))[([O^+]_o - y)e^{A_1}(E_1(A_1) - E_1(B_1))$$

$$\left. + ([N^+]_o + y)e^{A_2}(E_1(A_2) - E_1(B_2))] \right\} / (1 + \alpha_r' n_o t)^{k_7/\alpha_r'} \qquad (21)$$

where $A_1 = \beta_0/(\alpha_r' n_o)$, $B_1 = A_1(1 + \alpha_r' n_o t)$, $A_2 = \beta_N/(\alpha'_r n_o)$, $B_2 = A_2(1 + \alpha_r' n_o t)$, and $E_1(A)$ is the exponential integral $\int_A^\infty \frac{e^{-x}}{x} dx$ which is calculated by FUNCTION EIF. Equation (21) has been modified during the development of the analytic treatment to assure the best possible agreement with numerical solutions. In particular, the denominator $(1 + \alpha_r' n_o t)^{k_7/\alpha_r'}$ has been replaced by $(1 + \alpha_r n_o t)$, resulting in a more even performance of the solution over a wide range of α_r' values.

The inclusion of a continuous source term in Eq (19) results in the full equation

$$d[N_2^+]/dt = Q_{N_2^+} - k_7 n_e [N_2^+] - \beta_{N_2}[N_2^+] \quad (22)$$

which may be regrouped if n_e is assumed to be a constant

$$d[N_2^+]/dt = Q_{N_2^+} - \beta[N_2^+] \quad (23)$$

where $\beta = k_7 n_e + \beta_{N_2}$.

The solution to Eq (23) is found as for N^+ and O^+ using the FUNCTION WQX with $[N_2^+]_o = 0$.

The final concentration of N_2^+ at t_c is considered to be the maximum of the instantaneous and continuous source solutions.

5. MOLECULAR OXYGEN ION (O_2^+)

Next in the charge exchange chain, O_2^+ is involved in Reactions 8, 10, 11, 13, 17, and 20. Of these, Reactions 8, 11 and 13 produce $[O_2^+]$ and are treated as increasing $[O_2^+]$ at t = 0 by an amount

$$X_{O_2^+} = k_8[O_2]\int_o^t [N_2^+]dt' + k_{11}[O_2]\int_o^t [O^+]dt' + k_{13}[O_2]\int_o^t [N^+]dt' \quad (24)$$

where $I_{O^+} = \int_o^t [O^+]dt'$ and $I_{N^+} = \int_o^t [N^+]dt'$ can be found by integrating Eq (11) and Eq (4) respectively.

The integral $I_{N_2^+} = \int_o^t [N_2^+]dt'$ can not be performed exactly, therefore, an integrable form is assumed

$$[N_2^+] = [N_2^+]_o e^{-\beta_e^{N_2} t}/(1+\alpha_r n_o t) \qquad (25)$$

where $\beta_e^{N_2}$ is calculated by setting Eq (25) equal to the results of Eq (21). The integral may now be evaluated

$$I_{N_2^+} = [N_2^+]_o (e^{A_3}/(\alpha_r n_o))[E_1(A_3) - E_1(B_3)] \qquad (26)$$

where $A_3 = \beta_e^{N_2}/(\alpha_r n_o)$ and $B_3 = A_3(1 + \alpha_r n_o t)$ and Eq (24) is condensed to

$$X_{O_2^+} = [O_2]\left\{k_8 I_{N_2^+} + k_{11} I_{O^+} + k_{13} I_{N^+}\right\} \qquad (27)$$

The remaining Reactions 10, 17, and 20 define the differential equation for $[O_2^+]$

$$d[O_2^+]/dt = -k_{10}[O_2^+]n_e - k_{17}[NO][O_2^+] - k_{20}[N][O_2^+] \qquad (28)$$

or substituting Eq (16) and defining $\beta_{O_2} = k_{17}[NO] + k_{20}[N]$

$$d[O_2^+]/dt = -\left\{k_{10}[[A^+] + (n_o - [A^+])/(1+\alpha_r' n_o t)] + \beta_{O_2}\right\}[O_2^+] \qquad (29)$$

Treating Eq (29) in the same manner as Eq (20), the final instantaneous solution for $[O_2^+]$ is

$$[O_2^+] = [O_2^+]_o \exp\left\{-\beta_{O_2} t - k_{10} I_{A^+} + k_{10}/(\alpha_r' n_o)[([O^+]_o - y)e^{A_1}(E_1(A_1) - E_1(B_1))\right.$$

$$+ (([N^+]_o + y)e^{A_2}(E_1(A_2) - E_1(B_2)))\Big\} / (1+\alpha_r' n_o t)^{k_{10}/\alpha_r'} \qquad (30)$$

where $I_{A^+} = I_{O^+} + I_{N^+} = (([O^+]_o - y)/\beta_O)(1-e^{-\beta_O t}) + (([N^+]_o + y)/\beta_N)(1-e^{-\beta_N t})$;

A_1, B_1, A_2, and B_2 have been defined; and $[O_2^+]_o$ includes $X_{O_2^+}$.

The above treatment has been modified to take into account some of the errors introduced by the approximations made. Since $[O_2^+]_o$ is increased by an amount $X_{O_2^+}$ at t = 0 allowing that additional concentration to recombine from t = 0 and not from the actual time of creation, Eq (27) is modified to correct for the recombination of N_2^+ by the factor

$$C_{N_2} = [N_2^+]_o / \Big\{ [N_2^+] + (k_8[O_2] + k_9[O] + k_{18}[NO])I_{N_2^+} \Big\} \qquad (31)$$

where the latter term is the N_2^+ lost to all processes except recombination. Equation (27) then has the form

$$X_{O_2^+} = [O_2] \Big\{ k_8 C_{N_2} I_{N_2^+} + k_{11} I_{O^+} + k_{13} I_{N^+} \Big\} \qquad (32)$$

Equation (30) has also been altered to improve agreement with numerically calculated solutions. If Eq (30) is rewritten as

$$[O_2^+] = [O_2^+]_o \exp\Big\{ -\beta_{O_2} t - k_{10}(I_{A^+} - I) \Big\} / (1 + \alpha_r' n_o t)^{k_{10}/\alpha_r'} \qquad (33)$$

the modification to Eq (33) is the denominator transformation

$$(1 + \alpha_r' n_o t)^{k_{10}/\alpha_r'} \rightarrow (1 + \alpha_r' n_o t(\exp(-k_{10}(I_{A^+} - I))))^{k_{10}/\alpha_r'}$$

The continuous source calculation for O_2^+ is handled in a similar manner to N_2^+. The full differential equation for O_2^+

$$d[O_2^+]/dt = Q_{O_2^+} + \left\{ k_8[N_2^+] + k_{11}[O^+] + k_{13}[N^+] \right\} [O_2]$$
$$- \left\{ k_{10}n_e + \beta_{O_2} \right\} [O_2^+] \quad (34)$$

can be regrouped into the familiar form

$$d[O_2^+]/dt = Q - \beta[O_2^+] \quad (35)$$

where $Q = Q_{O_2^+} + \left\{ k_8[N_2^+] + k_{11}[O^+] + k_{13}[N^+] \right\} [O_2]$

and $\beta = k_{10}n_e + \beta_{O_2}$. Eq (35) is solved in the usual way using FUNCTION WQX with $[O_2^+]_o = 0$.

The final concentration of O_2^+ at t_c is considered to be the maximum of the instantaneous and continuous source solutions.

6. NITRIC OXIDE ION (NO+)

The final species in the charge exchange chain, NO^+, is involved in Reactions 9, 12, 14, 15, 16, 17, 18, 19, and 20. All these reactions except 12 may be viewed as increasing $[NO^+]$ at t = 0 by an amount

$$X_{NO^+} = k_9[O]I_{N_2^+} + k_{14}[O_2]I_{N^+} + k_{15}[N_2]I_{O^+} + k_{16}[NO]I_{O^+} + k_{17}[NO]I_{O_2^+}$$
$$+ k_{18}[NO]I_{N_2^+} + k_{19}[NO]I_{N^+} + k_{20}[N]I_{O_2^+} \quad (36)$$

where $I_{O_2^+} = \int_o^t [O_2^+]dt'$. In analogy to the calculation of $I_{N_2^+}$, an integrable form is assumed for $\left[O_2^+\right]$

$$[O_2^+] = [O_2^+]_o e^{-\beta_e^{O_2} t} / (1+\alpha_r n_o t) \quad (37)$$

where $\beta_e^{O_2}$ is calculated by setting Eq (37) equal to the results of Eq (30)

Thus

$$I_{O_2^+} = [O_2^+]_o e^{A_4}/(\alpha_r n_o)(E_1(A_4) - E_1\ (B_4))$$

where $A_4 = \beta_e^{O_2}/(\alpha_r n_o)$ and $B_4 = A_4(1+\alpha_r n_o t)$. (38)

This approach leaves the differential equation for the instantaneous solutions of $[NO^+]$ in the form

$$d[NO^+]/dt = -\ k_{12} n_e [NO^+] \tag{39}$$

Substituting Eq (16) for n_e and assuming α_r' a constant, the equation is integrated to give the solution

$$[NO^+] = [NO]_o^+ \exp\{-k_{12} I_{A^+} + k_{12}/(\alpha_r' n_o)[(([O^+]_o - y)e^{A_1}(E_1(A_1) - E_1(B_1)) + ([N^+]_o + y)e^{A_2}(E_1(A_2) - E_1(B_2))]\}/(1+\alpha_r' n_o t)^{k_{12}/\alpha_r'} \tag{40}$$

where A_1, B_1, A_2, and B_2 have been defined previously, and $[NO^+]_o$ includes X_{NO^+}.

Again, as for $[O_2^+]$, Eq (36) and Eq (40) must be modified to correct approximation errors. In Eq (36), all terms involving $I_{N_2^+}$ are multiplied by the factor C_{N_2} and all involving $I_{O_2^+}$, by the factor

$$C_{O_2} = [O_2^+]_o/([O_2^+] + (k_{17}[NO] + k_{20}[N])I_{O_2^+}) \tag{41}$$

to correct for the fact that these concentrations did not recombine from $t = 0$.

Eq (40) is not only modified but is also passed through an iteration process along with the continuous source solution. First, if Eq (40) is rewritten as

$$[NO^+] = [NO^+]_o \exp\left\{-k_{12}(I_{A^+} - I)\right\} /(1 + \alpha_r' n_o t)^{k_{12}/\alpha_r'} \qquad (42)$$

the denominator is modified to give the first iteration instantaneous solution form

$$[NO^+] = [NO^+]_o \exp\left\{-k_{12}(I_{A^+}-I)\right\} /(1+\alpha_r' n_o t(\exp(-k_{12}(I_{A^+} - I)))) \qquad (43)$$

The first iteration continuous source solution solves the full differential equation for $[NO^+]$ which is analogous to Eq (34) and may be reduced to

$$d[NO^+]/dt = Q - \beta[NO^+] \qquad (44)$$

which is solved using FUNCTION WQX with $[NO^+]_o = 0$ and $\beta = k_{12}n_e$.

The maximum of the instantaneous and continuous source solutions of Eq (43) and Eq (44) constitute the first iteration solution of $[NO^+]$.

Having calculated concentrations at t_c for all the positive molecular ions, a new α_r and α_r' are calculated and the formalism for the calculation of n_e in Section IV-3 is repeated to update the electron (i.e. negative ion) concentration at t_c.

The second iteration on $[NO^+]$ then uses the new α_r' to recalculate the instantaneous solution of Eq (42) modified as

$$[NO^+] = [NO^+]_o \exp\left\{-k_{12}(I_{A^+} + I)\right\} /(1 + \alpha_r' n_o t(\exp(-k_{12}(I_{A^+} - I))))^{k_{12}/\alpha_r'} \qquad (45)$$

with I not being recalculated. Likewise, the continuous solution is recalculated using the new n_e. Finally, the maximum of the two solutions is taken to give the ultimate $[NO^+]$ concentration at t_c.

7. SPECIES AND TEMPERATURE UPDATING

Throughout the above treatment all neutral species concentrations were assumed to be constant. This approximation alone is insufficient, however, and intermediate updating of some neutral species concentrations is accomplished between the solutions for $[N_2^+]$ and $[O_2^+]$ (i.e., Sections IV-4 and IV-5). Likewise, the neutral species concentrations and the temperature are ultimately modified after the entire treatment to account for production by the fast ion chemistry.

a. Intermediate Updating of NO, N, and O

Intermediate updating is accomplished for [N], [O], and [NO]. [N] and [O] created or destroyed by an ion-neutral reaction are accounted for by additions to their initial concentrations, $[N]_o$ or $[O]_o$

$$[Y]_o = [Y]_o \pm bk[X]I_{m^+} \tag{46}$$

where I_{m^+} is either I_{N^+}, I_{O^+}, or $I_{N_2^+}$, b is a branching ratio, k is the reaction rate constant, and X is the reacting neutral whose concentration is assumed to be constant. The increase in [N] due to the dissociative recombination of N_2^+ additionally requires the more complex integral $k_7 \int_o^t n_e[N_2^+]dt'$ where neither term of the product can be assumed to be constant. This integral is calculated by substituting Eq (16) and Eq (25) for n_e and $[N_2^+]$ respectively and solving.

$$I_{N_2^+}^{n_e} = \int_o^t [N_2^+]n_e dt' = \int_o^t \frac{[N_2^+]_o e^{-\beta_e^{N_2} t'}}{1+\alpha_r n_o t'} \left\{[A^+] + \frac{n_o - [A^+]}{1+\alpha_r' n_o t'}\right\} dt' \tag{47}$$

$$I_{N_2^+}^{n_e} = [N_2^+]_o \left\{\int_o^t \frac{[A^+] e^{-\beta_e^{N_2} t'}}{1+\alpha_r n_o t'} dt' + \int_o^t \frac{(n_o - [A^+]) e^{-\beta_e^{N_2} t'}}{(1+\alpha_r n_o t')(1+\alpha_r' n_o t')} dt'\right\} \tag{48}$$

The denominator in the second integral is approximated by $(1 + \gamma n_o t')^2$ where the constant $\gamma = \sqrt{\alpha_r \alpha_r'}$. Integrating yields

$$\begin{aligned} I^{n_e}_{N_2^+} = [N_2^+]_o \Bigg\{ & \frac{([O^+]_o - y)}{\alpha_r n_o} e^{A_5} (E_1(A_5) - E_1(B_5)) + \frac{([N^+]_o + y)}{\alpha_r n_o} e^{A_6} (E_1(A_6) - E_1(B_6)) \\ & + \frac{1}{\gamma} [(1 - \frac{e^{-\beta_e^{N_2} t}}{1+\gamma n_o t}) - A_7 e^{A_7} (E_1(A_7) - E_1(B_7))] - \frac{([O^+]_o - y)}{\gamma n_o} [(1 - \frac{e^{-\delta t}}{1+\gamma n_o t} \\ & - A_8 e^{A_8} (E_1(A_8) - E_1(B_8))] - \frac{([N^+]_o + y)}{\gamma n_o} [(1 - \frac{e^{-\sigma t}}{1+\gamma n_o t}) - A_9 e^{A_9} (E_1(A_9) - E_2(B_9))] \Bigg\} \end{aligned} \tag{49}$$

where $\delta = \beta_e^{N_2} + \beta_O$, $\sigma = \beta_e^{N_2} + \beta_N$, $A_5 = \frac{\delta}{\alpha_r n_o}$, $B_5 = A_5(1+\alpha_r n_o t)$, $A_6 = \frac{\sigma}{\alpha_r n_o}$

$B_6 = A_6\ (1+\alpha_r n_o t)$, $A_7 = \frac{\beta_e^{N_2}}{\gamma n_o}$, $B_7 = A_7(1+\gamma n_o t)$, $A_8 = \frac{\delta}{\gamma n_o}$, $B_8 = A_8(1+\gamma n_o t)$,

$A_9 = \frac{\sigma}{\gamma n_o}$, and $B_9 = A_9(1+\gamma n_o t)$.

Having calculated $I^{n_e}_{N_2}$, [N] can be updated using the recombination term $k_7 I^{n_e}_{N_2^+}$. However, since several approximations were made in the calculation, a further modification is necessary. The total amount of N_2^+ that has been removed by the several reactions in which it participates is

$$\Delta N_2^+ = [N_2^+]_o - [N_2^+]_t \tag{50}$$

which if no approximations had been made in calculating $I_{N_2^+}$ and $I^{n_e}_{N_2^+}$ would be equivalent to

$$A_{N_2} = (k_8[O_2] + k_9[O] + k_{18}[NO]) I_{N_2^+} + k_7\ I^{n_e}_{N_2^+} \tag{51}$$

Since the two terms will not be equal, the concentration of N_2^+ which has recombined is calculated as the total change in $[N_2^+]$ multiplied by the ratio of that which has recombined to the total that has reacted. Thus the concentration of N_2^+ which has recombined is

$$R_{N_2^+} = \Delta N_2^+ \; (k_7 I_{N_2^+}^{n_e} / A_{N_2^+}) \tag{52}$$

which is used along with the appropriate branching ratios to update the N concentrations.

The intermediate updating of [NO] is accomplished in a very approximate fashion. Reactions 1, 2, 3, 4, 24, 25, 26, 28, and 31 involve [NO], but only the first four are considered, resulting in the differential equation

$$\frac{d[NO]}{dt} = [NSP](k_1[O_2] - k_3[NO]) + [N(^2D)](k_2[O_2] - k_4[NO]) \tag{53}$$

where $[NSP] = [N(^4S)] + [N(^2P)]$. The number of variables in Eq (53) can be reduced by assuming that an increase in [NO] is reflected as a decrease in $[O_2]$ such that

$$[O_2] = [O_2]_o - ([NO] - [NO]_o) \tag{54}$$

Substituting into Eq (53)

$$\frac{d[NO]}{dt} = [NSP] \left\{ k_1([O_2]_o + [NO]_o) - (k_1+k_3)[NO] \right\} + [N(^2D)] \left\{ k_2([O_2]_o + [NO]_o) - (k_2+k_4)[NO] \right\} \tag{55}$$

If reactions involving $N(^2D)$ are more rapid than those of $N(^4S)$ and $N(^2P)$, the two halves of Eq (55) may be solved sequentially. First, the solution for $[N(^2D)]$ is assumed to have the form

$$[N(^2D)] = [N(^2D)]_o e^{-\beta_1 t} \tag{56}$$

where $\beta_1 = k_2[O_2]_o + k_4[NO]_o$. And the solution to the second half of Eq (55) is

$$[NO]_1 = k_2([O_2]_o + [NO]_o)/(k_2+k_4) - \left\{k_2([O_2]_o + [NO]_o)/(k_2+k_4) - [NO]_o\right\} \exp\left\{-(k_2+k_4)[N(^2D)]_o(1-e^{-\beta_1 t})/\beta_1\right\} \tag{57}$$

The result of Eq (57) is then used as the initial condition for [NO] in the solution to the first half of Eq (55). Thus, the intermediate updated concentration for NO is

$$[NO] = k_1([O_2]_o + [NO]_o)/(k_1+k_3) - \left\{k_1([O_2]_o + [NO]_o)/(k_1+k_3) - [NO]_1\right\} \exp\left\{-(k_1+k_3)[NSP]_o(1-e^{-\beta_2 t})/\beta_2\right\} \tag{58}$$

where $\beta_2 = k_1[O_2]_o + k_3[NO]_1$ and the time dependence of [NSP] has the form of Eq (56).

b. FINAL UPDATING OF N AND O

After completion of the fast ion chemistry, the concentrations of N and O are updated to account for production by the reactions of O_2^+ and NO^+. Procedures similar to those for the intermediate updating are followed. In particular for the recombination of O_2^+, the integral is needed

$$I^{n_e}_{O_2^+} = \int_o^t [O_2^+] n_e dt' = [O_2^+]_o \left\{ \int_o^t \frac{[A^+] e^{-\beta_e^{O_2} t'}}{(1+\alpha_r n_o t')} dt' + \int_o^t \frac{(n_o - [A^+]) e^{-\beta_e^{O_2} t'}}{(1+\gamma n_o t')^2} dt' \right\} \qquad (59)$$

which can be solved in analogy to N_2^+ in Eq (48) to give the solution of Eq (49) where $[O_2^+]_o$ is substituted for $[N_2^+]_o$ and $\beta_e^{O_2}$ for $\beta_e^{N_2}$. A similar integral for $[NO^+]$, however is not required since the only loss mechanism for NO^+ is recombination and the integral is simply

$$k_{12} \int_o^t n_e [NO^+] dt' = \Delta NO^+ = [NO^+]_o - [NO^+]_t \qquad (60)$$

Again in analogy to the N_2^+, the recombination integral for O_2^+ is corrected for the approximations made throughout the calculation and the final concentration of O_2^+ which has recombined is calculated as

$$R_{O_2^+} = \Delta O_2^+ \quad (k_{10} I^{n_e}_{O_2^+} / A_{O_2^+}) ([O_2^+]'_o / [O_2^+]_o) \qquad (61)$$

where a second correction term $([O_2^+]'_o/[O_2^+]_o)$ has been added to account for the effects of $[O_2^+]_o$ having been increased by $X_{O_2^+}$, Eq (32), and the approximations made there. Similarly, the final concentration of NO^+ which has recombined is calculated as

$$R_{NO^+} = \Delta NO^+ \quad ([NO^+]'_o / [NO^+]_o) \qquad (62)$$

where the correction term has been added to account for the approximations made in updating $[NO^+]_o$ with X_{NO^+}.

The branching ratios of Reactions 10 and 12 are used with $R_{O_2^+}$ and R_{NO^+} respectively, to update the N and O concentrations.

c. FINAL UPDATING OF TEMPERATURE AND REACTION RATES

The final step in the fast ion chemistry treatment is the recomputation of the gas temperature and reaction rates. For the temperature calculation, the specific heat of the sample volume is recalculated as is the total heat of formation for all species in the volume. The internal energy of the volume is then recalculated as its former value plus the change in the total heat of formation for all species. This new internal energy is finally converted to an updated gas temperature using the new specific heat. The new temperature is then used in RATE to recalculate the reaction rates for all reactions of Table II.

8. NEUTRAL SPECIES CHEMISTRY

The slower neutral chemistry is much simpler in its mathematics, but is intricate in the ordering of species and reactions for solution. The subsequent discussion, therefore, follows the programmed logic rather than segmentation by species.

In general, the treatment follows four steps. In the first, the continuous source production rates are neglected and [O], $[O_2(^3\Sigma)]$, [N], [NO], and $[O_3]$ are addressed. In the second the continuous source rates are included in the solutions for most species. The reactions involving [OH] and [H] are treated separately in the third. And the metal/metal oxide chemistry is handled in an uncoupled manner in the fourth.

a. Decay of Oxygen Excited States

Reactions 33 and 34 involve the decay of $[O(^1S)]$ and $[O(^1D)]$. The $O(^1S)$ decay is simply expressed as

$$[O(^1S)] = [O(^1S)]_o \, e^{-k_{33}t} \tag{63}$$

and the differential equation for $O(^1D)$

$$\frac{d[O(^1D)]}{dt} = -k_{34}[O(^1D)] - d[O(^1S)]/dt \tag{64}$$

has the solution

$$[O(^1D)] = \left\{[O(^1D)]_o - k_{33}[O(^1S)]_o/(k_{34}-k_{33})\right\} e^{-k_{34}t} + k_{33}[O(^1S)]_o/(k_{34}-k_{33})e^{-k_{33}t} \tag{65}$$

where the initial values $[O(^1D)]_o$ and $[O(^1S)]_o$ are those updated at the end of the charged species treatment. At the same time, $[O_2(^3\Sigma)]$ is decayed according to Reaction 23

$$[O_2(^3\Sigma)] = [O_2(^3\Sigma)]_o e^{-k_{23}[O_2]t} \tag{66}$$

b. Nitrogen-Nitric Oxide

The interplay of [N] and [NO] is handled by dividing the solution for [N] into two parts separated by an updating of [NO].

The first set of nitrogen Reactions 1, 2, and 32 are faster and do not involve [NO]. $N(^2P)$ decays in a simple exponential manner according to Reactions 1 and 32, in analogy to $O(^1S)$ in Eq (63). The differential equation for $N(^2D)$, derived from Reactions 2 and 32, is solved as for $O(^1D)$ and the solution is of the same form as Eq (65). And $N(^4S)$ is expotentially decayed according to Reaction 1.

For the updating of [NO], the pertinent reactions of Table II are divided into two groups: Reactions 1, 2, 3, 4 and Reactions 24, 25, 26, 28, and 31. The solution to the first group of four reactions is found in Eq (57) and Eq (58) as used in Section IV-7. The second group of five are divided into a formation term, $F = k_{26}[O][NO_2] + k_{31}[N(^4S)][O_3]$, and a destruction term, $D = k_{24}[O_3] + k_{25}[O] + k_{28}[N]$, for [NO] and FUNCTION WQX is used to evaluate $[NO]_t$. Once both solutions have been found, the maximum of the two is adopted as the final value of [NO] at t_c.

With [NO] updated, the second set of nitrogen Reactions 3, 4, 27, 28, 29, and 31 are considered. Each atomic state of nitrogen suffers a simple exponential decay with exponents derived from: Reactions 3, 27, 28, and 29 for $N(^2P)$, Reactions 4, 27, 28, and 29 for $N(^2D)$, and Reactions 3, 27, 28, 29, and 31 for $N(^4S)$. The total change in [N] over the two part treatment is calculated and added to [O] since the major reactions in the nitrogen treatment involve production of atomic oxygen.

C. Ozone and Atomic Oxygen

Ozone is involved in Reactions 5, 6, 21, 23, 24, 30, 31, and photo dissociation. Neglecting Reactions 21 and 30, the differential equation for $[O_3]$ may be written

$$d[O_3]/dt = - [O_3]\left\{k_6[O] + k_{24}[NO] + k_{31}[N(^4S)] + \phi\right\} + k_5[O_2][O] + k_{23}[O_2][O_2(^3\Sigma)] \qquad (67)$$

where ϕ is the photodissociation rate constant for ozone and Eq(66) can be substituted for $[O_2(^3\Sigma)]$. The value of [O] in the second term is replaced by $[O]e^{-k_5[O_2]t}$ and Eq (67) is solved to give the final value for $[O_3]$

$$[O_3] = \left\{[O_3]_o + \gamma[O_2(^3\Sigma)]_o/(\gamma-\beta) + \delta[O]/(\delta-\beta)\right\} e^{-\beta t} - \left\{\gamma[O_2(^3\Sigma)]_o/(\gamma-\beta)\right\} e^{-\gamma t} - \left\{\delta[O]/(\delta-\beta)\right\} e^{-\delta t} \qquad (68)$$

where $\beta = k_6[O] + k_{24}[NO] + k_{31}[N(^4S)] + \phi$, $\gamma = k_{23}[O_2]$, and $\delta = k_5[O_2]$.

With Reactions 33 and 34 already addressed, atomic oxygen is involved in Reactions 5, 6, 23, 25, 26, and 29 for which the differential equation is

$$\frac{d[O]}{dt} = - [O]\left\{k_5[O_2] + k_6[O_3] + k_{25}[NO] + k_{26}[NO_2]\right\} + \left\{k_{29}[NO_2][N] + \phi\right\} + k_{23}[O_2][O_2(^3\Sigma)] \tag{69}$$

If $[O_2(^3\Sigma)]$ is replaced by Eq (66), the solution to Eq (69) using the updated value for $[O_3]$ is

$$[O] = \left\{[O]_o + \gamma[O_2(^3\Sigma)]_o/(\gamma-\beta)\right\} e^{-\beta t} + \delta/\beta(1-e^{-\beta t}) - \left\{\gamma[O_2(^3\Sigma)]_o/(\gamma-\beta)\right\} e^{-\gamma t} \tag{70}$$

where $\beta = k_5[O_2] + k_6[O_3] + k_{25}[NO] + k_{26}[NO_2]$, $\gamma = k_{23}[O_2]$, and $\delta = k_{29}[NO_2][N] + \phi$. The above solution is applied to $[O(^3P)]$ and the values of $[O(^1S)]$ and $[O(^1D)]$ are adjusted in proportion to the resultant change in $[O(^3P)]$.

d. Inclusion of Continuous Source Production

The second step of the neutral chemistry includes continuous energy deposition contributions in the species time dependent solutions. The species and their reactions from step one are addressed again here. For each species, formation rates (sec^{-1}) and destruction rates ($cc^{-1}sec^{-1}$) are calculated using the continuous source rates from ENQDEP and the appropriate reaction rate constants and current species concentration values. Then, in sequence, the solutions for $O(^3P)$, $O(^1D)$, $O(^1S)$, $N(^4S)$, $N(^2D)$, $N(^2P)$, $O_2(^3\Sigma)$, and O_3 are systematically calculated using FUNCTION WQX, with the calculational time, t_c, and concentrations at $t = 0$ assumed to be zero. The final value for each species concentration at t_c is computed as the sum of the solutions from the first and second steps of the neutral species chemistry.

e. NO_2, N_2O, and $O_2(^1\Delta)$

The NO_2 and N_2O concentrations are calculated using an approach to equilibrium with the FUNCTION WQX. NO_2 is formed in Reactions 24 and 25 and destroyed in Reaction 26, 27, and 29. N_2O is formed in Reactions 28 and 29 and destroyed in Reaction 30. Appropriate formation and destruction terms are computed for each species and FUNCTION WQX is applied to calculate their concentrations at t_c.

Having updated $[N_2O]$, $O_2\ (^1\Delta)$ is now addressed. It's only source of production is from the continuous energy deposition and its only form of destruction is by way of Reaction 30. FUNCTION WQX is utilized twice to solve for $[O_2(^1\Delta)]$ and the final value of the concentration is taken as the sum of the two results. In the first, both production and destruction terms are considered and $[O_2(^1\Delta)]_o$ is set equal to zero; and in the second, the production term is deleted and $[O_2(^1\Delta)]_o$ is its initial value.

f. Hydrogen

The final neutral system to be addressed before the metal oxides is the H, OH equilibrium of Reactions 21 and 22. Again the FUNCTION WQX is employed in an ad hoc fashion to solve this cyclic set of equations. In this case, the value of [OH] at t_c, is calculated using the production term $k_{21}[O_3]\left\{[H] + [OH]\right\}$, the destruction term $k_{21}[O_3] + k_{22}[O(^3P)]$, and the initial value $[OH]_o$. The value of [H] is then taken as that free hydrogen which has not been converted to OH.

g. Metal Oxides

The metal and metal oxide reactions are uncoupled from the rest of the analytical algorithm. The light metals such as Li, Be, Mg, Al, Si, Ti, Fe, and Cu, presently carried in WORRY, are treated in the same manner; therefore, in the following discussion the symbol X will be used to describe any one of these eight metals. The reactions and rate constants for the formation of the metal oxides are

$$X+O_2 \rightarrow XO+O. \qquad (k_1)$$

$$X+O+M \rightarrow XO+M \qquad (k_2)$$

$$X+O_3 \rightarrow XO+O_2 \qquad (k_3)$$

The reactions and rate constants for the destruction of the metal oxides are

$$XO+O \rightarrow X+O_2 \qquad (k_4)$$

$$XO+O_3 \rightarrow X+O_2+O_2 \quad (k_5)$$

The differential equation for [XO] is

$$\frac{\partial\,[XO]}{\partial\,t} = \left\{k_1[O_2] + k_2[O][M] + k_3[O_3]\right\}[X] - [XO]\left\{k_4[O] + k_5[O_3]\right\} \qquad (71)$$

But the total number of metal atoms does not change

$$[X] + [XO] = A \qquad (72)$$

and A is a constant, whose value is $[X]_o$ if all metal atoms are unoxidized at $t = 0$.

Thus Eq (71) can be rewritten as

$$\frac{d[XO]}{dt} = F(A-[XO]) - D[XO] \qquad (73)$$

where $F = k_1[O_2] + K_2[O][M] + k_3[O_3]$ and $D = k_4[O] + k_5[O_3]$. F and D are computed for each species using the final values of [O], $[O_2]$, and $[O_3]$, which are assumed to be constant.

Reordering Eq (73) gives

$$\frac{d[XO]}{dt} = FA - (F+D)[XO] \tag{74}$$

which may be solved for [XO] at t_c using FUNCTION WQX with a formation term of FA, a destruction term of F + D, and $[XO]_o$.

Because of the unique chemistry of U, only the following reaction is treated and in a simple exponential fashion:

$$U+O \rightarrow UO^+ + e$$

With all species concentrations now calculated and stored in the CMD array, the analytic algorithm is complete and new formation and destruction rates for all species are calculated where needed, to be used in subroutine RRCRT.

SECTION V

ACCESSORIAL SUBROUTINES AND FUNCTIONS

1. ROUTINES SHARED BY BOTH ALGORITHMS

a. ENTDEP and ENDQDEP

The routine ENTDEP calculates the initial distribution of ions and neutrals produced at t = 0 by the prompt energy deposition, while its entry point ENQDEP partitions the continuous energy deposition (ion pairs/cc/sec) among the same set of species. ENTDEP also calculates the specific heat of the sample volume, the internal kinetic energy of the gas, and adjusts the gas temperature accordingly.

ENTDEP requires inputs of the gas temperature, the total density, and the total number of ion pairs produced by the prompt energy deposition. The latter two are converted to a fractional ionization and ionized fractions of $[N_2]$, $[O_2]$, and $[O]$ are calculated. Then the concentration for each of the following species is adjusted for its production or depletion by ionization of N_2, O_2, and O: N_2, O_2, $O(^3P)$, $O(^1D)$, $O(^1S)$, $N(^4S)$, $N(^2D)$, $N(^2P)$, $O_2(^1\Delta)$, $O_2(^3\Sigma)$, N^+, O^+, N_2^+, O_2^+, and e^-.

ENQDEP likewise calculates the continuous ionization rates of N_2, O_2, and O and converts these to formation and destruction rates for the same set of product species.

b. RATE

The RATE routine simply calculates the rate constants for the reactions of table II and stores them in the R array. RATE requires inputs of the gas temperature (°K) and the total density (cc^{-1}). All three body reactions are provided with pseudo-second-order rate constants by including [M] in the constant.

c. RRCRT

This routine stores the necessary species destruction rates in RCRT and transforms the species formation rates into vibrational level formation rates which are stored in the RR array and used by the WORRY calculation of chemiluminescence. Because the product vibrational level branching ratios for the various reactions are not known, equal partition to the highest accessable level is presently assumed.

2. FUNCTIONS OF THE ANALYTIC ALGORITHM

a. FUNCTION WQX (A, B, XO, T)

This function solves the differential equation

$$\frac{d[X]}{dt} = A - B[x] \tag{75}$$

to give [x] at time, T, with $[x]_0$ = XO.

b. FUNCTION WR(A, B, XO, T)

This function solves the differential equation

$$\frac{d[x]}{dt} = A - B[x]^2 \tag{76}$$

to give [x] at time, T, with $[x]_0$ = XO.

c. FUNCTION SHXOX (X)

This function evaluates the expression

$$\frac{e^x - 1}{x}$$

d. FUNCTION X1IGL (A, B, C, T)

This function evaluates the integral

$$\int_0^T \frac{e^{-Bt}}{(1 + ACt)} dt$$

e. FUNCTION X2IGL (A, B, C, T)

This function evaluates the integral

$$\int_0^T \frac{e^{-Bt}}{(1 + ACt)^2} dt$$

f. FUNCTION E1F (X)

This function evaluates the integral

$$\int_X^\infty \frac{e^{-x}}{x} dx$$

SECTION VI

COMPARISONS OF ALGORITHMS

Figures 2, 3, 4, and 5 demonstrate the agreement between the analytic and numerical algorithms. A large number of such comparisons were presented at the DNA 1973 Atmospheric Effects Symposium at San Diego (ref 1). The problem definitions for figures 2, 3, and 4 were taken from Ory and Gilmore (ref 2), while that for figure 5 was taken from Scheibe (ref 3).

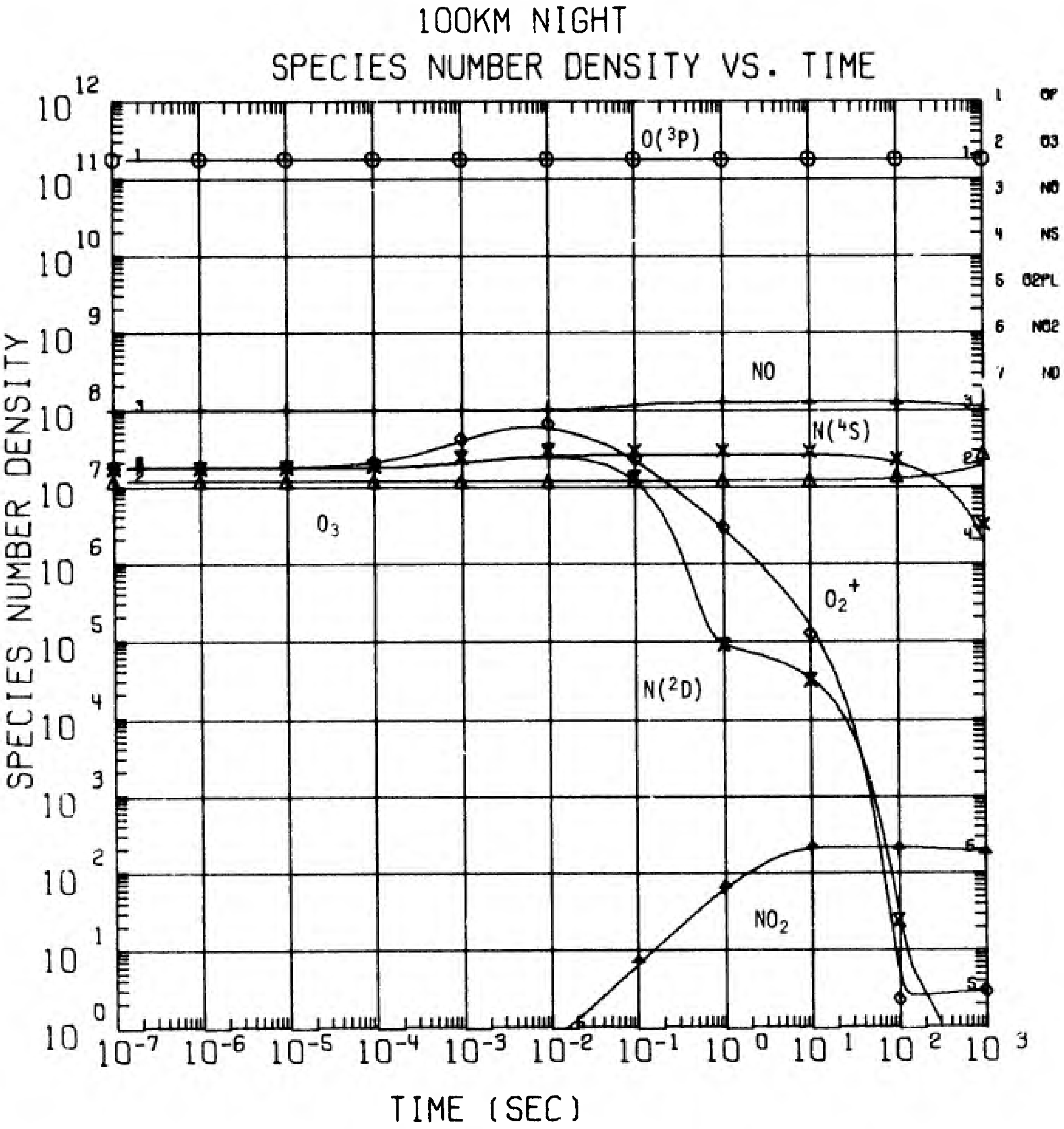

Figure 2. Comparison of Numerical (———) and Analytic (symbols) Algorithms (Altitude of 100 km, energy deposition of 10^8 ion pairs/cc during the night).

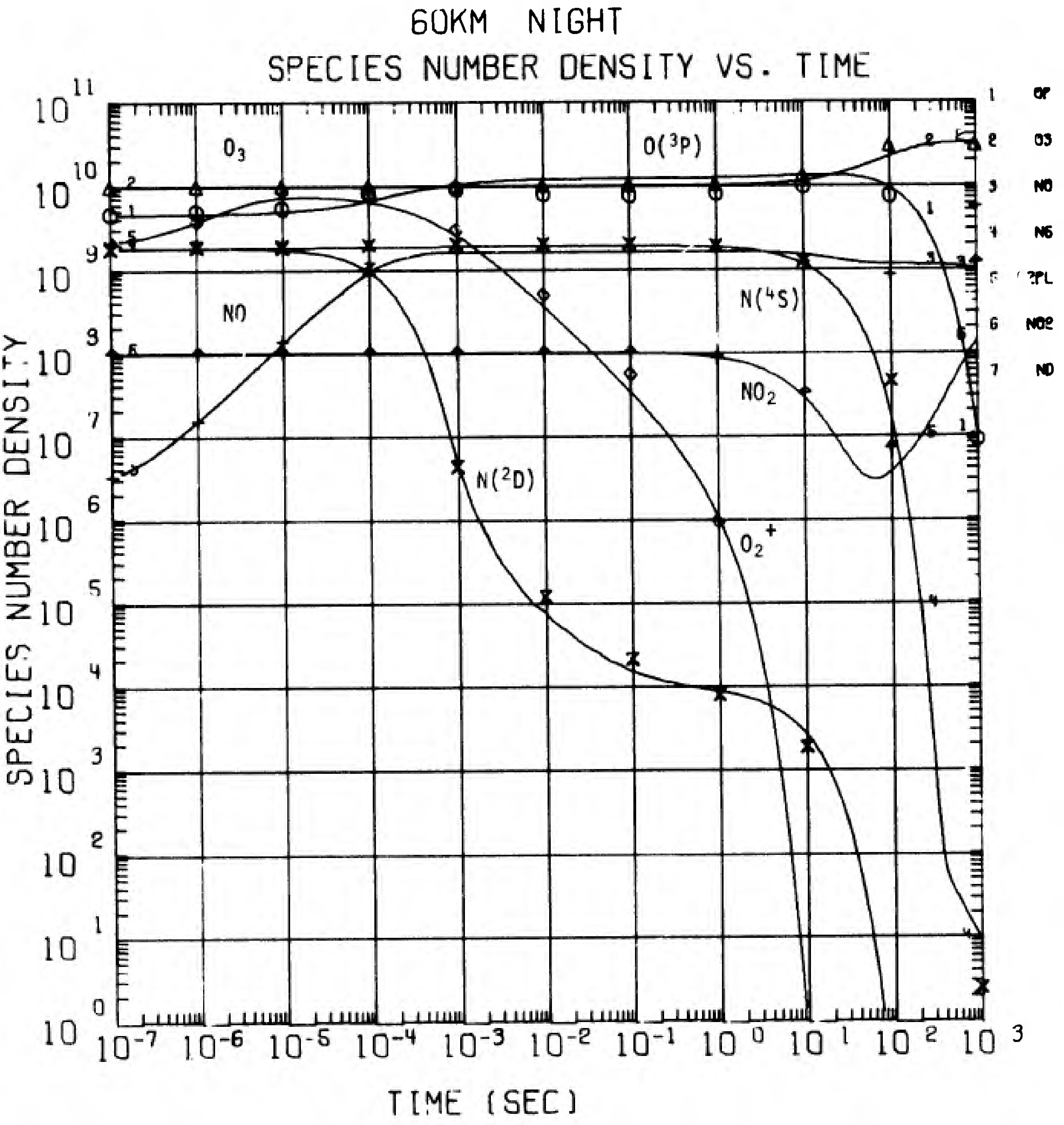

Figure 3. Comparison of Numerical and Analytic Algorithms (Altitude of 60 km, energy deposition of 10^{10} ion pairs/cc during the night).

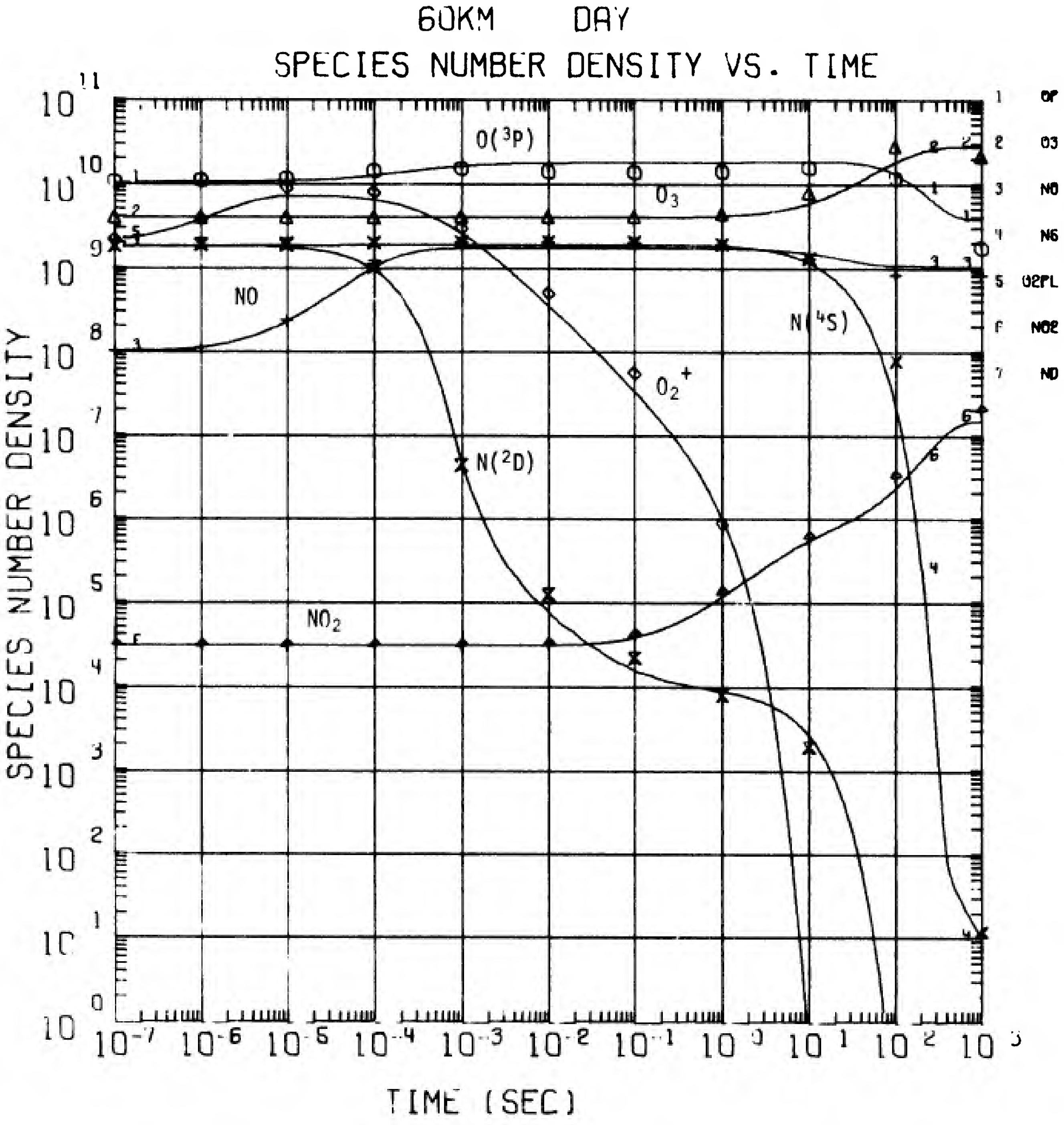

Figure 4. Comparison of Numerical and Analytic Algorithms (Altitude of 60 km, energy deposition of 10^{10} ion pairs/cc during the day).

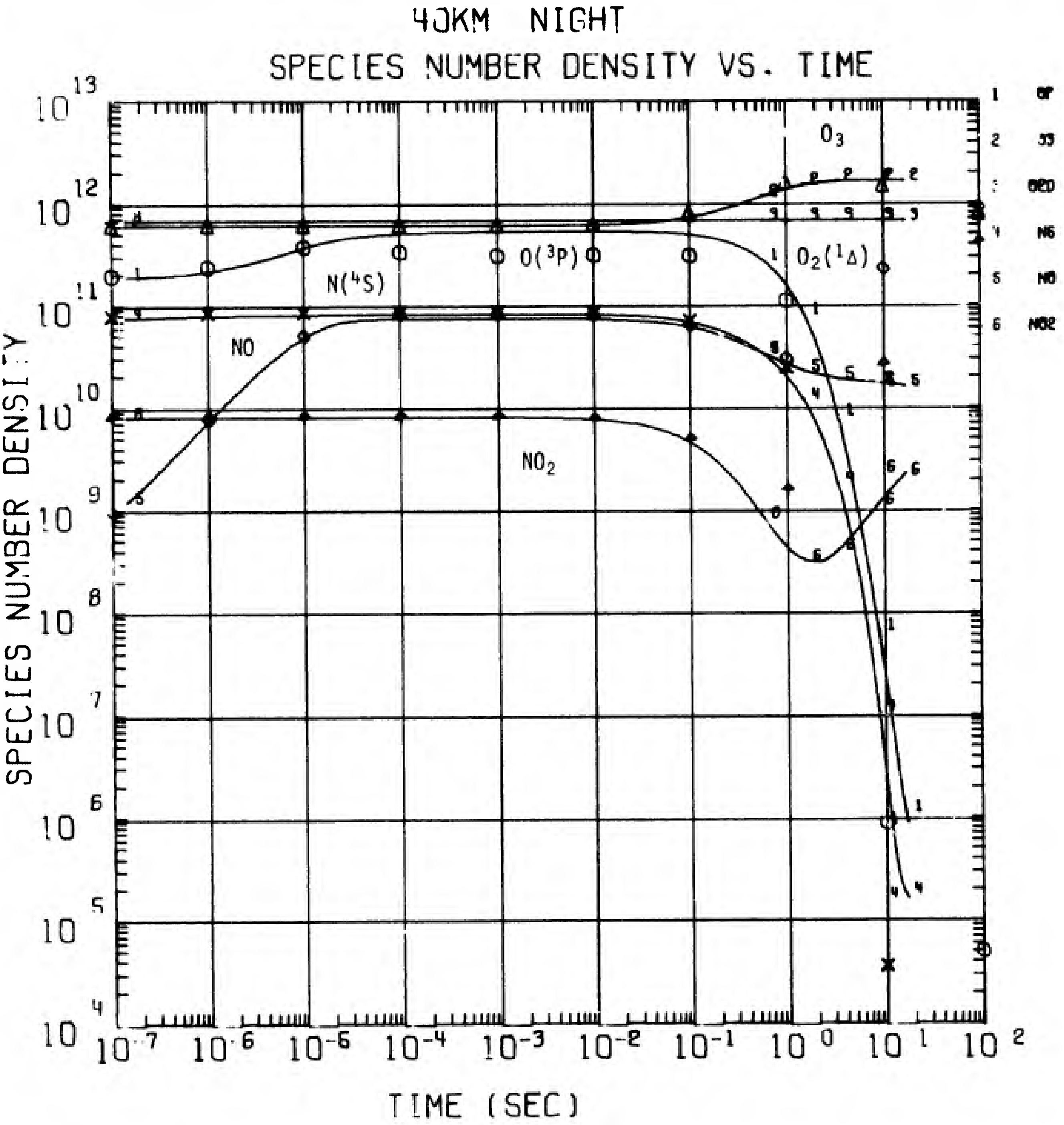

Figure 5. Comparison of Numerical and Analytic Algorithms (Altitude of 40 km, Energy Deposition of 4 x 10^{11} ion pairs/cc, and continuous ionization of 10^7 ion pairs/cc/sec during the night).

SECTION VII

CODE LISTING

This section lists the chemistry package as it is run outside WORRY. The first two routines constitute the external diver which decodes the users problem and prepares the necessary inputs for a chemistry package calculation by either the analytic or numerical algorithms. The diver also uses two plotting routines (not listed) to prepare comparison plots between the two methods. Since the external running of the chemistry package requires diagnostics which are otherwise unnecessary, the routines as listed contain some statements which are not standard in the operational version of WORRY. These statements are identified by a CH prefix in columns 73 and 74 of the card containing the statement.

When the chemistry package is used within WORRY, explicit phenomenology calculations provide a description of the continuous energy deposition as a function of time. When running in an external mode, the chemistry package as listed must assume a form for the time dependence of the continuous energy deposition. That form is

$$Q = QI*(1 + t)** \ 1.2$$

where t is the time after prompt energy deposition and QI is the energy deposition rate at t = 0.

```
************************************************************************
*                                                                      *
*     PACKAGE CHEM74                 01 JUL 74 VERSION          PAGE  1 *
*                                                                      *
************************************************************************

      PROGRAM CHEM(INPUT,OUTPUT,PUNCH,FILMPL,TAPE2,TAPE3=INPUT,TAPE4,TAP
     1E5,TAPE6=OUTPUT,TAPE7=PUNCH,TAPE1,TAPE8)
C     ******************************************************************
C
C        EXTERNAL DRIVER FOR WORRY CHEMISTRY PACKAGE
C
C     ******************************************************************
C
C     NOTE THAT TAPE3=INPUT
C     CALCOMP PLOT TAPE IS TAPE5
C     PROGRAM RETURNS BOTH MICROFILM AND CALCOMP
C
      COMMON /BANDS/ MSTATE(20),NSTATE(20)
      COMMON /BURST/ DAY
      COMMON /BUR2/ DYMETL(10)
      COMMON /PLTS/ XPLOTS(7,54),NPPL(54),IPL,NO(7)
      COMMON /QIN/ QI,QA
      COMMON /SWR/ SWICH(80)
      COMMON /TITLE/ TITL(7)
      COMMON /XUX/ RR(200),CMD(90),RCRT(90),NSPEC
      DIMENSION TI(70), TEST(10), ALPH(80), X(7)
      DIMENSION CMO0(90), YDMETL(10)
      DIMENSION AO3(11), ANO(11), AOH(11), FO3(11), FNO(11)
      DIMENSION XI(7), NSR(7)
      EQUIVALENCE (CMD(1),CH), (CMD(2),CLI), (CMD(3),CBE), (CMD(4),CMG),
     1 (CMD(5),CAL), (CMD(6),CSI), (CMD(7),CTI), (CMD(8),CFE), (CMD(9),C
     2CU), (CMD(10),CU), (CMD(11),COH), (CMD(12),CLIO), (CMD(13),CBEO),
     3(CMD(14),CMGO), (CMD(15),CALO), (CMD(16),CSIO), (CMD(17),CTIO), (C
     4MD(18),CFEO), (CMD(19),CCUO), (CMD(20),CUOPL), (CMD(21),CNOPL), (C
     5MD(22),CNO), (CMD(23),CNO2), (CMD(24),CN2O), (CMD(25),CCO), (CMD(2
     66),CCO2), (CMD(27),CO3), (CMD(28),CH2O), (CMD(30),CEL), (CMD(31),C
     7N2), (CMD(32),CN2A), (CMD(33),CN2B), (CMD(34),CNS), (CMD(35),CND),
     8 (CMD(36),CNP), (CMD(38),COP), (CMD(39),COD), (CMD(40),COS), (CMD(
     941),CN2PL), (CMD(42),CO2PL), (CMD(43),CNPL), (CMD(44),COPL), (CMD(
     $45),CN2APL), (CMD(46),CN2BPL), (CMD(50),CEN), (CMD(51),CO2), (CMD(
     $52),CO2D), (CMD(53),CO2B), (CMD(54),CO2SG)
      DATA BLANK/5H     /
      DATA NSPEC/54/
      DATA MSTATE/0,10,14,18,22,26,30,34,38,42,46,50,59,63,67,71,77,94,1
     104,0/
      DATA NSTATE/10,4,4,4,4,4,4,4,4,4,4,9,4,4,4,6,17,10,4,0/
      DATA TEST/6H      ,6HSWITCH,6HCONTRO,6HCMD   ,6HALTTEM,6HENERGY,6H
     1NUCLEA,6HPLOT  ,6HEND DA,6HEND FI/
      DATA AO3/1.E10,5.E10,1.E11,2.6E12,6.2E11,5.0E10,7.9E9,6.3E8,1.E8,1
     1.E8,1.E7/
      DATA ANO/1.,1.,5.E7,1.6E8,2.5E8,4.E8,6.6E8,3.4E8,1.7E8,1.E8,9.6E7/
      DATA AOH/1.,1.,1.,5.E6,1.E7,1.E7,1.6E6,7.9E5,1.6E5,2.5E3,4.0E1/
      DATA FO3/1.E7,2.E5,1.E5,1.E4,1.E3,1.E2,1.E1,1.,1.,1.,1./
      DATA FNO/9.E7,1.E8,9.E7,7.3E7,5.5E7,4.1E7,2.9E7,2.0E7,1.4E7,1.E7,6
     1.7E6/
C     ******************************************************************
C
C                    COMMENTS ON INPUT CARDS
C
C     CONTROL TM,CMD,ALTTEM,NUCLEARM1(M2),PLOT CARDS MUST BE REPEATED
C      FOR EACH INTERNAL PROB -- I.E. PROBLEMS DIVIDED BY END DATA CARDS
C     NUCLEAR M1 AND M2 CARDS ARE NOT NECESSARY BUT MUST BE IN ORDER.
C     A NEGATIVE TEMPERATURE INPUT KEEPS THE TEM FROM BEING UPDATED
C
C
C     ED    PROMPT ENERGY DEP (ERG/CC)
C     QI    CONT SOURCE AT TIME=0. (ION PAIRS/CC/SEC)
C           DECAYS AT Q=QI/(1.+T)**1.2 UNLESS SWICH(55) IS ON
C     DP    DIRECTION COSINE OF SUN,    NIGHT IF(DP.LE.0.)
C     QA    AMBIENT CONT SOURCE  (ION PAIRS/CC/SEC)
```

```
          PACKAGE CHEM74                  01 JUL 74 VERSION                PAGE   2

C                                                                        A  68
C                                                                        A  69
C                     SWITCHES CARD                                      A  70
C                                                                        A  71
C    SWTCH(12) = 1HN  ONLY ONE CALL TO DECAYR PER TIME                   A  72
C    SWTCH(13) = 1HR  READ IN CMD ARRAY AFTER END DATA  (8E10.2)         A  73
C                     REPLACES ALL OTHER INITIALIZATION OF SPECIES       A  74
C                     BEFORE FIRST CALL TO DECAYR.                       A  75
C    SWTCH(14) = 1HR  READ IN CMD ARRAY FOR PLOTTING (SOLID LINES)       A  76
C                     ARRAY IS READ ONTO TAPE8 FOR PLOTTING ,(58 ON)     A  77
C                     IF USED, NUMERICAL CHEM RUN (TAPE4) CAN NOT BE     A  78
C                     PLOTTED SINCE TAPE8 OVERRIDES TAPE4 PLOTTING.      A  79
C                     BUT A TAPE8-TAPE1 (ANALYTIC CHEM) COMPARISON MAY   A  80
C                     BE MADE BY USE OF SWTCH(61).                       A  81
C                     DATA READ AFTER  END DATA  CARD                    A  82
C                     FIRST CARD IS NO. OF TIMES TO BE READ,NTI, AND     A  83
C                     SPECIES POSITIONS IN CMD ARRAY (MAX OF 7). 8I10    A  84
C                     NEXT NTI CARDS ARE TIME, T, AND CONC OF SPECIES.   A  85
C    SWTCH(15) = 1HS  USED ONLY IN CONJUCTION WITH SWTCH(14)             A  86
C                     PLOT TAPE8 FOR OVERLAY USING TAPE4 GRID.           A  87
C                     THEREFORE NUML CHEM RUN MUST HAVE BEEN MADE PREV   A  88
C                     SWTCH(61) MAY NOT BE USED IF SWTCH(15) IS USED.    A  89
C    SWTCH(55) = 1HQ  Q DOES NOT VARY WITH TIME, REMAINS AT QI VALUE     A  90
C    SWTCH(56) = 1HY  DETAILED PRINT IN NUML CHEMISTRY                   A  91
C    SWTCH(57) = 1HY  PRINT CHARGE AND PARTICAL NO. BEFORE AND AFTER E   A  92
C                     EACH TIME.                                         A  93
C    SWTCH(58) = 1HP  PLOT CHEMISTRY CONCENTRATIONS VS TIME              A  94
C                     PLOT CARDS ARE NECESSARY                           A  95
C                     THE NUMBER OF PLOTS = THE NUMBER OF PLOT CARDS     A  96
C    SWTCH(59) = 1HF  DO NUML CHEMISTRY                                  A  97
C    SWTCH(60)        USED INTERNALLY                                    A  98
C    SWTCH(61) = 1HC  DO PLOT COMPARISON OF ANALYTIC AND NUML CHEMISTR   A  99
C                     PLOT CARDS AND SWTCH(61) NEED ONLY BE INCLUDED     A 100
C                     IN THE SECOND OF THE TWO INTERNAL PROBLEMS WHICH   A 101
C                     MUST BE RUN.  SWTCH(61) MUST BE ONLY ON THE        A 102
C                     SWITCHES CARD OF THE SECOND PROBLEM I.E. PLACING   A 103
C                     A SWTCH(61) IN THE FIRST PROB WILL RESULT IN       A 104
C                     GARBAGE.   ALSO SWTCH(58) MUST BE ON IN THE        A 105
C                     SECOND PROBLEM, IT MAY OR MAY NOT BE ON IN THE     A 106
C                     FIRST IF AN INDIVIDUAL PLOT IS DESIRED.            A 107
C                     EITHER NUML OR ANALYTIC MAY BE RUN FIRST           A 108
C                                                                        A 109
C                                                                        A 110
C                     EXAMPLE RUN                                        A 111
C                                                                        A 112
C                                                                        A 113
C1234567890         0         0         0         0         0         0         9
C
CTITLE                      100KM NIGHT
CSWITCHES   NR                                            Y
CCONTROL TM   1.0E-7    1.0E-6    1.0E-5    1.0E-4    1.0E-3    1.0E-2    1.0E-
CCONTROL TM       1.       10.      100.    9.9E2
CALTTEM         100.     200.0
CENERGY DEP  .535E-2        0.        0.    3.1E-1
CEND DATA
C        0.        0.        0.        0.        0.        0.        0.        0
C        0.        0.        0.        0.        0.        0.        0.        0
C        0.        0.        0.        0.        0.     1.0E8    6.0E-2       0
C        0.        0.     1.2E7        0.        0.        0.   6.18E12       0
C        0.     2.4E4        0.        0.        0.    1.6E11        0.       0
C        0.        0.        0.        0.        0.        0.        0.       0
C        0.        0.   1.99E12        0.        0.        0.
CTITLE                      100KM NIGHT
CSWITCHES   NR                                        YPF C
CCONTROL TM    9.9E2
CALTTEM         100.     200.0
CENERGY DEP  .535E-2        0.        0.    3.1E-1
CPLOT             OP        O3        NO        NS      O2PL       NO2         N
CEND DATA
C        0.        0.        0.        0.        0.        0.        0.        0
C        0.        0.        0.        0.        0.        0.        0.        0
C        0.        0.        0.        0.        0.     1.0E8    6.0E-2       0
C        0.        0.     1.2E7        0.        0.        0.   6.18E12       0
C        0.     2.4E4        0.        0.        0.    1.6E11        0.       0
C        0.        0.        0.        0.        0.        0.        0.       0
```

```
          PACKAGE CH_M74                    01 JUL 74 VERSION                   PAGE   3

C        0.        0.   1.99E12        0.        0.        0.
CTITLE                     60KM     NIGHT
CSWITCHES   NR                                           Y
CCONTROL TM    1.0E-7    1.0E-6    1.0E-5    1.0E-4    1.0E-3    1.0E-2     1.0E-
CCONTROL TM        1.       10.      100.     9.9E2
CALTTEM           60.     260.0
CENERGY DEP      .535        0.        0.    1.7E-2
CEND DATA
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.     2.0E6     1.0E8      4.0E
C        0.        0.    1.0E10        0.        0.        0.    5.0E15         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.   1.33E15        0.        0.        0.
CTITLE                     60KM     NIGHT
CSWITCHES   NR                                          YPF C
CCONTROL TM     9.9E2
CALTTEM           60.     260.0
CENERGY DEP      .535        0.        0.    1.7E-2
CPLOT             OP        O3        NO        NS      O2PL       NO2         N
CEND DATA
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.     2.0E6     1.0E8      4.0E
C        0.        0.    1.0E10        0.        0.        0.    5.0E15         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.   1.33E15        0.        0.        0.
CTITLE                     60KM       DAY
CSWITCHES   NR                                           Y
CCONTROL TM    1.0E-7    1.0E-6    1.0E-5    1.0E-4    1.0E-3    1.0E-2     1.0E-
CCONTROL TM        1.       10.      100.     9.9E2
CALTTEM           60.     260.0
CENERGY DEP      .535        0.        1.    4.2E-2
CEND DATA
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.     1.0E8     3.0E4      3.0E
C        0.        0.     4.0E9        0.        0.        0.    5.0E15         0
C        0.     3.0E3        0.        0.        0.     6.0E9        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.   1.33E15    2.0E10        0.        0.
CTITLE                     60KM       DAY
CSWITCHES   NR                                          YPF C
CCONTROL TM     9.9E2
CALTTEM           60.     260.0
CENERGY DEP      .535        0.        1.    4.2E-2
CPLOT             OP        O3        NO        NS      O2PL       NO2         N
CEND DATA
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.        0.        0.        0.     1.0E8     3.0E4      3.0E
C        0.        0.     4.0E9        0.        0.        0.    5.0E15         0
C        0.     3.0E3        0.        0.        0.     6.0E9        0.         0
C        0.        0.        0.        0.        0.        0.        0.         0
C        0.        0.   1.33E15    2.0E10        0.        0.
CTITLE                     40KM     NIGHT
CSWITCHES                                                Y
CCONTROL TM    1.0E-7    1.0E-6    1.0E-5    1.0E-4    1.0E-3    1.0E-2     1.0E-
CCONTROL TM        1.       10.      100.
CCMD         6.488E16  1.741E15        1.
CALTTEM           40.     250.4
CENERGY DEP    21.4E0     1.0E7      -.68    2.2E-1
CEND DATA
CTITLE                     40KM     NIGHT
CSWITCHES                                               YPF C
CCONTROL TM      1.E2
CCMD         6.488E16  1.741E16        1.
CALTTEM           40.     250.4
CENERGY DEP    21.4E0     1.0E7      -.68    2.2E-1
CPLOT             OP        O3       O2D        NS        NO       NO2
CEND DATA
CEND FILE                                                                   A 216
C
```

```
C     ***************************************************************
C
 1    CONTINUE
      REWIND 4
      REWIND 1
      REWIND 3
      DO 2 I=1,10
      YOMETL(I)=0.
 2    OYMETL(I)=0.
      DO 3 I=1,70
 3    TI(I)=0.
      DO 4 I=1,NSPEC
 4    CMD(I)=0.
      IPL=0
      ITM=0
      INM=0
      PRINT 36
 5    CONTINUE
      REWIND 2
      READ (3,37) ALPH
      WRITE (6,35) ALPH
      IF (ALPH(1).EQ.1HS) GO TO 7
      WRITE (2,37) ALPH
      IF (ALPH(1).EQ.1HT) GO TO 6
      IF (ALPH(1).EQ.1HP) GO TO 17
      REWIND 2
      READ (2,39) TYPE,(X(L),L=1,7)
      JUMP=LOGIC(9,TYPE,TEST)
      GO TO (5,7,9,11,12,13,15,17,19,14), JUMP
 6    CONTINUE
C
C     TITLE   FOR PLOTS--USES ONLY COLUMNS 10 TO 60
C
      REWIND 2
      READ (2,40) TYPE,(TITL(L),L=1,7)
      GO TO 5
 7    CONTINUE
C
C     SWITCHES
C
      DO 8 I=1,60
 8    SWTCH(I)=ALPH(I)
      GO TO 5
 9    CONTINUE
C
C     CONTROL TM    TIME CARDS
C
      DO 10 I=1,7
      III=I+ITM
 10   TI(III)=X(I)
      ITM=ITM+7
      GO TO 5
 11   CONTINUE
C
C     CHD CONCENTRATIONS OF N2,O2,O,(AND N)
C
      CN2=X(1)
      CO2=X(2)
      COP=X(3)
      CNS=X(4)
      GO TO 5
 12   CONTINUE
C
C     ALTITUDE AND TEMPERATURE
C
      ALT=X(1)
      TEM=X(2)
      GO TO 5
 13   CONTINUE
C
C     ENERGY DEPOSITION   ED,QI,QP,QA
C
      ED=X(1)
      QI=X(2)
      QP=X(3)
```

```
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      QA=X(4)
      DAY=DP
      GO TO 5
   14 CONTINUE
      CALL PLOT (XP,YP,40)
      STOP
   15 CONTINUE
C
C     METALS CARD M1
C
      INM=INM+1
      IF (INM.EQ.2) GO TO 16
      YDMETL(1)=X(2)
      YDMETL(2)=X(3)
      YDMETL(3)=X(4)
      YDMETL(4)=X(5)
      YDMETL(5)=X(6)
      YDMETL(6)=X(7)
      GO TO 5
C
C     METALS CARD M2
C
   16 YDMETL(7)=X(2)
      YDMETL(8)=X(3)
      YDMETL(9)=X(4)
      YDMETL(10)=X(5)
      GO TO 5
   17 CONTINUE
C
C     SPECIES TO BE PLOTTED
C
      JPL=0
      IPL=IPL+1
      REWIND 2
      READ (2,41) TYPE,(X(L),L=1,7)
      DO 18 IP=1,7
      IF (X(IP).EQ.BLANK) GO TO 18
      JPL=JPL+1
      XPLOTS(JPL,IPL)=X(IP)
   18 CONTINUE
      NPPL(IPL)=JPL
      GO TO 5
   19 CONTINUE
C
C     PREPARE INPUTS FOR CHEMISTRY PACKAGE
C
      IF (SWTCH(14).EQ.1HR) GO TO 30
      TN=CN2+CO2+COP
      RHO=TN/4.E22
      IF (ALT-100.) 20,20,21
   20 CONTINUE
      HQ=AMAX1((ALT-60.),0.)/20.
      HQ=EXP(-HQ)
      CH=2.E8*(1.-HQ)
      CCO2=TN*3.3E-4
      IHA=ALT/10.
      IF (IHA.GE.10) IHA=9
      THA=(ALT-IHA*10.)/10.
      IHA=IHA+1
      GO3=ALOG(AO3(IHA))*(1.-THA)+ALOG(AO3(IHA+1))*THA
      GNO=ALOG(ANO(IHA))*(1.-THA)+ALOG(ANO(IHA+1))*THA
      GOH=ALOG(AOH(IHA))*(1.-THA)+ALOG(AOH(IHA+1))*THA
      CO3=EXP(GO3)
      CNO=EXP(GNO)
      COH=EXP(GOH)
      GO TO 22
   21 CONTINUE
      CH=1.E-5*TN
      CCO2=3.3E-4*TN
      IHA=ALT/10.-10
      IF (IHA.GE.10) IHA=9
      THA=((ALT-100.)-(FLOAT(IHA)*10.))/10.
      IHA=IHA+1
      GO3=ALOG(FO3(IHA))*(1.-THA)+ALOG(FO3(IHA+1))*THA
      GNO=ALOG(FNO(IHA))*(1.-THA)+ALOG(FNO(IHA+1))*THA
```

```
      CO3=EXP(GO3)
      CNO=EXP(GNO)
 22   CONTINUE
      IF (SWTCH(13).NE.1HR) GO TO 23
      READ (3,42) (CMO(I),I=1,NSPEC)
 23   CONTINUE
      IF (SWTCH(12).EQ.1HN) GO TO 24
      SWTCH(60)=1.
      CALL SECOND (CTIME)
      PRINT 43, CTIME
      TEMI=-TEM
      IF (TEMI.GE.0.) TEMI=-TEMI
C
C     INITIALIZATION CALL TO DECAYR
C
      CALL DECAYR (1.E-30,QA,DP,TEMI,10000.,RHO)
      CALL SECOND (CTIME)
      PRINT 43, CTIME
      SWTCH(60)=0.
 24   CONTINUE
      DO 25 I=1,90
 25   CMOO(I)=CMO(I)
      LTM=0
      DO 28 II=1,70
      DT=TI(II)
      IF (DT.EQ.0.) GO TO 29
      LTM=LTM+1
      DO 26 I=1,90
 26   CMO(I)=CMOO(I)
      DO 27 I=1,10
 27   DYMETL(I)=YOMETL(I)
      WRITE (6,44) DT
      TEW=TEM
      CALL SECOND (CTIME)
      PRINT 43, CTIME
C
C     CALCULATION OF CONTINUOUS ENERGY DEPOSITION AT TIME DT
C
      Q=QI/((1.+DT)**1.2)
      IF (SWTCH(55).EQ.1HQ) Q=QI
      Q=Q+QA
C
C     CALL TO THE CHEMISTRY PACKAGE
C
      CALL DECAYR (ED,Q,DP,TEW,DT,RHO)
      CALL SECOND (CTIME)
      PRINT 43, CTIME
      PRINT 48
      WRITE (6,47) ED,Q,QA,DP,TEM,TEW,DT,RHO
      PRINT 48
      WRITE (6,45) (CMO(I),I=1,54)
      PRINT 48
      WRITE (6,46) (RR(I),I=1,110)
 28   CONTINUE
 29   CONTINUE
      IF (SWTCH(56).NE.1HP) GO TO 35
      START=1.E-7
      END=TI(LTM)
 30   CONTINUE
      IF (SWTCH(14).NE.1HR) GO TO 33
      START=1.E-7
      END=TI(1)
      READ (3,49) NTI,(NSR(J),J=1,7)
      DO 32 I=1,NTI
      READ (3,50) T,(XI(J),J=1,7)
      DO 31 K=1,7
      NSRR=NSR(K)
 31   CMO(NSRR)=XI(K)
      WRITE (3,51) T,(CMO(K),K=1,NSPEC)
 32   CONTINUE
 33   CONTINUE
      DO 34 I=1,IPL
      CALL PLOTPK (START,END,I)
 34   CONTINUE
 35   CONTINUE
```

```
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        GO TO 1                                                        A 442
C                                                                      A 443
C                                                                      A 444
   36   FORMAT (55H1123456789012345678901234567890123456789012345678901234 A 445
       1,26H56789012345678901234567890//)                              A 446
   37   FORMAT (80A1)                                                  A 447
   38   FORMAT (1X,80A1)                                               A 448
   39   FORMAT (A6,4X,7E10.0)                                          A 449
   40   FORMAT (A6,4X,7A10)                                            A 450
   41   FORMAT (A6,4X,7(5X,A5))                                        A 451
   42   FORMAT (6E10.2)                                                A 452
   43   FORMAT (1X,10HCP TIME = ,E12.3)                                A 453
   44   FORMAT (1H1,8H TIME = ,E15.6)                                  A 454
   45   FORMAT (1X,4HCMO 10E13.4)                                      A 455
   46   FORMAT (1X,4HRR  10E13.4)                                      A 456
   47   FORMAT (1X,25HED,Q,QA,DP,TEM,TEW,UT,RHO,8E11.3)                A 457
   48   FORMAT (///)                                                   A 458
   49   FORMAT (8I10)                                                  A 459
   50   FORMAT (8E10.2)                                                A 460
   51   FORMAT (E13.6,(6E13.6,/))                                      A 461
        END                                                            A 462-
```

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                 PACKAGE CHEM74                01 JUL 74 VERSION                  PAGE    8

 464             FUNCTION LOGIC (N,X,TEST)                                         8    1        464
 465    C                                                                          8    2        465
 466             DIMENSION TEST(2)                                                 8    3        466
 467             DO 1 K=1,N                                                        8    4        467
 468             IF (X-TEST(K)) 1,2,1                                              8    5        468
 469    1        CONTINUE                                                          8    6        469
 470             K=N+1                                                             8    7        470
 471    2        LOGIC=K                                                           8    8        471
 472             RETURN                                                            8    9        472
 473             END                                                               8   10-       473
```

```
      SUBROUTINE DECAYR (ED,Q,DP,TEM,DT,RHO)
C     ******************************************************************
C
C       DECAYR
C             PRIMARY ANALYTICAL ALGORITHM ROUTINE
C
C     ******************************************************************
C
      COMMON /BUR2/ DYMETL(10)
      COMMON /FU/ Y(90),P(90),S(90),R(90),CHT,TGEV,QQ,TNUM,NFLAG,NTG
      COMMON /ININ/ XNTG,QN2PL,QO2PL,QOPL,QNPL,QNS1,QND1,QNP1,QFO,QDO,QO
     1D1,QOS1,QO2D,QO2S,QDN2,QDO2,QNOPL
      COMMON /SWR/ SWTCH(80)
      COMMON /XUX/ RR(200),CMD(90),RCRT(90),NSPEC
      DIMENSION ENERX(90)
      EQUIVALENCE (CMD(1),CH), (CMD(2),CLI), (CMD(3),CBE), (CMD(4),CMG),
     1 (CMD(5),CAL), (CMD(6),CSI), (CMD(7),CTI), (CMD(8),CFE), (CMD(9),C
     2CU), (CMD(10),CU), (CMD(11),COH), (CMD(12),CLIO), (CMD(13),CBEO),
     3(CMD(14),CMGO), (CMD(15),CALO), (CMD(16),CSIO), (CMD(17),CTIO), (C
     4MD(18),CFEO), (CMD(19),CCUO), (CMD(20),CUOPL), (CMD(21),CNOPL), (C
     5MD(22),CNO), (CMD(23),CNO2), (CMD(24),CN2O), (CMD(25),CCO), (CMD(2
     66),CCO2), (CMD(27),CO3), (CMD(28),CH2O), (CMD(30),CEL), (CMD(31),C
     7N2), (CMD(32),CN2A), (CMD(33),CN2B), (CMD(34),CNS), (CMD(35),CND),
     8 (CMD(36),CNP), (CMD(38),COP), (CMD(39),COD), (CMD(40),COS), (CMD(
     941),CN2PL), (CMD(42),CO2PL), (CMD(43),CNPL), (CMD(44),COPL), (CMD(
     $45),CN2APL), (CMD(46),CN2BPL), (CMD(50),CEN), (CMD(51),CO2), (CMD(
     $52),CO2D), (CMD(53),CO2B), (CMD(54),CO2SG)
      EQUIVALENCE (Y(80),CMTL), (Y(61),CMTLO)
      EQUIVALENCE (P(1),FH), (P(2),FLI), (P(3),FBE), (P(4),FMG), (P(5),F
     1AL), (P(6),FSI), (P(7),FTI), (P(8),FFE), (P(9),FCU), (P(10),FU), (
     2P(11),FOH), (P(12),FLIO), (P(13),FBEO), (P(14),FMGO), (P(15),FALO)
     3, (P(16),FSIO), (P(17),FTIO), (P(18),FFEO), (P(19),FCUO), (P(20),F
     4UOPL), (P(21),FNOPL), (P(22),FNO), (P(23),FNO2), (P(24),FN2O), (P(
     525),FCO), (P(26),FCO2), (P(27),FO3), (P(28),FH2O), (P(30),FEL), (P
     6(31),FN2), (P(32),FN2A), (P(33),FN23), (P(34),FNS), (P(35),FND), (
     7P(36),FNP), (P(38),FO), (P(39),FOD), (P(40),FOS), (P(41),FN2PL), (
     8P(42),FO2PL), (P(43),FNPL), (P(44),FOPL), (P(45),FN2APL), (P(46),F
     9N2BPL), (P(50),FEN), (P(51),FO2), (P(52),FO2D), (P(53),FO2B), (P(5
     $4),FO2SG)
      EQUIVALENCE (P(70),FLIO2), (P(71),FLIO3), (P(72),FBEO2), (P(73),FB
     1EO3), (P(74),FMGO2), (P(75),FMGO3), (P(76),FALO2), (P(77),FALO3),
     2(P(78),FSIO2), (P(79),FSIO3), (P(80),FTIO2), (P(81),FTIO3), (P(82)
     3,FFEO2), (P(83),FFEO3), (P(84),FCUO2), (P(85),FCUO3), (P(86),G), (
     4P(87),H), (P(88),FO3A), (P(89),FO3S), (S(70),DMTLO)
      EQUIVALENCE (S(1),DH), (S(2),DLI), (S(3),DBE), (S(4),DMG), (S(5),D
     1AL), (S(6),DSI), (S(7),DTI), (S(8),DFE), (S(9),DCU), (S(10),DU), (
     2S(11),DOH), (S(12),DLIO), (S(13),DBEO), (S(14),DMGO), (S(15),DALO)
     3, (S(16),DSIO), (S(17),DTIO), (S(18),DFEO), (S(19),DCUO), (S(20),D
     4UOPL), (S(21),DNOPL), (S(22),DNO), (S(23),DNO2), (S(24),DN2O), (S(
     525),DCO), (S(26),DCO2), (S(27),DO3), (S(28),DH2O), (S(30),DEL), (S
     6(31),DN2), (S(32),DN2A), (S(33),DN23), (S(34),DNS), (S(35),DND), (
     7S(36),DNP), (S(38),DO), (S(39),DOD), (S(40),DOS), (S(41),DN2PL), (
     8S(42),DO2PL), (S(43),DNPL), (S(44),DOPL), (S(45),DN2APL), (S(46),D
     9N2BPL), (S(50),DEN), (S(51),DO2), (S(52),DO2D), (S(53),DO2B), (S(5
     $4),DO2SG)
      EQUIVALENCE (R(1),RNSO2), (R(2),RNDO2), (R(3),RNSNO), (R(4),RNDNO)
     1, (R(5),TO2O), (R(6),RO3O), (R(7),RN2PEL), (R(8),XN2PO2), (R(9),RN
     22PLO), (P(10),RO2PEL), (R(11),XOPLO2), (R(12),RNOPEL), (R(13),XO2N
     3PL), (R(14),RO2NPL), (R(15),RN2OPL), (R(16),XOPLNO), (R(17),XO2PNO
     4), (R(18),XN2PNO), (R(19),XNPLNO), (R(20),RO2PLN), (R(21),RHO3), (
     5R(22),ROHO), (R(23),RO2SO2), (R(24),RO3NO), (R(25),TONO), (R(26),R
     6ONO2), (R(27),RNO2NA), (R(28),TNON), (R(29),RNO2NB), (R(30),RO2N2O
     7), (R(31),RNSO3), (R(32),RNPHV), (R(33),ROSHV), (R(34),RODHV), (R(
     835),RNPLO)
      EQUIVALENCE (R(50),RLIO2), (R(51),TLIO), (R(52),ROLIO), (R(53),RBE
     1O2), (R(54),TBEO), (R(55),ROBEO), (R(56),RMGO2), (R(57),TMGO), (R(
     258),ROMGO), (R(59),RALO2), (R(60),TALO), (R(61),ROALO), (R(62),RSI
     3O2), (R(63),TSIO), (R(64),ROSIO), (R(65),RTIO2), (R(66),TTIO), (R(
     467),ROTIO), (R(68),RFEO2), (R(69),TFEO), (R(70),ROFEO), (R(71),RCU
     5O2), (R(72),TCUO), (R(73),ROCUO), (R(74),RUO)
      EQUIVALENCE (R(75),RMTLO3), (R(76),RO3LIO), (R(77),RO3BEO), (R(78)
     1,RO3MGO), (R(79),RO3ALO), (R(80),RO3SIO), (R(81),RO3TIO), (R(82),R
     2O3FEO), (R(83),RO3CUO)
      EQUIVALENCE (R(90),PDISO3)
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          DATA CONV/1.16E4/                                                   C   76
          DATA (ENERX(I),I=1,54)/2.*0.0,10.198,0.931,0.372,0.081,-1.179,-4.0  C   77
         173,1.506,-2.476,0.0,0.0,0.0,5.169,7.354,4.880,7.264,6.456,0.0,2.55  C   78
         28,4.525,6.748,15.580,12.063,19.412,16.175,16.580,18.750,5*0.0,0.97  C   79
         37,1.627,4.340/                                                      C   80
          DATA CO2NG/0./                                                      C   81
    C                                                                         C   82
          PRINT 22, ED,Q,DP,TEM,DT,RHO                                      CHC   83
          PRINT 23, CMD                                                     CHC   84
          QQ=Q                                                                C   85
          CON=CN2+CO2+COP                                                     C   86
    C                                                                         C   87
    C --- ADD METALS TO CMD ARRAY                                             C   88
    C                                                                         C   89
          DO 1 K=1,10                                                         C   90
          CMD(K)=CMD(K)+DYMETL(K)                                             C   91
    1     DYMETL(K)=0.                                                        C   92
          DO 2 K=1,90                                                         C   93
          P(K)=0.                                                             C   94
          S(K)=0.                                                             C   95
    2     CONTINUE                                                            C   96
          CMTL=CLI+CBE+CMG+CAL+CSI+CFE+CCU+CTI                                C   97
          CMTLO=CLIO+CBEO+CMGO+CALO+CSIO+CFEO+CCUO+CTIO                       C   98
          IF (SWTCH(60).EQ.1.) GO TO 3                                        C   99
    C                                                                         C  100
    C --- BRANCH TO NUMERICAL CHEMISTRY                                       C  101
    C                                                                         C  102
          IF (SWTCH(59).EQ.1HF) GO TO 21                                      C  103
    3     CONTINUE                                                            C  104
          IF (SWTCH(57).NE.1HY) GO TO 4                                     CHC  105
          CHG=CN2PL+COPL+CNOPL+CNPL+CO2PL+CUOPL+CN2APL+CN2BPL-CEL           CHC  106
          PNUM=CNS+CND+CNP+COP+COS+COD+CNPL+COPL+CH+CMTL+CU+2.*(CO2+CO2D+CO2CHC  107
         1B+CO2SG+CN2+CN2A+CN2B+CN2PL+CN2APL+CN2BPL+CO2PL+CNO+CNOPL+COH+CCO+CHC  108
         2CMTLO+CUOPL)+3.0*(CO3+CNO2+CN2O+CCO2+CH2O)                        CHC  109
          PRINT 24, CHG,PNUM                                                CHC  110
    4     CONTINUE                                                          CHC  111
    C                                                                         C  112
    C --- CONVERT ED(ERGS/CM3) TO ION PAIRS/CM3                               C  113
    C     AND CALL ENTDEP TO ACCOUNT FOR PROMT ENERGY DEPOSITION EFFECTS      C  114
    C                                                                         C  115
          DEX=1.87E13*ED+1.E-30                                               C  116
          CALL ENTDEP (DEX,CON,TEM)                                           C  117
    C                                                                         C  118
    C --- CALCULATE TOTAL ENERGY FROM HEATS OF FORMATION AND TOTAL INTERNAL    C  119
    C     KINETIC ENERGY                                                      C  120
    C                                                                         C  121
          CENT=CEN                                                            C  122
          DO 5 I=1,NSPEC                                                      C  123
          CENT=CENT+ENERX(I)*CMD(I)                                           C  124
    5     CONTINUE                                                            C  125
    C                                                                         C  126
    C --- FILL R ARRAY WITH RATE CONSTANTS                                    C  127
    C                                                                         C  128
          CALL RATE (TEM,CON)                                                 C  129
    C                                                                         C  130
    C --- CALL ENQDEP FOR CONTINUOUS SOURCE TERMS                              C  131
    C                                                                         C  132
          CALL ENQDEP (DEX,CON,TEM)                                           C  133
    C                                                                         C  134
    C --- BEGIN FAST ION CHEMISTRY                                            C  135
    C                                                                         C  136
    C ---      N+                                                             C  137
    C                                                                         C  138
          CNPL0=CNPL                                                          C  139
          CO=COP+COD+COS                                                      C  140
          BN=XNPLNO*CNO+XO2NPL*CO2+RNPLO*CO+RO2NPL*CO2                        C  141
          EXPBNT=EXP(-BN*DT)                                                  C  142
          CNPLT=CNPL0*EXPBNT                                                  C  143
          CNPLQ=WQX(QNPL,BN,0.0,DT)                                           C  144
          CNPL=CNPLT+CNPLQ                                                    C  145
          XNIGL=(1.-EXPBNT)/BN                                                C  146
    C                                                                         C  147
    C ---      O+                                                             C  148
    C                                                                         C  149
          BO=XOPLO2*CO2+XOPLNO*CNO+RN2OPL*CN2                                 C  150
```

```
      EXPBOT=EXP(-BO*DT)
      COPL0=COPL
      GM=RNPLO*CO
      YAE=GM*CNPL0/(BO-BN)
      COPLT=(COPL0-YAE)*EXPBOT+YAE*EXPBNT
      QQCPL=QOPL+GM*CNPL
      COPLQ=WQX(QQOPL,BO,0.0,DT)
      COPL=COPLQ+COPLT
C
C ---    ATOMIC IONS
C
      ATMPLT=COPLT+CNPLT
      ATMPL0=COPL0+CNPL0
      XOGL=(1.-EXP(-BO*DT))/BO
      COPL01=COPL0-YAE
      COPL02=CNPL0+YAE
      XOIGL=COPL01*XOGL+YAE*XNIGL
      XAGLP=COPL01*XOGL+COPL02*XNIGL
      GOPLO2=XOIGL*CO2*XOPLO2
C
C ---    NEGATIVE CHARGE
C
      ALPHAR=(RN2PEL*CN2PL+RO2PEL*CO2PL+RNOPEL*CNOPL)/(CN2PL+CO2PL+CNOPL
     1+COPL+CNPL)
      AB=ALPHAR*ATMPLT*DT
      ALPHRP=ALPHAR*SHXOX(AB)
      CNEG=CEL+CO2NG
      CNEG0=CNEG
      ANG0P=ALPHRP*CNEG0
      ANG0PT=ANG0P*DT
      OANOPT=1.+ANG0PT
      CNEG=ATMPLT+(CNEG0-ATMPLT)/OANOPT
      CNEGQ=WR(QQ,ALPHAR,0.0,DT)
      CNEG=AMAX1(CNEG,CNEGQ)
      XOGLP1=X1IGL(ALPHRP,BO,CNEG0,DT)
      XOGLP2=X1IGL(ALPHRP,BN,CNEG0,DT)
      XOGLP=COPL01*XOGLP1+COPL02*XOGLP2
C
C ---    N2+
C
      CN2PL0=CN2PL
C
C --- FACTOR OF 2 DUE TO SEPARATION OF REACTION 9 INTO TWO PARTS
C
      BN2=XN2PO2*CO2+XN2PNO*CNO+RN2PLO*CO*2.0
      CN2PLT=CN2PL0*EXP(-BN2*DT-RN2PEL*(XAGLP-XOGLP))/(1.+ALPHAR*CNEG0*D
     1T)+1.E-50
      BN2EFF=BN2+(RN2PEL*(XAGLP-XOGLP))/DT
      IF (CN2PLT.LE.2.E-50) BN2EFF=BN2
      GAMMA=SQRT(ALPHAR*ALPHRP)
      XN2IGL=X1IGL(ALPHAR,BN2EFF,CNEG0,DT)
      B=RN2PEL*CNEG+BN2
      CN2PLQ=WQX(QN2PL,B,0.0,DT)
      CN2PL=AMAX1(CN2PLT,CN2PLQ)
      GN2PO2=CN2PL0*XN2IGL*XN2PO2*CO2
      GN2PNO=CN2PL0*XN2IGL*XN2PNO*CNO
      GN2PLO=CN2PL0*XN2IGL*RN2PLO*CO*2.0
      DELTA1=BN2EFF+BO
      DELTA2=BN2EFF+BN
      GN2PEL=RN2PEL*CN2PL0*(COPL01*X1IGL(ALPHAR,DELTA1,CNEG0,DT)+COPL02*
     1X1IGL(ALPHAR,DELTA2,CNEG0,DT)+CNEG0*X2IGL(GAMMA,BN2EFF,CNEG0,DT)-C
     2OPL01*X2IGL(GAMMA,DELTA1,CNEG0,DT)-COPL02*X2IGL(GAMMA,DELTA2,CNEG0
     3,DT))
      ADELN2=GN2PO2+GN2PNO+GN2PLO+GN2PEL+1.E-30
      DELN2P=CN2PL0-CN2PLT
      DN2TR=DELN2P/ADELN2
C
C --- UPDATE N AND O
C
      GOPLN2=RN2OPL*CN2*XOIGL
      GNPLO2=XO2NPL*CNPL0*CO2*XNIGL
      GNPRO2=RO2NPL*CO2*XNIGL*CNPL0
      GNPLO=GM*CNPL0*XNIGL
      GNPLNO=XNPLNO*CNO*CNPL0*XNIGL
      GOPLNO=XOPLNO*CNO*XOIGL
```

```
      CNS=CNS+0.33*GN2PEL*DN2TR+0.5*GN2PLO*DN2TR+0.5*GNPLO2+GOPLN2+0.5*G
     1NPLNO+GNPLO
      CND=CND+0.33*GN2PEL*DN2TR+0.5*GN2PLO*DN2TR+0.5*GNPLO2+0.5*GNPLNO
      CNP=CNP+0.02*GN2PEL*DN2TR
      CN=CNS+CND+CNP
      COP=COP+GOPLO2+GNPRO2+GOPLNO
      CO=COP+COD+COS
      DELO=GN2PLO+GNPLO
      COP=COP-DELO*(COP/CO)
      COD=COD-DELO*(COD/CO)
      COS=COS-DELO*(COS/CO)
      CO=COP+COD+COS
      CNO=CNO-GOPLNO-GN2PNO-GNPLNO
      ZNS=CNS
      ZND=CND
      ZNP=CNP
C
C --- INTERMEDIATE UPDATING OF NO
C
      CO20=CO2
      CNO0=CNO
      CO2NO0=CO20+CNO0
      XKAY=RNOO2+RNONO
      BTA=CO2*RNOO2+RNONO*CNO
      BTAT=-BTA*DT
      RTO=CO2NO0*RNOO2/XKAY
      CNOG=RTO-(RTO-CNO0)*EXP(-XKAY*ZND*DT*SHXOX(BTAT))
      GMA=RNSO2*CO2+RNSNO*CNOG
      GMAT=-GMA*DT
      ALMO=RNSO2+RNSNO
      RT1=RNSO2*CO2NOG/ALMO
      CNOG=RT1-(RT1-CNOG)*EXP(-ALMO*(ZNS+ZNP)*DT*SHXOX(GMAT))
      CNO=CNOG
C
C ---     O2+
C
      BO2=XO2PNO*CNO+RO2PLN*(CN)+1.E-30
      GN2PNO=CN2PLO*XN2IGL*XN2PNO*CNO
      XCN2PL=GN2PO2+GN2PLO+GN2PNO
      CO2PLO=CO2PL+GOPLO2+GNPLO2+GN2PO2*(CN2PLO/(CN2PL+XCN2PL))
      CO2POP=CO2PL+GN2PO2+GOPLO2+GNPLO2
      EXPGL=EXP(-RO2PEL*(XAGLP-XOGLP))
      CO2PLT=CO2PLO*EXP(-BO2*DT)*EXPGL*(1.+ANGOPT*EXPGL)**(-RO2PEL/ALPHR
     1P)+1.E-50
      BO2EFF=ALOG(CO2PLO/((1.+ALPHAR*CNEGO*DT)*CO2PLT))/DT
      IF (CO2PLT.LE.2.E-30) BO2EFF=BO2
      XO2IGL=X1IGL(ALPHAR,BO2EFF,CNEGO,DT)
      GO2PNO=XO2PNO*CO2PLO*XO2IGL*CNO
      DELTA1=BO2EFF+BO
      DELTA2=BO2EFF+BN
      GO2PEL=RO2PEL*CO2PLO*(COPLO1*X1IGL(ALPHAR,DELTA1,CNEGO,DT)+COPLO2*
     1X1IGL(ALPHAR,DELTA2,CNEGO,DT)+CNEGO*X2IGL(GAMMA,BO2EFF,CNEGO,DT)-C
     2OPLO1*X2IGL(GAMMA,DELTA1,CNEGO,DT)-COPLO2*X2IGL(GAMMA,DELTA2,CNEGO
     3,DT))
      GO2PLN=RO2PLN*CN*CO2PLO*XO2IGL
      ADELO2=GO2PNO+GO2PEL+GO2PLN+1.E-30
      DELO2P=CO2PLO-CO2PLT
      DO2TR=GO2PEL*DELO2P/ADELO2
      DO2TR=DO2TR*CO2POP/CO2PLO
      QQO2PL=QO2PL+(XN2PO2*CN2PL+XOPLO2*COPL+XO2NPL*CNPL)*CO2
      B=RO2PEL*CNEG+BO2
      CO2PLQ=WQX(QQO2PL,B,0.0,DT)
      CO2PL=AMAX1(CO2PLT,CO2PLQ)
C
C ---     NO+
C
      GOPLNO=XOIGL*CNO*XOPLNO
      GNPLNO=XNPLNO*CNO*CNPLO*XNIGL
      GN2PLO=CO*RN2PLO*XN2IGL*CN2PLO*2.0
      XCO2PL=GO2PNO+GO2PLN
      CNOPLO=CNOPL+GOPLNO+GNPLNO+GNPRO2+GOPLN2+(GN2PNO+GN2PLO)*CN2PLO/(C
     1N2PL+XCN2PL)+XCO2PL*CO2PLO/(CO2PL+XCO2PL)+1.E-50
      CNOPOP=CNOPL+GOPLNO+GNPLNO+GNPRO2+GOPLN2+GN2PNO+GN2PLO+XCO2PL
      EXPGL=EXP(-RNOPEL*(XAGLP-XOGLP))
      CNOPLT=CNOPLO*EXPGL/(1.+ALPHRP*CNEGO*EXPGL*DT)
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      QQNOPL=QNOPL+CNO*(CN2PL*XN2PNO+CO2PL*XO2PNO+COPL*XOPLNO+CNPL*XNPLN
     10)+2.0*CN2PL*CO*RN2PLO+COPL*CN2*RN2OPL+CNPL*RO2NPL*CO2+RO2PLN*CO2P
     2L*CN
      B=RNOPEL*CNEG
      CNCPLQ=WQX(QQNOPL,B,0.0,DT)
      CNOPL=AMAX1(CNOPLT,CNOPLQ)
C
C --- REEVALUATE ALPHAR AND ALPHRP AND THEN CEL AND CNOPL
C
      ALPHAR=(RN2PEL*CN2PL+RO2PEL*CO2PL+RNOPEL*CNOPL)/(CN2PL+CO2PL+CNOPL
     1+COPL+CNPL)
      ALPHRP=ALPHAR*SHXOX(AB)
      OANOPT=1.+ALPHRP*CNEGC*DT
      CNEG=ATMPLT+(CNEG0-ATMPLT)/OANOPT
      CNEGQ=WR(QQ,ALPHAR,0.0,DT)
      CNEG=AMAX1(CNEG,CNEGQ)
      CEL=CNEG
      CNOPLT=CNOPL0*EXPGL*(1.+ALPHRP*CNEG0*EXPGL*DT)**(-RNOPEL/ALPHRP)+1
     1.E-30
      B=RNOPEL*CNEG
      CNOPLQ=WQX(QQNOPL,B,0.0,DT)
      CNOPL=AMAX1(CNOPLT,CNOPLQ)
      DNOTR=CNOPL0-CNOPLT
      DNOTR=DNOTR*CNCP0P/CNOPL0
C
C --- UPDATE N AND O
C
      CNS=CNS+0.25*DNOTR-GO2PLN*(CNS/CN)
      CND=CND+0.75*DNOTR-GO2PLN*(CND/CN)
      CNP=CNP-GO2PLN*(CNP/CN)
      CN=CNS+CND+CNP
      COP=COP+0.8*CO2TR+0.75*DNOTR+GO2PLN
      COD=COD+0.8*DO2TR+0.25*DNOTR
      COS=COS+0.4*DO2TR
      CO=COP+COD+COS
      CNC=CNO-GO2PNO
      IF (NTG.EQ.0) GO TO 7
C
C --- UPDATE TEMPERATURE AND RECALCULATE THE RATE CONSTANTS
C
      CHT=1.5*(CNS+CND+CNP+COP+COD+COS+CNPL+COPL)+2.5*(CNOPL+CNO+CCO+CN2
     1+CN2A+CN2B+CN2PL+CO2PL+CN2APL+CN2BPL+CO2+CO2D+CO2B+CO2SG)+3.0*(CNO
     22+CN2O+CCO2+CO3+CH2O)
      SUME=0.0
      DO 6 I=1,NSPEC
      SUME=SUME+CMO(I)*ENERX(I)
    6 CONTINUE
      CEN=ABS(CENT-SUME)
      TGEV=CEN/CHT
      TEM=TGEV*CONV
      IF (TEM.GT.11000.) TEM=11000.
      CALL RATE (TEM,CON)
    7 CONTINUE
C
C --- PREPARE PRODUCT TERMS FOR CONTINUOUS SOURCE CALCULATIONS
C
      DOQX1=RN2PLO*CO*CN2PL
      DOQX2=XOPLO2*COPL*CO2+XOPLNO*CNO*COPL
      DN2QR=RN2PEL*CEL*CN2PL
      DO2QX=RO2PLN*CO2PL*CN
      DO2QR=RO2PEL*CEL*CO2PL
      DNOQR=RNOPEL*CEL*CNOPL
      DNQX1=XO2NPL*CO2*CNPL
      DOQR=RN2OPL*CN2*COPL
      DNQX2=XNPLNO*CNO*CNPL
      DNQX3=RNPLO*CO*CNPL
      DNQR=RO2NPL*CO2*CNPL
      QNS=QNS1+0.99*DN2QR+0.25*DNOQR+DOQX1+.5*DNQX1+DOQR+.5*DNQX2+DNQX3
      QND=QND1+0.99*DN2QR+0.75*DNOQR+DOQX1+.5*DNQX1+.5*DNQX2
      QNP=QNP1+0.02*DN2QR
      QO=QFO-QCO*COP+0.50*DO2QR+0.75*DNOQR+DO2QX+DOQX2+DNQR
      QOD=QOD1+0.6*DO2QR+0.25*DNOQR
      QOS=QOS1+0.4*DO2QR
C
C --- PREPARE USEFUL RATE TERMS FOR SUBSEQUENT CALCULATIONS
```

```
C                                                                         C 376
C                                                                         C 377
C ---    O     +    O2    +    M              O3    +     M               C 378
C                                                                         C 379
      B1=TO2O*CO2                                                         C 380
C                                                                         C 381
C ---    O2    +    O2*(S)                    O3    +     O               C 382
C                                                                         C 383
      B11=RO2SO2*CO2                                                      C 384
C                                                                         C 385
C ---    O(1S)                               O(1D)+     HV               C 386
C                                                                         C 387
      B13=ROSHV                                                           C 388
C                                                                         C 389
C ---    O(1D)                               O(3P)+     HV               C 390
C                                                                         C 391
      B14=RODHV                                                           C 392
C                                                                         C 393
C ---    N(4S)+     O3                        NO** +     O2               C 394
C                                                                         C 395
      B16=RNSO3*CO3                                                       C 396
C                                                                         C 397
C --- DECAY O(1S) AND O(1D) AND O2*(S)                                    C 398
C                                                                         C 399
      XCOSD=COS*EXP(-B13*DT)                                              C 400
      COD=(COD+B13/(B13-B14)*COS)*EXP(-B14*DT)-B13/(B13-B14)*XCOSD        C 401
      COS=XCOSD                                                           C 402
      COP=CO-COD-COS                                                      C 403
      OCO2S=CO2SG                                                         C 404
      CO2SG=CO2SG*EXP(-B11*DT)                                            C 405
C                                                                         C 406
C ---    N(4S)+     O2                        NO** +     O                C 407
C        N(2P)+     O2                        NO** +     O                C 408
C                                                                         C 409
      B3=RNSO2*CO2                                                        C 410
C                                                                         C 411
C ---    N(2D)+     O2                        NO** +     O                C 412
C                                                                         C 413
      B4=RNDO2*CO2                                                        C 414
C                                                                         C 415
C ---    N(2P)                                N(2D)+     HV               C 416
C                                                                         C 417
      B5=RNPHV                                                            C 418
      ONP=CNP                                                             C 419
      OND=CND                                                             C 420
      ONS=CNS                                                             C 421
C                                                                         C 422
C --- DECAY STATES OF N                                                   C 423
C                                                                         C 424
      CNP=CNP*EXP(-(B5+B3)*DT)                                            C 425
      CND=(CND+B5/(B5-B4)*ONP)*EXP(-B4*DT)-B5/(B5-B4)*CNP                 C 426
      CNS=CNS*EXP(-B3*DT)                                                 C 427
      CN=CNP+CND+CNS                                                      C 428
C                                                                         C 429
C --- RECALCULATION OF NO                                                 C 430
C                                                                         C 431
      BALL=RO3NO*CO3+TONO*CO+TNON*CN                                      C 432
      CALL=B16*CNS+RONO2*CO*CNO2                                          C 433
      CNOG=WQX(CALL,BALL,CNOG,DT)                                         C 434
      XKAY=RNOO2+RNDNO                                                    C 435
      BTA=B4+RNDNO*CNO                                                    C 436
      BTAT=-BTA*DT                                                        C 437
      RTO=CO2NOO*RNDO2/XKAY                                               C 438
      CNO=RTO-(RTO-CNOO)*EXP(-XKAY*ZNO*DT*SHXOX(BTAT))                    C 439
      GMA=B3+RNSNO*CNO                                                    C 440
      GMAT=-GMA*DT                                                        C 441
      ALMD=RNSO2+RNSNO                                                    C 442
      RT1=RNSO2*CO2NOO/ALMD                                               C 443
      CNO=RT1-(RT1-CNO)*EXP(-ALMD*(ZNS+ZNP)*DT*SHXOX(GMAT))               C 444
      CNO=AMAX1(CNO,CNOG)                                                 C 445
C                                                                         C 446
C --- DECAY OF STATES OF N                                                C 447
C                                                                         C 448
      BALL=(RNO2NA+RNO2NB)*CNO2+TNON*CNO                                  C 449
      BB=RNSNO*CNO                                                        C 450
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      B9=RNDNO*CNO                                                      C 451
      CNS=CNS*EXP(-(B8+B16+BALL)*DT)                                    C 452
      CND=CND*EXP(-(B9+BALL)*DT)                                        C 453
      CNP=CNP*EXP(-(B8+BALL)*DT)                                        C 454
      CN=CNS+CND+CNP                                                    C 455
      DEALLN=ONS+OND+ONP-CN                                             C 456
C                                                                       C 457
C --- INCREASE O FOR LOSS OF N                                          C 458
C                                                                       C 459
      COP=COP+DEALLN                                                    C 460
      CO=CO+DEALLN                                                      C 461
      XOC=COP                                                           C 462
C                                                                       C 463
C --- CALCULATION OF O3 AND O                                           C 464
C                                                                       C 465
      BTO3=R030*CO+RNSO3*CNS+RO3NO*CNO+PDISO3                           C 466
      CO3=(CO3+B11*OCO2S/(B11-BTO3)+B1*CO/(B1-BTO3))*EXP(-BTO3*DT)-B11/(C 467
     1B11-BTO3)*OCO2S*EXP(-B11*DT)-B1/(B1-BTO3)*CO*EXP(-B1*DT)          C 468
      BTO=B1+R030*CO3+TONO*CNO+RONO2*CNO2                               C 469
      AYE=RNO2N3*CNO2*CN+PDISO3                                         C 470
      PROD=(B11*OCO2S)/(B11-BTO)                                        C 471
      EXPBTA=EXP(-BTO*DT)                                               C 472
      COP=(COP+PROD)*EXPBTA+(AYE/BTO)*(1.-EXPBTA)-PROD*EXP(-B11*DT)     C 473
      COS=COS*COP/XOC                                                   C 474
      COD=COD*COP/XOC                                                   C 475
      CO=COP+COD+COS                                                    C 476
C                                                                       C 477
C --- PREPARE USEFUL RATE TERMS FOR SUBSEQUENT CALCULATIONS             C 478
C                                                                       C 479
C                                                                       C 480
C ---     O     +     O3                          O2    +    O2         C 481
C                                                                       C 482
      B2=R030*CO3                                                       C 483
      C2=B2*CO                                                          C 484
C                                                                       C 485
C ---     O2    +     O2*(S)                      O3    +    O          C 486
C                                                                       C 487
      C11=B11*CO2SG                                                     C 488
C                                                                       C 489
C ---     N(4S)+      O3                          NO**  +    O2         C 490
C                                                                       C 491
      B16=RNSO3*CO3                                                     C 492
C                                                                       C 493
C ---     N(4S)+      O2                          NO**  +    O          C 494
C                                                                       C 495
      C1A=B3*CNS                                                        C 496
C                                                                       C 497
C ---     N(2P)+      O2                          NO**  +    O          C 498
C                                                                       C 499
      C1B=B3*CNP                                                        C 500
C                                                                       C 501
C ---     N(2D)+      O2                          NO**  +    O          C 502
C                                                                       C 503
      C2A=B4*CND                                                        C 504
C                                                                       C 505
C ---     N(4S)+      NO                          N2    +    O          C 506
C                                                                       C 507
      B3A=RNSNO*CNO                                                     C 508
      C3A=B3A*CNS                                                       C 509
C                                                                       C 510
C ---     N(2P)+      NO                          N2    +    O          C 511
C                                                                       C 512
      C3B=B3A*CNP                                                       C 513
C                                                                       C 514
C ---     N(2D)+      NO                          N2    +    O          C 515
C                                                                       C 516
      B4A=RNDNO*CNO                                                     C 517
      C4A=B4A*CND                                                       C 518
C                                                                       C 519
C ---     NO    +     O     +     M               NO2   +    M          C 520
C                                                                       C 521
      B140=TONO*CO                                                      C 522
      C140=B140*CNO                                                     C 523
C                                                                       C 524
C ---     NO    +     O3                          NO2   +    O2         C 525
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C                                                                       C 526
      B141=RO3NO*CO3                                                    C 527
      C141=B141*CNO                                                     C 528
C                                                                       C 529
C ---    NO2    +    O                       NO    +    O2              C 530
C                                                                       C 531
      B144=RONO2*CO                                                     C 532
C                                                                       C 533
C ---    N      +    NO     +    M           N2O   +    M               C 534
C                                                                       C 535
      B110=TNON*CN                                                      C 536
      C110=B110*CNO                                                     C 537
C                                                                       C 538
C ---    N      +    NO2                     N2    +    O2              C 539
C                                                                       C 540
      B112=RNO2NA*CN                                                    C 541
C                                                                       C 542
C ---    N      +    NO2                     N2O   +    O               C 543
C                                                                       C 544
      B111=RNO2NB*CN                                                    C 545
      C111=B111*CNO2                                                    C 546
C                                                                       C 547
C ---    N2O    +    O2(1D)                  N2    +    O3              C 548
C                                                                       C 549
      B143=RO2N2O*CO2D                                                  C 550
C                                                                       C 551
C ---    U      +    O                       UO+   +    E               C 552
C                                                                       C 553
C                                                                       C 554
C --- CALCULATIONS INCLUDING THE CONTINUOUS SOURCE                      C 555
C                                                                       C 556
      QQO=QO+C1A+C1B+C2A+C3A+C3B+C4A+C11+C111+PDISO3*CO3                C 557
      QW=B1+B2+TONO*CNO+RONO2*CNO2+RUO*CU+RN2PLO*CN2PL+RNPLO*CNPL+1.E-30 C 558
      COPQ=WQX(QQO,QW,0.0,DT)                                           C 559
      COP=COP+COPQ                                                      C 560
      QW1=B14+QW                                                        C 561
      CODQ=WQX(QOD,QW1,0.0,DT)                                          C 562
      COD=COD+CODQ                                                      C 563
      QW1=B13+QW                                                        C 564
      COSQ=WQX(QOS,QW1,0.0,DT)                                          C 565
      COS=COS+COSQ                                                      C 566
      CO=COP+COD+COS                                                    C 567
      B28R=TNON*CNO+1.E-30                                              C 568
      B20=RO2PLN*CO2PL                                                  C 569
      B27=RNO2NA*CNO2                                                   C 570
      B29=RNO2NB*CNO2                                                   C 571
      BALL=B20+B27+B28R+B29                                             C 572
      DENS=B3+B3A+BALL+B15                                              C 573
      CNSQ=WQX(QNS,DENS,0.0,DT)                                         C 574
      CNS=CNS+CNSQ                                                      C 575
      DEND=B4+B4A+BALL                                                  C 576
      CNDQ=WQX(QND,DEND,0.0,DT)                                         C 577
      CND=CND+CNDQ                                                      C 578
      DENP=B3+B3A+BALL+B5                                               C 579
      CNPQ=WQX(QNP,DENP,0.0,DT)                                         C 580
      CNP=CNP+CNPQ                                                      C 581
      CN=CNS+CND+CNP                                                    C 582
      CO2SGQ=WQX(QO2S,B11,0.0,DT)                                       C 583
      CO2SG=CO2SG+CO2SGQ                                                C 584
      QO3=B1*CO+B11*CO2SG+B143*CN2O                                     C 585
      DO3=RO3O*CO+RNSO3*CNS+RO3NO*CNO+PDISO3                            C 586
      CO3Q=WQX(QO3,DO3,0.0,DT)                                          C 587
      CO3=CO3+CO3Q                                                      C 588
      B2=RO3O*CO3                                                       C 589
      B110=TNON*CN                                                      C 590
      B111=RNO2NB*CN                                                    C 591
      B112=RNO2NA*CN                                                    C 592
      B140=TONO*CO                                                      C 593
      B141=RO3NO*CO3                                                    C 594
      B144=RONO2*CO                                                     C 595
      C110=B110*CNO                                                     C 596
      C140=B140*CNO                                                     C 597
      C141=B141*CNO                                                     C 598
C                                                                       C 599
C --- CALCULATION OF NO2 AND N2O                                        C 600
```

```
C                                                                               C 601
      FNO2=C140+C141                                                            C 602
      DNO2=B144+B111+B112                                                       C 603
      CNO2=WQX(FNO2,DNO2,CNO2,DT)                                               C 604
      C111=B111*CNO2                                                            C 605
      FN2O=C110+C111                                                            C 606
      DN2O=B143                                                                 C 607
      CN2O=WQX(FN2O,DN2O,CN2O,DT)                                               C 608
C                                                                               C 609
C ---    N2O  +    O2(1D)                     N2    +    O3                    C 610
C                                                                               C 611
      B145=RO2N2O*CN2O                                                          C 612
C                                                                               C 613
C --- CALCULATION OF O2(1D)                                                     C 614
C                                                                               C 615
      CO2DQ=WQX(QO2D,B145,0.0,DT)                                               C 616
      CO2D=WQX(0.0,B145,CO2D,DT)                                                C 617
      CO2D=CO2DQ+CO2D                                                           C 618
C                                                                               C 619
C ---    H    +    O3                        OH    +    O2                    C 620
C                                                                               C 621
      B21=RHO3*CO3                                                              C 622
C                                                                               C 623
C ---    OH   +    O                         H     +    O2                    C 624
C                                                                               C 625
      B22=ROHO*CO                                                               C 626
C                                                                               C 627
C --- CALCULATION OF H AND OH                                                   C 628
C                                                                               C 629
      QX=B21                                                                    C 630
      QY=B22                                                                    C 631
      CHOH=CH+COH                                                               C 632
      QZ=CHOH*QX                                                                C 633
      COH=WQX(QZ,(QX+QY),COH,DT)                                                C 634
      CH=AMAX1((CHOH-COH),0.)                                                   C 635
C                                                                               C 636
C --- BEGIN METAL-METAL OXIDE CALCULATION                                       C 637
C                                                                               C 638
      IF (CMTL.LE.0.) GO TO 17                                                  C 639
C                                                                               C 640
C ---    X    +    O3                        XO    +    O2                    C 641
C                                                                               C 642
      FMTLOZ=RMTLO3*CO3                                                         C 643
C                                                                               C 644
C ---    LITHIUM                                                                C 645
C                                                                               C 646
      NMT=1                                                                     C 647
      IF (CLI.LE.0.) GO TO 8                                                    C 648
C                                                                               C 649
C ---    LI   +    O    +    M               LIO   +    M                     C 650
C                                                                               C 651
      B211=TLIO*COP                                                             C 652
      C211=B211*CLI                                                             C 653
C                                                                               C 654
C ---    LI   +    O2                        LIO   +    O                     C 655
C                                                                               C 656
      B212=RLIO2*CO2                                                            C 657
      C212=B212*CLI                                                             C 658
C                                                                               C 659
C ---    LIO  +    O                         LI    +    O2                    C 660
C                                                                               C 661
      B213=ROLIO*COP                                                            C 662
C                                                                               C 663
C ---    LIO  +    O3                        LI    +    O2    +     O2        C 664
C                                                                               C 665
      B214=RO3LIO*CO3                                                           C 666
C                                                                               C 667
C ---    LI   +    O3                        LIO   +    O2                    C 668
C                                                                               C 669
      C215=FMTLOZ*CLI                                                           C 670
      QX=B211+B212+FMTLOZ                                                       C 671
      QY=B213+B214                                                              C 672
      GO TO 15                                                                  C 673
8     CONTINUE                                                                  C 674
C                                                                               C 675
```

```
C ---    BERYLLIUM
C
      NMT=NMT+1
      IF (CBE.LE.0.) GO TO 9
C
C ---    BE   +    O    +    M                BEO  +    M
C
      C221=B211*CBE
C
C ---    BE   +    O2                         BEO  +    O
C
      B222=RBEO2*CO2
      C222=B222*CBE
C
C ---    BEO  +    O                          BE   +    O2
C
C ---    BEO  +    O3                         BE   +    O2   +    O2
C
      B224=RO3BEO*CO3
C
C ---    BE   +    O3                         BEO  +    O2
C
      C225=FMTLOZ*CBE
      QX=B211+B222+FMTLOZ
      QY=B213+B224
      GO TO 15
    9 CONTINUE
C
C ---    MAGNESIUM
C
      NMT=NMT+1
      IF (CMG.LE.0.) GO TO 10
C
C ---    MG   +    O    +    M                MGO  +    M
C
      C231=B211*CMG
C
C ---    MG   +    O2                         MGO  +    O
C
      B232=RMGO2*CO2
      C232=B232*CMG
C
C ---    MGO  +    O                          MG   +    O2
C
C ---    MGO  +    O3                         MG   +    O2   +    O2
C
      B234=RO3MGO*CO3
C
C ---    MG   +    O3                         MGO  +    O2
C
      C235=FMTLOZ*CMG
      QX=B211+B232+FMTLOZ
      QY=B213+B234
      GO TO 15
   10 CONTINUE
C
C ---    ALUMINUM
C
      NMT=NMT+1
      IF (CAL.LE.0.) GO TO 11
C
C ---    AL   +    O    +    M                ALO  +    M
C
      C241=B211*CAL
C
C ---    AL   +    O2                         ALO  +    O
C
      B242=RALO2*CO2
      C242=B242*CAL
C
C ---    ALO  +    O                          AL   +    O2
C
      B243=ROALO*COP
C
C ---    ALO  +    O3                         AL   +    O2   +    O2
```

```
      C
            B244=RO3ALO*CO3
      C
      C ---    AL    +    O3                         ALO   +    O2
      C
            C245=FMTLOZ*CAL
            QX=B242+B211+FMTLOZ
            QX1=QX
            QY=B243+B244
            GO TO 15
   11       CONTINUE
      C
      C ---    SILICON
      C
            NMT=NMT+1
            IF (CSI.LE.0.) GO TO 12
      C
      C ---    SI    +    O    +    M                SIO   +    M
      C
            C251=B211*CSI
      C
      C ---    SI    +    O2                         SIO   +    O
      C
            C252=B242*CSI
      C
      C ---    SIO   +    O                          SI    +    O2
      C
            B253=ROSIO*COP
      C
      C ---    SIO   +    O3                         SI    +    O2    +    O2
      C
            B254=RO3SIO*CO3
      C
      C ---    SI    +    O3                         SIO   +    O2
      C
            C255=FMTLOZ*CSI
            QX=QX1
            QY=B253+B254
            GO TO 15
   12       CONTINUE
      C
      C ---    TITANIUM
      C
            NMT=NMT+1
            IF (CTI.LE.0.) GO TO 13
      C
      C ---    TI    +    O    +    M                TIO   +    M
      C
            C261=B211*CTI
      C
      C ---    TI    +    O2                         TIO   +    O
      C
            C262=B242*CTI
      C
      C ---    TIO   +    O                          TI    +    O2
      C
            B263=ROTIO*COP
      C
      C ---    TIO   +    O3                         TI    +    O2    +    O2
      C
            B264=RO3TIO*CO3
      C
      C ---    TI    +    O3                         TIO   +    O2
      C
            C265=FMTLOZ*CTI
            QX=QX1
            QY=B263+B264
            GO TO 15
   13       CONTINUE
      C
      C ---    IRON
      C
            NMT=NMT+1
            IF (CFE.LE.0.) GO TO 14
      C
```

```
C ---     FE    +    O     +    M               FEO   +    M
C
      C271=B211*CFE
C
C ---     FE    +    O2                         FEO   +    O
C
      B272=RFEO2*CO2
      C272=B272*CFE
C
C ---     FEO   +    O                          FE    +    O2
C
C ---     FEO   +    O3                         FE    +    O2    +    O2
C
      B274=RO3FEO*CO3
C
C ---     FE    +    O3                         FEO   +    O2
C
      C275=FMTLOZ*CFE
      QX=B211+B272+FMTLOZ
      QY=B213+B274
      GO TO 15
14    CONTINUE
C
C ---     COPPER
C
      NMT=NMT+1
      IF (CCU.LE.0.) GO TO 16
C
C ---     CU    +    O     +    M               CUO   +    M
C
      C281=B211*CCU
C
C ---     CU    +    O2                         CUO   +    O
C
      B282=RCUO2*CO2
      C282=B282*CCU
C
C ---     CUO   +    O                          CU    +    O2
C
C ---     CUO   +    O3                         CU    +    O2    +    O2
C
      B284=RO3CUO*CO3
C
C ---     CU    +    O3                         CUO   +    O2
C
      C285=FMTLOZ*CCU
      QX=B211+B282+FMTLOZ
      QY=B213+B284
15    CONTINUE
      NM=NMT+1
      CYD=CMD(NM)+CMO(NM+10)
      QZ=CYD*QX
      CMD(NM+10)=WQX(QZ,(QX+QY),CMO(NM+10),DT)
      CMD(NM)=AMAX1(CYD-CMO(NM+10),0.0)
      GO TO (8,9,10,11,12,13,14,16), NMT
16    CONTINUE
17    CONTINUE
C
C --- CALCULATION OF UO+
C
      IF (CU.LE.0.) GO TO 18
C
C ---     U     +    O                          UO+   +    E
C
      B210=RUO*CO
      XCUD=CU
      CU=CU*EXP(-B210*DT)
      CUOPL=CUOPL+(XCUD-CU)
18    CONTINUE
C
C --- RECALCULATE NECESSARY FORMATION AND DESTRUCTION RATES
C
      CMTL=CLI+CBE+CMG+CAL+CSI+CTI+CFE+CCU
      CMTLO=CLIO+CBEO+CMGO+CALO+CSIO+CFEO+CCUO+CTIO
      C1=B1*CO
```

```
      C1A=B3*CNS                                                          C 901
      C1B=B3*CNP                                                          C 902
      C2A=B4*CND                                                          C 903
      C144=B144*CNO2                                                      C 904
      C16=RNSO3*CO3*CNS                                                   C 905
      B21R=RHO3*CH                                                        C 906
      FOH=B21R*CO3                                                        C 907
      FUOPL=RUO*CO*CU                                                     C 908
      H=C1B+C2A+C16                                                       C 909
      FO3X=C1                                                             C 910
      FO3S=B11*CO2SG+B145*CO2D                                            C 911
      G=C1A+C144                                                          C 912
      DOH=B22                                                             C 913
      DLIO=B213+B214                                                      C 914
      DBEO=B213+B224                                                      C 915
      DMGO=B213+B234                                                      C 916
      DALO=B243+B244                                                      C 917
      DSIO=B253+B254                                                      C 918
      DTIO=B263+B264                                                      C 919
      DFEO=B213+B274                                                      C 920
      DCUO=B213+B284                                                      C 921
      DNO=B140+B141+B110+RNSNO*(CNS+CNP)+RNDNO*CND                        C 922
      DO3=RO30*CO+B21R+RO3NO*CNO+RNSO3*CNS+DIS                            C 923
      DOD=B1+B2+TONO*CNO+RONO2*CNO2+ROHO*COH+TLIO*CMTL+ROLIO*CLIO+ROBEO*  C 924
     1CBEO+ROMGO*CMGO+ROALO*CALO+ROSIO*CSIO+ROTIO*CTIO+ROFEO*CFEO+ROCUO*  C 925
     2CCUO+RUO*CU                                                         C 926
      DOS=DOD                                                             C 927
      DOD=DOD+RODHV                                                       C 928
      DOS=DOS+ROSHV                                                       C 929
      DN2O=RO2N2O*CO2D                                                    C 930
      DNOPL=RNOPEL*CEL                                                    C 931
      FNOPL=RN2PLO*CO*CN2PL+DNQR+DOQR+(XOPLNO*COPL+XO2PNO*CO2PL+XN2PNO*C  C 932
     1N2PL+XNPLNO*CNPL)*CNO+RO2PLN*CN*CO2PL                               C 933
      FLIO3=C211+C215                                                     C 934
      FLIO2=C212                                                          C 935
      FBEO3=C221+C225                                                     C 936
      FBEO2=C222                                                          C 937
      FMGO3=C231+C235                                                     C 938
      FMGO2=C232                                                          C 939
      FALO3=C241+C245                                                     C 940
      FALO2=C242                                                          C 941
      FSIO3=C251+C255                                                     C 942
      FSIO2=C252                                                          C 943
      FTIO3=C261+C265                                                     C 944
      FTIO2=C262                                                          C 945
      FFEO3=C271+C275                                                     C 946
      FFEO2=C272                                                          C 947
      FCUO3=C281+C285                                                     C 948
      FCUO2=C282                                                          C 949
      CALL RRCRT (TEM)                                                    C 950
      IF (SWTCH(60).EQ.1.) GO TO 19                                     CHC 951
      WRITE (1,25) DT,(CMO(I),I=1,NSPEC)                                CHC 952
19    CONTINUE                                                          CHC 953
      IF (SWTCH(57).NE.1HY) GO TO 20                                    CHC 954
      CHG=CN2PL+COPL+CNOPL+CNPL+CO2PL+CUOPL+CN2APL+CN2BPL-CEL           CHC 955
      PNUM=CNS+CNO+CNP+COP+COS+COD+CNPL+COPL+CH+CMTL+CU+2.*(CO2+CO2D+CO2CHC 956
     1B+CO2SG+CN2+CN2A+CN2B+CN2PL+CN2APL+CN2BPL+CO2PL+CNO+CNOPL+COH+CCO+CHC 957
     2CMTLO+CUOPL)+3.0*(CO3+CNO2+CN2O+CCO2+CH2O)                        CHC 958
      PRINT 26, CHG,PNUM                                                CHC 959
20    CONTINUE                                                          CHC 960
      RETURN                                                              C 961
21    CONTINUE                                                            C 962
      CALL DECAR (ED,Q,DP,TEM,DT,RHO)                                     C 963
      RETURN                                                              C 964
C                                                                         C 965
C                                                                         C 966
C                                                                         C 967
22    FORMAT (1X,31HED,Q,DP,TEM,DT,RHO--INTO DECAYR,6E14.7)               C 968
23    FORMAT (1X,21HCMD GOING INTO DECAYR/(1X,10E12.5))                   C 969
24    FORMAT (29H INITIAL CHARGE AND PARTICLES,2E25.15)                   C 970
25    FORMAT (E13.6,(6E13.6,/))                                           C 971
26    FORMAT (29H FINAL   CHARGE AND PARTICLES,2E25.15)                   C 972
      END                                                                 C 973-
```

```
      SUBROUTINE ENTDEP (TIONPR,CON,TG)
C**********************************************************************
C
C        ENTDEP (AND ENQDEP)
C              INITIALIZATION DUE TO PROMPT ENERGY DEPOSITION
C              CALCULATION OF CONTINUOUS SOURCE RATES
C
C**********************************************************************
C
      COMMON /FU/ Y(90),P(90),S(90),R(90),CHT,TGEV,QQ,TNUM,NFLAG,NTG
      COMMON /KEN/ CONV,DT,N
      COMMON /ININ/ XNTG,QN2PL,QO2PL,QOPL,QNPL,QNS1,QND1,QNP1,QFO,QDO,QO
     1O1,QOS1,QO2D,QO2S,QDN2,QDO2,QNOPL
      COMMON /XUX/ RR(200),CMD(90),RCRT(90),NSPEC
      EQUIVALENCE (CMD(1),CH), (CMD(2),CLI), (CMD(3),CBE), (CMD(4),CMG),
     1 (CMD(5),CAL), (CMD(6),CSI), (CMD(7),CTI), (CMD(8),CFE), (CMD(9),C
     2CU), (CMD(10),CU), (CMD(11),COH), (CMD(12),CLIO), (CMD(13),CBEO),
     3(CMD(14),CMGO), (CMD(15),CALO), (CMD(16),CSIO), (CMD(17),CTIO), (C
     4MD(18),CFEO), (CMD(19),CCUO), (CMD(20),CUOPL), (CMD(21),CNOPL), (C
     5MD(22),CNO), (CMD(23),CNO2), (CMD(24),CN2O), (CMD(25),CCO), (CMD(2
     66),CCO2), (CMD(27),CO3), (CMD(28),CH2O), (CMD(30),CEL), (CMD(31),C
     7N2), (CMD(32),CN2A), (CMD(33),CN2B), (CMD(34),CNS), (CMD(35),CND),
     8 (CMD(36),CNP), (CMD(36),COP), (CMD(39),COD), (CMD(40),COS), (CMD(
     941),CN2PL), (CMD(42),CO2PL), (CMD(43),CNPL), (CMD(44),COPL), (CMD(
     $45),CN2APL), (CMD(46),CN2BPL), (CMD(50),CEN), (CMD(51),CO2), (CMD(
     $52),CO2D), (CMD(53),CO2B), (CMD(54),CO2SG)
      DATA PFNS,PFND/2*0.224/,PFNP/0.112/,PFN2PL,PFO2PL/2*0.94/,PFNPL/0.
     106/,PFOPL1/1.0/,PFOPL2/0.06/,PFOP2/2.125/,PFOP3/0.051/,PFOD1/0.2/,
     2PFOS1/0.05/,PFOD2/0.25/,PFOD3/0.006/,PFOS2/0.125/,PFOS3/0.003/,PFO
     32D/8.0/,PFO2SG/0.02/
      DATA FO2I/2.25/
      DATA EVINPR/5.0/
C
      NTG=1
      IF (TG.GE.0.) GO TO 1
      NTG=0
      TG=-TG
    1 CONTINUE
      XNTG=NTG
      TGEV=TG/CONV
      FRION=TIONPR/CON
      IF (FO2I*FRION.GT.1.) FRION=1./FO2I
      TIONPR=FRION*CON
      FRIN2=CN2*FRION
      FRIO2=CO2*FRION
      FRIO=COP*FRION
      CNS=CNS+PFNS*FRIN2
      CND=CND+PFND*FRIN2
      CNP=CNP+PFNP*FRIN2
      CN2PL=CN2PL+PFN2PL*FRIN2
      CO2PL=CO2PL+PFO2PL*FRIO2
      CNPL=CNPL+PFNPL*FRIN2
      COPL=COPL+FRIO*PFOPL1+FRIO2*PFOPL2
      COP=COP+(PFOP2+PFOP3)*FRIO2-(PFOPL1+PFOD1+PFOS1)*FRIO
      COD=COD+(PFOD2+PFOD3)*FRIO2+PFOD1*FRIO
      COS=COS+(PFOS2+PFOS3)*FRIO2+PFOS1*FRIO
      CO2D=CO2D+PFO2D*FRIO2
      CO2SG=CO2SG+PFO2SG*FRIO2
      CN2=CN2-FRIN2*(PFN2PL+0.5*(PFNS+PFND+PFNP+PFNPL))
      CO2=CO2-FO2I*FRIO2
      CEL=CEL+TIONPR
      CHT=1.5*(CNS+CND+CNP+COP+COD+COS+CNPL+COPL)+2.5*(CNOPL+CNO+CCO+CN2
     1+CN2A+CN2B+CN2PL+CO2PL+CN2APL+CN2BPL+CO2+CO2D+CO2B+CO2SG)+3.0*(CNO
     22+CN2O+CCO2+CO3+CH2O)
      CEN=TGEV*CHT+EVINPR*TIONPR*XNTG
      TGEV=CEN/CHT
      TG=TGEV*CONV
      IF (TG.GT.11000.) TG=11000.
      RETURN
      ENTRY ENQDEP
      FRON=QQ/CON
      FRN2=FRON*CN2
      FRO2=FRON*CO2
      FRO=FRON*COP
```

```
                PACKAGE CHEM74              01 JUL 74 VERSION                 PAGE  23

1522            QNPL=PFNPL*FRN2                                                        0  76     1522
1523            QOPL=PFOPL1*FRO+PFOPL2*FRO2                                            0  77     1523
1524            QN2PL=PFN2PL*FRN2                                                      0  78     1524
1525            QO2PL=PFO2PL*FRO2                                                      0  79     1525
1526            QNOPL=0.0                                                              0  80     1526
1527            QNS1=PFNS*FRN2                                                         0  81     1527
1528            QND1=PFND*FRN2                                                         0  82     1528
1529            QNP1=PFNP*FRN2                                                         0  83     1529
1530            QFO=(PFOP2+PFOP3)*FRO2                                                 0  84     1530
1531            QDO=(PFOPL1+PFOD1+PFOS1)*FRON                                          0  85     1531
1532            QOD1=(PFOD2+PFOD3)*FRO2+PFOD1*FRO                                      0  86     1532
1533            QOS1=(PFOS2+PFOS3)*FRO2+PFOS1*FRO                                      0  87     1533
1534            QO2D=PFO2D*FRO2                                                        0  88     1534
1535            QO2S=PFO2SG*FRO2                                                       0  89     1535
1536            QDN2=(PFN2PL+0.5*(PFNS+PFND+PFNP+PFNPL))*FRON                          0  90     1536
1537            QDO2=FO2I*FRON                                                         0  91     1537
1538            RETURN                                                                 0  92     1538
1539            END                                                                    0  93-    1539
```

```
      PACKAGE CHEM7+                  21 JUL 74 VERSION            PAGE  24

      FUNCTION X1IGL (A,B,C,T)
C
C --- INTEGRAL OF EXP(-B*T)*DT/(1.+A*C*T)
C
      CC=A*C
      AA=B/CC
      IF  (AA.LE.0.0) GO TO 1
      IF  (AA.GT.700.) AA=700.
      BB=AA*(1.+CC*T)
      X1IGL=EXP(AA)*(EIF(AA)-EIF(BB))/CC
      RETURN
    1 CONTINUE
      X1IGL=0.0
      RETURN
      END
```

```
      FUNCTION X2IGL (A,B,C,T)
C
C ---  INTEGRAL OF EXP(-B*T)*DT/(1.+A*C*T)**2
C
      CC=A*C
      AA=B/CC
      IF (AA.LE.0.0) GO TO 1
      IF (AA.GT.700.0) AA=700.0
      BB=AA*(1.+CC*T)
      XIGL=AA*EXP(AA)*(EIF(AA)-EIF(BB))
      GO TO 2
    1 CONTINUE
      XIGL=0.0
    2 CONTINUE
      X2IGL=(1.-EXP(-B*T)/(1.+CC*T)-XIGL)/CC
      RETURN
      END
```

```
            PACKAGE CHEM74                      01 JUL 74 VERSION                  PAGE  26

            FUNCTION EIF (X)
      C
      C --- INTEGRAL OF  EXP(-X)/X  FROM X TO INF
      C
            IF (X-1.) 1,1,2
      1     EIF=-ALOG(X)+((((0.00107857*X-0.00976004)*X+0.05519968)*X-0.249910
           155)*X+0.99999193)*X-0.57721566
            GO TO 3
      2     EIF=EXP(-X)*((X+2.334733)*X+0.250621)/((X+3.330657)*X+1.681534)/X
      3     RETURN
            END
```

```
        PACKAGE CHEM74              01 JUL 74 VERSION             PAGE  27

              FUNCTION SHXOX (X)                                           H   1      1583
      C                                                                    H   2      1584
      C --- EVALUATION OF (EXP(X)-1.)/X                                    H   3      1585
      C                                                                    H   4      1586
              IF (ABS(X).LE.1.E-7) GO TO 1                                 H   5      1587
              IF (X.GT.700.) X=700.                                        H   6      1588
              SHXOX=(EXP(X)-1.)/X                                          H   7      1589
              RETURN                                                       H   8      1590
      1       CONTINUE                                                     H   9      1591
              SHXOX=1.+X/2.                                                H  10      1592
              RETURN                                                       H  11      1593
              END                                                          H  12-     1594
```

```
                PACKAGE CHEM74                 01 JUL 74 VERSION               PAGE   26

 1595                 FUNCTION WR (Q,A,X0,T)                                            I    1          1595
 1596       C                                                                           I    2          1596
 1597       C ---      SOLUTION OF DX/DT=Q-A*X**2                                       I    3          1597
 1598       C                                                                           I    4          1598
 1599                 IF (Q.LE.0.) GO TO 1                                              I    5          1599
 1600                 SQ1=SQRT(Q/A)                                                     I    6          1600
 1601                 SQ2=SQRT(Q*A)                                                     I    7          1601
 1602                 EXQA=EXP(-SQ2*2.*T)                                               I    8          1602
 1603                 B=(X0-SQ1)/(X0+SQ1)                                               I    9          1603
 1604                 WR=SQ1*(1.+B*EXQA)/(1.-B*EXQA)                                    I   10          1604
 1605                 RETURN                                                            I   11          1605
 1606       1         CONTINUE                                                          I   12          1606
 1607                 WR=X0/(1.+A*X0*T)                                                 I   13          1607
 1608                 RETURN                                                            I   14          1608
 1609                 END                                                               I   15-         1609
```

```
      FUNCTION WQX (A,B,X0,T)
C
C ---  SOLUTION OF DX/DT=A-B*X
C
      BT=B*T
      IF (BT.GT.1.E-3) GO TO 1
      WQX=A*T+X0*(1.-BT)
      RETURN
1     CONTINUE
      IF (BT.GT.200.) GO TO 2
      EXBT=EXP(-BT)
      WQX=A*(1.-EXBT)/B+X0*EXBT
      RETURN
2     CONTINUE
      WQX=A/B
      RETURN
      END
```

```
      SUBROUTINE DECAR (ED,Q,DP,TG,END,RHO)
C     ****************************************************************
C
C        DECAR
C              EXECUTIVE FOR THE NUMERICAL ALGORITH
C
C     ****************************************************************
C
      COMMON /FU/ Y(90),P(90),S(90),R(90),CHT,TGEV,QQ,TNUM,NFLAG,NTG
      COMMON /KEN/ CONV,DT,N
      COMMON /QIN/ QI,QA
      COMMON /SWR/ SWTCH(80)
      COMMON /XUX/ RR(200),CMD(90),RCRT(30),NSPEC
      DIMENSION X(90), Z(90), F(90), D(90), B(90)
      DIMENSION SR(200)
      DIMENSION U(60,54), SS(60,6), TXX(60), V(60), DV(60)
      EQUIVALENCE (X,CMD)
      EQUIVALENCE (X(1),CH), (X(2),CLI), (X(3),CBE), (X(4),CMG), (X(5),C
     1AL), (X(6),CSI), (X(7),CTI), (X(8),CFE), (X(9),CCU), (X(10),CU), (
     2X(11),COH), (X(12),CLIO), (X(13),CBEO), (X(14),CMGO), (X(15),CALO)
     3, (X(16),CSIO), (X(17),CTIO), (X(18),CFEO), (X(19),CCUO), (X(20),C
     4UOPL), (X(21),CNOPL), (X(22),CNO), (X(23),CNO2), (X(24),CN2O), (X(
     525),CCO), (X(26),CCO2), (X(27),CO3), (X(28),CH2O), (X(30),CEL), (X
     6(31),CN2), (X(32),CN2A), (X(33),CN2B), (X(34),CNS), (X(35),CND), (
     7X(36),CNP), (X(38),COP), (X(39),COD), (X(40),COS), (X(41),CN2PL),
     8(X(42),CO2PL), (X(43),CNPL), (X(44),COPL), (X(45),CN2APL), (X(46),
     9CN2BPL), (X(50),CEN), (X(51),CO2), (X(52),CO2D), (X(53),CO2B), (X(
     $54),CO2SG)
      EQUIVALENCE (Y(80),CMTL), (Y(81),CMTLO)
      DATA CONV/1.16E4/
C
      N=NSPEC
      TIONPR=1.37E10*ED
      CON=CN2+CO2+COP
      TNUM=CON
      QQ=Q
C
C --- NOTE THAT THE CMD ARRAY IS MODIFYIED SLIGHTLY BEFORE PRINTING PNUM
C
      CALL ENTDEP (TIONPR,CON,TG)
      DT=1.E5/CON
      IF (SWTCH(56).NE.1HY) GO TO 1
      PRINT 25, ED,TIONPR,FRION,TG,END,QQ,QXT,NFLAG
    1 CONTINUE
      T=0.0
      IF (CNO.EQ.0.) CNO=1.
      IF (CNOPL.EQ.0.) CNOPL=1.0
      IF (CO3.EQ.0.) CO3=1.0
      IF (CNO2.EQ.0.) CNO2=1.0
      IF (CN2O.EQ.0.) CN2O=1.0
      IF (CCO.EQ.0.) CCO=1.0
      IF (SWTCH(57).NE.1HY) GO TO 2
      CHG=CN2PL+COPL+CNOPL+CNPL+CO2PL+CUOPL+CN2APL+CN2BPL-CEL
      PNUM=CNS+CND+CNP+COP+COS+COD+CNPL+COPL+CH+CMTL+CU+2.*(CO2+CO2D+CO2
     1B+CO2SG+CN2+CN2A+CN2B+CN2PL+CN2APL+CN2BPL+CO2PL+CNO+CNOPL+COH+CCO+
     2CMTLO+CUOPL)+3.0*(CO3+CNO2+CN2O+CCO2+CH2O)
      PRINT 26, CHG,PNUM
    2 CONTINUE
    3 CONTINUE
      LL=0
      DO 16 K=1,60
      DO 4 I=1,N
      B(I)=X(I)
      Y(I)=X(I)
    4 CONTINUE
      IF (SWTCH(55).EQ.1HQ) GO TO 5
      QQ=(QI/((1.+T)**1.2))+QA
    5 CONTINUE
      CALL FUNG
      IF (NTG.EQ.10) GO TO 17
      DO 6 I=1,N
      F(I)=P(I)
      D(I)=S(I)
    6 CONTINUE
```

```
 7      CALL EVIL (B,F,D,Y)                                                   K   76
        DO 11 L=1,3                                                           K   77
        CALL FUNG                                                             K   78
        IF (NTG.EQ.10) GO TO 17                                               K   79
        CALL EVIL (B,P,S,Z)                                                   K   80
        DO 8 I=1,N                                                            K   81
        ERR=ABS(Z(I)-Y(I))/(X(I)+1.0E-5)-1.0E-4                               K   82
        IF (ERR.LE.0.) GO TO 8                                                K   83
        GO TO 9                                                               K   84
 8      CONTINUE                                                              K   85
        GO TO 12                                                              K   86
 9      DO 10 I=1,N                                                           K   87
 10     Y(I)=Z(I)                                                             K   88
 11     CONTINUE                                                              K   89
        DT=0.5*DT                                                             K   90
        IF (DT.LE.1.0E-25) STOP                                               K   91
        GO TO 7                                                               K   92
 12     CONTINUE                                                              K   93
        LL=LL+1                                                             CHK   94
        DO 13 J=1,N                                                           K   95
        U(K,J)=Z(J)                                                         CHK   96
        X(J)=Z(J)                                                             K   97
 13     CONTINUE                                                              K   98
        CEL=CN2PL+COPL+CNOPL+CNPL+CO2PL+CUOPL+CN2APL+CN2BPL                   K   99
        T=T+DT                                                                K  100
        U(K,30)=CEL                                                         CHK  101
        WRITE (4,27) T,(CMD(I),I=1,NSPEC)                                   CHK  102
        TG=TGEV*CONV                                                        CHK  103
        SS(K,1)=P(87)                                                       CHK  104
        SS(K,2)=P(86)                                                       CHK  105
        SS(K,3)=P(38)                                                       CHK  106
        SS(K,4)=P(89)                                                       CHK  107
        SS(K,5)=P(23)                                                       CHK  108
        SS(K,6)=P(24)                                                       CHK  109
        TXX(K)=TG                                                           CHK  110
        DV(K)=DT                                                            CHK  111
        V(K)=T                                                              CHK  112
        DT=2.0*DT                                                             K  113
        IF (T-END) 14,17,17                                                   K  114
 14     IF ((T+DT)-END) 16,16,15                                              K  115
 15     DT=END-T+1.E-10                                                       K  116
 16     CONTINUE                                                              K  117
 C      GO TO 1                                                             CHK  118
 17     CONTINUE                                                              K  119
 C                                                                          CHK  120
 C      THE FOLLOWING ARE CHEM SPECIAL PRINTS  *************               CHK  121
 C                                                                          CHK  122
        IF (SWTCH(56..NE.1HY) GO TO 22                                        K  123
        PRINT 28                                                              K  124
        DO 18 K=1,LL                                                          K  125
        PRINT 29, V(K),DV(K),U(K,39),U(K,40),U(K,25),(SS(K,I),I=1,6),TXX(K    K  126
       1)                                                                     K  127
 18     CONTINUE                                                              K  128
        PRINT 30                                                              K  129
        DO 19 K=1,LL                                                          K  130
        PRINT 34, V(K),U(K,34),U(K,35),U(K,51),U(K,22),U(K,31),U(K,38),U(K    K  131
       1,30),U(K,41),U(K,42),U(K,43),U(K,44)                                  K  132
 19     CONTINUE                                                              K  133
        PRINT 31                                                              K  134
        DO 20 K=1,LL                                                          K  135
        PRINT 34, V(K),U(K,21),U(K,27),U(K,1),U(K,11),U(K,36),U(K,23),U(K,    K  136
       124),U(K,10),U(K,20),U(K,52),U(K,54)                                   K  137
 20     CONTINUE                                                              K  138
        IF (CMTL.LE.0.) GO TO 22                                              K  139
        PRINT 32                                                              K  140
        PRINT 33                                                              K  141
        DO 21 K=1,LL                                                          K  142
        PRINT 35, V(K),U(K,2),U(K,12),U(K,4),U(K,14),U(K,5),U(K,15),U(K,6)    K  143
       1,U(K,16),U(K,8),U(K,18),U(K,9),U(K,19)                                K  144
 21     CONTINUE                                                              K  145
 C                                                                          CHK  146
 C      END OF SPECIAL PRINTS *********                                     CHK  147
 C                                                                          CHK  148
 22     CONTINUE                                                            CHK  149
        IF (T-END) 3,23,23                                                  CHK  150
```

```
23    CONTINUE                                                          CHK 151
      TG=TGEV*CONV                                                        K 152
      IF (NTG.EQ.10) RETURN                                               K 153
      CALL RRCRT (TG)                                                     K 154
      IF (SWTCH(57).NE.1HY) GO TO 24                                    CHK 155
      CHG=CN2PL+COPL+CNOPL+CNPL+CO2PL+CUOPL+CN2APL+CN2BPL-CEL           CHK 156
      CMTL=CLI+CBE+CMG+CAL+CSI+CFE+CCU+CTI                              CHK 157
      CMTLO=CLIO+CBEO+CMGO+CALO+CSIO+CFEO+CCUO+CTIO                     CHK 158
      PNUM=CNS+CND+CNP+COP+COS+COD+CNPL+COPL+CH+CMTL+CU+2.*(CO2+CO2D+CO2CHK 159
     1B+CO2SG+CN2+CN2A+CN2B+CN2PL+CN2APL+CN2BPL+CO2PL+CNO+CNOPL+COH+CCO+CHK 160
     2CMTLO+CUOPL)+3.0*(CO3+CNO2+CN2O+CCO2+CH2O)                        CHK 161
      PRINT 36, CHG,PNUM                                                CHK 162
24    CONTINUE                                                          CHK 163
      RETURN                                                              K 164
C                                                                         K 165
C                                                                         K 166
25    FORMAT (57H CHEMISTRY VARIABLES ED,TIONPR,FRION,TG,END,QQ,QXT,NFLA  K 167
     1G ,/,7E13.5,I5)                                                     K 168
26    FORMAT (29H INITIAL CHARGE AND PARTICLES,2E25.15)                   K 169
27    FORMAT (E13.6,(6E13.6,/))                                           K 170
28    FORMAT (131H1  TIME             DT            OD            OS           CO  K 171
     1        F-NO        F-NO        F-O3          F-O3          F-NO2        F-N2  K 172
     20       TEMP)                                                       K 173
29    FORMAT (E12.5,E10.3,10E11.3)                                        K 174
30    FORMAT (1H1,127H     TIME          N             N(D)          O2          NO  K 175
     1         N2           O            NE            N2+           O2+         N+  K 176
     2         O+)                                                        K 177
31    FORMAT (1H1,128H     TIME          NO+           O3            H          OH  K 178
     1        N(P)         NO2           N2O           U             UO+      O2(D)  K 179
     2        O2(D))                                                      K 180
32    FORMAT (1H1)                                                        K 181
33    FORMAT (125H   TIME          LI          LIO          MG          MGO       K 182
     1AL         ALO           SI          SIO          FE          FEO         CU   K 183
     2   CUO)                                                             K 184
34    FORMAT (12E11.3)                                                    K 185
35    FORMAT (13E10.3)                                                    K 186
36    FORMAT (29H FINAL   CHARGE AND PARTICLES,2E25.15)                   K 187
      END                                                                 K 188-
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      SUBROUTINE EVIL (X,P,R,Y)
C     ******************************************************************
C
C        EVIL
C                SOLUTION OF DX/DT = P - R*X  FOR NUMERICAL ALGORITHM
C
C     ******************************************************************
C
      DIMENSION X(1), P(1), R(1), Y(1)
      COMMON /KEN/ CONV,DT,N
      DO 3 I=1,N
      T=DT*R(I)
      IF (T.GT.1.E-3) GO TO 1
      Y(I)=X(I)*(1.-T)+DT*P(I)
      GO TO 3
    1 CONTINUE
      RX=P(I)/R(I)
      IF (T.LE.100.) GO TO 2
      Y(I)=RX
      GO TO 3
    2 Y(I)=(X(I)-RX)*EXP(-T)+RX
    3 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE FUNG
C     ******************************************************************
C
C         FUNG
C                 PREPARES SPECIES FORMATION AND DESTRUCTION RATES
C
C     ******************************************************************
C
      COMMON /FU/ Y(90),P(90),S(90),R(90),CHT,TGEV,QQ,TNUM,NFLAG,NTG
      COMMON /ININ/ XNTG,QN2PL,QO2PL,QOPL,QNPL,QNS1,QND1,QNP1,QFO,QDO,QO
     1D1,QOS1,QO2D,QO2S,QDN2,QDO2,QNOPL
      COMMON /KEN/ CONV,DT,N
      DIMENSION E(90)
      EQUIVALENCE (Y(1),CH), (Y(2),CLI), (Y(3),CBE), (Y(4),CMG), (Y(5),C
     1AL), (Y(6),CSI), (Y(7),CTI), (Y(8),CFE), (Y(9),CCU), (Y(10),CU), (
     2Y(11),COH), (Y(12),CLIO), (Y(13),CBEO), (Y(14),CMGO), (Y(15),CALO)
     3, (Y(16),CSIO), (Y(17),CTIO), (Y(18),CFEO), (Y(19),CCUO), (Y(20),C
     4UOPL), (Y(21),CNOPL), (Y(22),CNO), (Y(23),CNO2), (Y(24),CN2O), (Y(
     525),CCO), (Y(26),CCO2), (Y(27),CO3), (Y(28),CH2O), (Y(30),CEL), (Y
     6(31),CN2), (Y(32),CN2A), (Y(33),CN2B), (Y(34),CNS), (Y(35),CND), (
     7Y(36),CNP), (Y(38),COP), (Y(39),COD), (Y(40),COS), (Y(41),CN2PL),
     8(Y(42),CO2PL), (Y(43),CNPL), (Y(44),COPL), (Y(45),CN2APL), (Y(46),
     9CN2BPL), (Y(50),CEN), (Y(51),CO2), (Y(52),CO2D), (Y(53),CO2B), (Y(
     $54),CO2SG)
      EQUIVALENCE (Y(60),CMTL), (Y(61),CMTLO)
      EQUIVALENCE (P(1),FH), (P(2),FLI), (P(3),FBE), (P(4),FMG), (P(5),F
     1AL), (P(6),FSI), (P(7),FTI), (P(8),FFE), (P(9),FCU), (P(10),FU), (
     2P(11),FOH), (P(12),FLIO), (P(13),FBEO), (P(14),FMGO), (P(15),FALO)
     3, (P(15),FSIO), (P(17),FTIO), (P(18),FFEO), (P(19),FCUO), (P(20),F
     4UOPL), (P(21),FNOPL), (P(22),FNO), (P(23),FNO2), (P(24),FN2O), (P(
     525),FCO), (P(26),FCO2), (P(27),FO3), (P(28),FH2O), (P(30),FEL), (P
     6(31),FN2), (P(32),FN2A), (P(33),FN2B), (P(34),FNS), (P(35),FND), (
     7P(36),FNP), (P(38),FO), (P(39),FOD), (P(40),FOS), (P(41),FN2PL), (
     8P(42),FO2PL), (P(43),FNPL), (P(44),FOPL), (P(45),FN2APL), (P(46),F
     9N2BPL), (P(50),FEN), (P(51),FO2), (P(52),FO2D), (P(53),FO2B), (P(5
     $4),FO2SG)
      EQUIVALENCE (S(1),DH), (S(2),DLI), (S(3),DBE), (S(4),DMG), (S(5),D
     1AL), (S(6),DSI), (S(7),DTI), (S(8),DFE), (S(9),DCU), (S(10),DU), (
     2S(11),DOH), (S(12),DLIO), (S(13),DBEO), (S(14),DMGO), (S(15),DALO)
     3, (S(16),DSIO), (S(17),DTIO), (S(18),DFEO), (S(19),DCUO), (S(20),D
     4UOPL), (S(21),DNOPL), (S(22),DNO), (S(23),DNO2), (S(24),DN2O), (S(
     525),DCO), (S(26),DCO2), (S(27),DO3), (S(28),DH2O), (S(30),DEL), (S
     6(31),DN2), (S(32),DN2A), (S(33),DN2B), (S(34),DNS), (S(35),DND), (
     7S(36),DNP), (S(38),DO), (S(39),DOD), (S(40),DOS), (S(41),DN2PL), (
     8S(42),DO2PL), (S(43),DNPL), (S(44),DOPL), (S(45),DN2APL), (S(46),D
     9N2BPL), (S(50),DEN), (S(51),DO2), (S(52),DO2D), (S(53),DO2B), (S(5
     $4),DO2SG)
      EQUIVALENCE (P(70),FLIO2), (P(71),FLIO3), (P(72),FBEO2), (P(73),FB
     1EO3), (P(74),FMGO2), (P(75),FMGO3), (P(76),FALO2), (P(77),FALO3),
     2(P(78),FSIO2), (P(79),FSIO3), (P(80),FTIO2), (P(81),FTIO3), (P(82)
     3,FFEO2), (P(83),FFEO3), (P(84),FCUO2), (P(85),FCUO3), (P(86),G), (
     4P(87),H), (P(88),FO3X), (P(89),FO3S), (S(70),DMTLO)
      EQUIVALENCE (R(1),RNSO2), (R(2),RNDO2), (R(3),RNSNO), (R(4),RNDNO)
     1, (R(5),TO2O), (R(6),RO3O), (R(7),RN2PEL), (R(8),XN2PO2), (R(9),RN
     22PLO), (R(10),RO2PEL), (R(11),XOPLO2), (R(12),RNOPEL), (R(13),XO2N
     3PL), (R(14),RO2NPL), (R(15),RN2OPL), (R(16),XOPLNO), (R(17),XO2PNO
     4), (R(18),XN2PNO), (R(19),XNPLNO), (R(20),RO2PLN), (R(21),RHO3), (
     5R(22),ROHO), (R(23),RO2SO2), (R(24),RO3NO), (R(25),TONO), (R(26),R
     6ONO2), (R(27),RNO2NA), (R(28),TNON), (R(29),RNO2NB), (R(30),RO2N2O
     7), (R(31),RNSO3), (R(32),RNPHV), (R(33),ROSHV), (R(34),RODHV), (R(
     835),RNPLO)
      EQUIVALENCE (R(50),RLIO2), (R(51),TLIO), (R(52),ROLIO), (R(53),RBE
     1O2), (R(54),TBEO), (R(55),ROBEO), (R(56),RMGO2), (R(57),TMGO), (R(
     258),ROMGO), (R(59),RALO2), (R(60),TALO), (R(61),ROALO), (R(62),RSI
     3O2), (R(63),TSIO), (R(64),ROSIO), (R(65),RTIO2), (R(66),TTIO), (R(
     467),ROTIO), (R(68),RFEO2), (R(69),TFEO), (R(70),ROFEO), (R(71),RCU
     5O2), (R(72),TCUO), (R(73),ROCUO), (R(74),RUO)
      EQUIVALENCE (R(75),RMTLO3), (R(76),RO3LIO), (R(77),RO3BEO), (R(78)
     1,RO3MGO), (R(79),RO3ALO), (R(80),RO3SIO), (R(81),RO3TIO), (R(82),R
     2O3FEO), (R(83),RO3CUO)
      EQUIVALENCE (R(90),PDISO3)
      TGEV=CEN/CHT
      TG=CONV*TGEV
      IF (TG.LE.1.217) GO TO 5
```

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      CON=TNUM                                                          M  75
      CALL RATE (TG,CON)                                                M  76
      ALO=COP+COD+COS                                                   M  77
      ALO2=CO2+CO2D+CO2B+CO2SG                                          M  78
      ALN2=CN2+CN2A+CN2B                                                M  79
      ALN2PL=CN2PL+CN2APL+CN2BPL                                        M  80
      XN=CNS+CND+CNP                                                    M  81
      CMTL=CLI+CBE+CMG+CAL+CSI+CFE+CCU+CTI                              M  82
      CMTLO=CLIO+CBEO+CMGO+CALO+CSIO+CFEO+CCUO+CTIO                     M  83
      TATOM=XN+ALO+CNPL+COPL+CH+CMTL+CU                                 M  84
      TMOL5=ALO2+CNO+ALN2+ALN2PL+CO2PL+CNOPL+COH+CMTLO+CCO+CUOPL        M  85
      TMOL7=CO3+CNO2+CN2O+CCO2                                          M  86
      CHT=1.5*TATOM+2.5*TMOL5+3.0*TMOL7                                 M  87
      DMTLO=ROLIO*ALO                                                   M  88
      AA=0.99                                                           M  89
      FNS=RN2PEL*CEL*AA*ALN2PL+RN2PLO*ALN2PL*ALO+RNOPEL*CNOPL*CEL*.25+XOM  90
     12NPL*.5*CNPL*ALO2+RN2OPL*ALN2*COPL+XNPLNO*.5*CNPL*CNO+RNPLO*CNPL*AM  91
     2LO                                                                M  92
      DNS=RNSO2*ALO2+RNSNO*CNO+RNO2NA*CNO2+TNON*CNO+RNO2NB*CNO2+RO2PLN*CM  93
     1O2PL+RNSO3*CO3                                                    M  94
      FND=RN2PEL*CEL*ALN2PL*AA+RN2PLO*ALN2PL*ALO+RNOPEL*CNOPL*CEL*.75+RNM  95
     1PHV*CNP+XO2NPL*.5*CNPL*ALO2+XNPLNO*.5*CNPL*CNO                     M  96
      DND=RNDO2*ALO2+RNONO*CNO+RNO2NA*CNO2+TNON*CNO+RNO2NB*CNO2+RO2PLN*CM  97
     1O2PL                                                              M  98
      FO2=RO30*2.*ALO*CO3+XO2PNO*CO2PL*CNO+RHO3*CH*CO3+ROHO*COH*ALO+RO3NM  99
     1O*CNO*CO3+RONO2*ALO*CNO2+RNO2NA*CNO2*XN+RNSO3*CNS*CO3             M 100
      FO2M=ALO*(ROLIO*CLIO+ROBEO*CBEO+ROMGO*CMGO+ROALO*CALO+ROSIO*CSIO+RM 101
     1OFEO*CFEO+ROCUO*CCUO)+ALO*ROTIO*CTIO+2.0*CO3*(CLIO*RO3LIO+CBEO*RO3M 102
     2BEO+CMGO*RO3MGO+CALO*RO3ALO+CSIO*RO3SIO+CTIO*RO3TIO+CFEO*RO3FEO+CCM 103
     3UO*RO3CUO)+RMTLO3*CMTL*CO3                                        M 104
      FO2=FO2+FO2M+PDISO3*CO3                                           M 105
      DALO2=RNSO2*(CNS+CNP)+RNDO2*CND+XN2PO2*ALN2PL+XOPLO2*COPL+(RO2NPL+M 106
     12.*XO2NPL)*CNPL+TO2O*ALO+RO2SO2*CO2SG                             M 107
      DO2M=RLIO2*CLI+RBEO2*CBE+RMGO2*CMG+RALO2*CAL+RSIO2*CSI+RFEO2*CFE+RM 108
     1CUO2*CCU+RTIO2*CTI                                                M 109
      DO2=DALO2+DO2M                                                    M 110
      H=RNDO2*CND*ALO2+RNSO2*CNP*ALO2+RNSO3*CNS*CO3                     M 111
      G=RNSO2*CNS*ALO2+RONO2*ALO*CNO2                                   M 112
      FNO=H+G                                                           M 113
      DNO=RNSNO*CNS+RNDNO*CND+XOPLNO*COPL+XO2PNO*CO2PL+XN2PNO*ALN2PL+XNPM 114
     1LNO*CNPL+RO3NO*CO3+TONO*ALO+TNON*XN+RNSNO*CNP                     M 115
      FN2=RNSNO*CNS*CNO+RNDNO*CND*CNO+XN2PO2*ALN2PL*ALO2+XN2PNO*ALN2PL*CM 116
     1NO+RNO2NA*CNO2*XN+RO2N2O*CO2D*CN2O+RNSNO*CNP*CNO                  M 117
      DALN2=RN2OPL*COPL                                                 M 118
      DN2=DALN2                                                         M 119
      CE6=0.75*CEL                                                      M 120
      FO=RNSO2*CNS*ALO2+RNDO2*CND*ALO2+RNSNO*CNS*CNO+RNDNO*CND*CNO+.8*ROM 121
     12PEL*CEL*CO2PL+XOPLO2*COPL*ALO2+RNOPEL*CE6*CNOPL+RO2NPL*CNPL*ALO2+M 122
     2XOPLNO*COPL*CNO+RO2PLN*CO2PL*(CNS+CND)+RO2SO2*ALO2*CO2SG+RNO2NB*CNM 123
     3O2*XN+RNSO2*CNP*ALO2+RNSNO*CNP*CNO+RODHV*COD                      M 124
      FOM=ALO2*(RLIO2*CLI+RBEO2*CBE+RMGO2*CMG+RALO2*CAL+RSIO2*CSI+RFEO2*M 125
     1CFE+RCUO2*CCU+RTIO2*CTI)                                          M 126
      FO=FO+FOM+PDISO3*CO3                                              M 127
      DAOX=2.*RN2PLO*ALN2PL+ROHO*COH+TONO*CNO+RONO2*CNO2+TO2O*ALO2+RO30*M 128
     1CO3+RUO*CU+RNPLO*CNPL                                             M 129
      DOM=(TLIO*CMTL)+ROLIO*CLIO+ROBEO*CBEO+ROMGO*CMGO+ROALO*CALO+ROSIO*M 130
     1CSIO+ROFEO*CFEO+ROCUO*CCUO+ROTIO*CTIO                             M 131
      DO=DAOX+DOM                                                       M 132
      FEN=0.0                                                           M 133
      IF (NTG.EQ.0) GO TO 2                                             M 134
      FEN=0.0                                                           M 135
      E(1)=RN2PEL*CEL*((3.39+TE)*CN2PL+(4.49+TE)*CN2APL+(6.49+TE)*CN2BPLM 136
     1)                                                                 M 137
      E(2)=XN2PO2*(CO2*(3.52*CN2PL+4.62*CN2APL+6.62*CN2BPL)+CO2D*(4.5*CNM 138
     12PL+5.6*CN2APL+7.6*CN2BPL)+CO2SG*(7.82*CN2PL+8.92*CN2APL+10.92*CN2M 139
     2BPL)+CO2B*(5.12*CN2PL+6.22*CN2APL+8.22*CN2BPL))                   M 140
      E(3)=RN2PLO*(COP*(3.74*CN2PL+4.34*CN2APL+6.54*CN2BPL)+COD*(5.7*CN2M 141
     1PL+6.8*CN2APL+8.8*CN2BPL)+COS*(7.91*CN2PL+9.01*CN2APL+11.01*CN2BPLM 142
     2))                                                                M 143
      E(4)=RO2PEL*CEL*CO2PL*6.95                                        M 144
      E(5)=XOPLO2*COPL*(1.56*CO2+2.54*CO2D+3.16*CO2B+5.86*CO2SG)        M 145
      E(6)=RNOPEL*CNOPL*CEL*(0.98+TE)                                   M 146
      E(7)=XO2NPL*CNPL*(CO2*2.56+4.52*CO2D+11.16*CO2SG+5.76*CO2B)       M 147
      E(8)=RO2NPL*CNPL*(CO2*6.66+7.64*CO2D+10.96*CO2SG+8.26*CO2B)       M 148
      E(9)=RN2OPL*COPL*(CN2*1.1+7.3*CN2A+8.4*CN2B)                      M 149
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      E(11)=XOPLNO*COPL*CNO*4.05                                        M 150
      E(12)=XO2PNO*CNO*CO2PL*2.8                                        M 151
      E(13)=XN2PNO*CNO*(6.31*CN2PL+7.41*CN2APL+9.41*CN2BPL)             M 152
      E(14)=XNPLNO*CNO*CNPL*5.27                                        M 153
      E(15)=RO2PLN*CO2PL*(4.19*CNS+0.57*CND)                            M 154
      E(16)=RHO3*CH*CO3*3.34                                            M 155
      E(17)=ROHO*COH*(COP*0.72+2.68*COD+4.69*COS)                       M 156
      E(18)=RO2SO2*CO2SG*(0.24*CO2+1.22*CO2D+1.64*CO2B+4.54*CO2SG)      M 157
      E(19)=RO3NO*CNO*CO3*2.07                                          M 158
      E(20)=TONO*CNO*(3.12*COP+5.35*COD+7.29*COS)                       M 159
      E(21)=RONO2*CNO2*(2.*COP+3.96*COD+6.17*COS)                       M 160
      E(22)=RNO2NA*CNO2*(5.25*CNS+7.63*CND+6.62*CNP)                    M 161
      E(23)=TNON*CNO*(4.93*CNS+7.31*CND+8.5*CNP)                        M 162
      E(24)=RNO2NB*CNO2*(1.81*CNS+4.19*CND+5.36*CNP)                    M 163
      E(25)=RO2N2O*CN2O*CO2D*0.35                                       M 164
      E(26)=RNSO2*(CO2*(1.39*CNS+4.96*CNP)+CO2D*(2.37*CNS+5.94*CNP)+CO2B M 165
     1*(2.99*CNS+6.56*CNP)+CO2SG*(5.69*CNS+9.26*CNP))                   M 166
      E(27)=RNDO2*CND*(3.77*CO2+4.75*CO2D+5.37*CO2B+8.07*CO2SG)         M 167
      E(28)=RNSNO*CNO*(3.25*CNS+6.62*CNP)                               M 168
      E(29)=RNDNO*CNO*5.63*CND                                          M 169
      E(30)=TO2O*(COP*(1.05*CO2+2.03*CO2D+2.65*CO2B+5.35*CO2SG)+COD*(3.0 M 170
     11*CO2+3.99*CO2D+4.61*CO2B+7.31*CO2SG)+COS*(5.22*CO2+6.2*CO2D+6.82* M 171
     2CO2B+9.52*CO2SG))                                                 M 172
      E(31)=RO3O*CO3*(4.06*COP+6.02*COD+8.23*COS)                       M 173
      E(32)=TALO*CAL*(5.20*COP+7.16*COD+9.37*COS)                       M 174
      E(33)=RALO2*CAL*(0.38*CO2+1.06*CO2D+1.68*CO2B+4.38*CO2SG)         M 175
      E(34)=ROALO*CALO*(-0.06*COP+1.88*COD+4.09*COS)                    M 176
      E(35)=TBEO*CBE*(4.60*COP+6.56*COD+8.77*COS)                       M 177
      E(36)=RBEO2*CBE*(-0.52*CO2+0.46*CO2D+1.06*CO2B+3.76*CO2SG)        M 178
      E(37)=ROBEO*CBEO*(0.52*COP+2.46*COD+4.69*COS)                     M 179
      E(38)=TCUO*CCU*(4.03*COP+6.04*COD+8.25*COS)                       M 180
      E(39)=RCUO2*CCU*(-1.04*CO2-0.06*CO2D+0.56*CO2B+3.26*CO2SG)        M 181
      E(40)=ROCUO*CCUO*(1.04*COP+3.00*COD+5.21*COS)                     M 182
      E(41)=TFEO*CFE*(4.20*COP+6.16*COD+8.37*COS)                       M 183
      E(42)=RFEO2*CFE*(-0.92*CO2+0.06*CO2D+0.68*CO2B+2.36*CO2SG)        M 184
      E(43)=ROFEO*CFEO*(0.92*COP+2.88*COD+5.09*COS)                     M 185
      E(44)=TLIO*CLI*(3.40*COP+5.34*COD+7.57*COS)                       M 186
      E(45)=RLIO2*CLI*(-1.72*CO2-0.74*CO2D-0.12*CO2B+2.56*CO2SG)        M 187
      E(46)=ROLIO*CLIO*(1.72*COP+3.68*COD+5.89*COS)                     M 188
      E(47)=TSIO*CSI*(7.93*COP+9.89*COD+12.10*COS)                      M 189
      E(48)=RSIO2*CSI*(2.82*CO2+3.80*CO2D+4.42*CO2B+7.12*CO2SG)         M 190
      E(49)=ROSIO*CSIO*(-2.82*COP-0.86*COD+1.35*COS)                    M 191
      E(50)=TMGO*CMG*(3.50*COP+5.46*COD+7.67*COS)                       M 192
      E(51)=RMGO2*CMG*(-1.62*CO2-0.64*CO2D-0.02*CO2B+2.66*CO2SG)        M 193
      E(52)=ROMGO*CMGO*(1.52*COP+3.59*COD+5.79*COS)                     M 194
      E(53)=RNSO3*CNS*CO3*5.46                                          M 195
      E(54)=TTIO*CTI*(7.20*COP+9.16*COD+11.37*COS)                      M 196
      E(55)=RTIO2*CTI*(2.08*CO2+3.06*CO2D+3.68*CO2B+6.38*CO2SG)         M 197
      E(56)=ROTIO*CTIO*(-2.06*COP-0.12*COD+2.09*COS)                    M 198
      DO 1 I=1,56                                                       M 199
    1 FEN=FEN+E(I)                                                      M 200
    2 CONTINUE                                                          M 201
      FEL=0.                                                            M 202
      DEL=0.0                                                           M 203
      DEN=0.0                                                           M 204
      FN2PL=0.                                                          M 205
      DALN2PL=RN2PEL*CEL+XN2PO2*ALO2+RN2PLO*ALO*2.+XN2PNO*CNO           M 206
      DN2PL=DALN2PL                                                     M 207
      FO2PL=2.*XO2NPL*CNPL*ALO2+XOPLO2*COPL*ALO2+XN2PO2*ALN2PL*ALO2     M 208
      DO2PL=RO2PEL*CEL+XO2PNO*CNO+RO2PLN*(CNS+CND)                      M 209
      FNPL=0.                                                           M 210
      DNPL=RO2NPL*ALO2+2.*XO2NPL*ALO2+XNPLNO*CNO+RNPLO*ALO              M 211
      FOPL=RNPLO*CNPL*ALO                                               M 212
      DOPL=XOPLO2*ALO2+XOPLNO*CNO+RN2OPL*ALN2                           M 213
      FNOPL=RO2NPL*CNPL*ALO2+2.*RN2PLO*ALN2PL*ALO+XOPLNO*COPL*CNO+RN2OPL M 214
     1*ALN2*COPL+XO2PNO*CNO*CO2PL+XN2PNO*ALN2PL*CNO+XNPLNO*CNPL*CNO+RO2P M 215
     2LN*CO2PL*(CNS+CND)                                                M 216
      DNOPL=RNOPEL*CEL                                                  M 217
      FO3X=TO2O*ALO*ALO2+RO2N2O*CN2O*CO2D                               M 218
      FO3S=RO2SO2*CO2SG*ALO2                                            M 219
      FO3=FO3X+FO3S                                                     M 220
      DO3=RO3O*ALO+RHO3*CH+RO3NO*CNO+RNSO3*CNS+CLIO*RO3LIO+RO3BEO*CBEO+R M 221
     1O3MGO*CMGO+RO3ALO*CALO+RO3SIO*CSIO+RO3TIO*CTIO+RO3FEO*CFEO+RO3CUO* M 222
     2CCUO+RMTLO3*CMTL                                                  M 223
      DO3=DO3+PDISO3                                                    M 224
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      FN=ROHO*COH*ALO
      DH=RHO3*CO3
      FOH=RHO3*CH*CO3
      DOH=ROHO*ALO
      BB=0.02
      FNP=RN2PEL*CEL*ALN2PL*BB
      DNP=RNPHV+TNON*CNO+RNO2NA*CNO2+RNO2NB*CNO2+RNSO2*ALO2+RNSNO*CNO+RO
     12PLN*CO2PL
      FNO2=RO3NO*CNO*CO3+TONO*CNO*ALO
      DNO2=RONO2*ALO+RNO2NA*XN+RNO2NB*XN
      FN2O=TNON*CNO*XN+RNO2NB*CNO2*XN
      DN2O=RO2N2O*CO2D
      FCO2=0.
      DCO2=0.
      IF (CMTL.LE.0.) GO TO 3
      FMTLOZ=RMTLO3*CO3
      FLIO2=RLIO2*CLI*ALO2
      FLIO3=CLI*(TLIO*ALO+FMTLOZ)
      FLIO=FLIO2+FLIO3
      DLIO=ROLIO*ALO+RO3LIO*CO3
      FLI=ROLIO*ALO*CLIO+RO3LIO*CO3*CLIO
      DLI=TLIO*ALO+RLIO2*ALO2+FMTLOZ
      FBEO2=RBEO2*CBE*ALO2
      FBEO3=CBE*(TBEO*ALO+FMTLOZ)
      FBEO=FBEO2+FBEO3
      DBEO=ROBEO*ALO+RO3BEO*CO3
      FBE=ROBEO*ALO*CBEO+RO3BEO*CO3*CBEO
      DBE=TBEO*ALO+RBEO2*ALO2+FMTLOZ
      FMGO2=RMGO2*CMG*ALO2
      FMGO3=CMG*(TMGO*ALO+FMTLOZ)
      FMGO=FMGO2+FMGO3
      DMGO=ROMGO*ALO+RO3MGO*CO3
      FMG=ROMGO*ALO*CMGO+RO3MGO*CO3*CMGO
      DMG=TMGO*ALO+RMGO2*ALO2+FMTLOZ
      FALO2=RALO2*CAL*ALO2
      FALO3=CAL*(TALO*ALO+FMTLOZ)
      FALO=FALO2+FALO3
      DALO=ROALO*ALO+RO3ALO*CO3
      FAL=ROALO*ALO*CALO+RO3ALO*CO3*CALO
      DAL=TALO*ALO+RALO2*ALO2+FMTLOZ
      FSIO2=RSIO2*CSI*ALO2
      FSIO3=CSI*(TSIO*ALO+FMTLOZ)
      FSIO=FSIO2+FSIO3
      DSIO=ROSIO*ALO+RO3SIO*CO3
      FSI=ROSIO*ALO*CSIO+RO3SIO*CO3*CSIO
      DSI=TSIO*ALO+RSIO2*ALO2+FMTLOZ
      FTIO2=RTIO2*CTI*ALO2
      FTIO3=CTI*(TTIO*ALO+FMTLOZ)
      FTIO=FTIO2+FTIO3
      DTIO=ROTIO*ALO+RO3TIO*CO3
      FTI=ROTIO*ALO*CTIO+RO3TIO*CO3*CTIO
      DTI=TTIO*ALO+RTIO2*ALO2+FMTLOZ
      FFEO2=RFEO2*CFE*ALO2
      FFEO3=CFE*(TFEO*ALO+FMTLOZ)
      FFEO=FFEO2+FFEO3
      DFEO=ROFEO*ALO+RO3FEO*CO3
      FFE=ROFEO*ALO*CFEO+RO3FEO*CO3*CFEO
      DFE=TFEO*ALO+RFEO2*ALO2+FMTLOZ
      FCUO2=RCUO2*CCU*ALO2
      FCUO3=CCU*(TCUO*ALO+FMTLOZ)
      FCUO=FCUO2+FCUO3
      DCUO=ROCUO*ALO+RO3CUO*CO3
      FCU=ROCUO*ALO*CCUO+RO3CUO*CO3*CCUO
      DCU=TCUO*ALO+RCUO2*ALO2+FMTLOZ
3     CONTINUE
      FOD=ROSHV*COS+0.25*RNOPEL*CNOPL*CEL+0.6*RO2PEL*CO2PL*CEL
      DOD=DAOX+DOM+RODHV
      FOS=0.4*RO2PEL*CO2PL*CEL
      DOS=DAOX+DOM+ROSHV
      FO2D=0.
      DO2D=DALO2+DO2M+RO2N2O*CN2O
      DO2M=DALO2+DO2M
      FO2SG=0.
      DO2SG=DALO2+DO2M+RO2SG2*ALO2
      FCO=0.
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                DCO=0.                                                    M  300
                FU=0.                                                     M  301
                DU=RUO*ALO                                                M  302
                FUOPL=RUO*CU*ALO                                          M  303
                DUOPL=0.                                                  M  304
                DN2A=DALN2                                                M  305
                DN2B=DALN2                                                M  306
                DN2APL=DALN2PL                                            M  307
                DN2BPL=DALN2PL                                            M  308
                IF (QQ.LE.0.0) GO TO 4                                    M  309
                CALL ENQDEP (TIONPR,CON,TG)                               M  310
                FEN=FEN+5.0*QQ                                            M  311
                FNS=FNS+QNS1                                              M  312
                FND=FND+QND1                                              M  313
                FNP=FNP+QNP1                                              M  314
                FN2PL=FN2PL+QN2PL                                         M  315
                FO2PL=FO2PL+QO2PL                                         M  316
                FNPL=FNPL+QNPL                                            M  317
                FOPL=FOPL+QOPL                                            M  318
                FO=FO+QFO                                                 M  319
                DO=DO+QDO                                                 M  320
                FOD=FOD+QOD1                                              M  321
                FOS=FOS+QOS1                                              M  322
                FO2D=FO2D+QO2D                                            M  323
                FO2SG=FO2SG+QO2S                                          M  324
                DN2=DN2+QDN2                                              M  325
                DO2=DO2+QDO2                                              M  326
          4     CONTINUE                                                  M  327
                RETURN                                                    M  328
          5     NTG=10                                                    M  329
                PRINT 6, TG                                               M  330
                RETURN                                                    M  331
          C                                                               M  332
          C                                                               M  333
          6     FORMAT (34H TG IS TOO SMALL OR NEGATIVE AND = ,E14.7)     M  334
                END                                                       M  335-
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```
      SUBROUTINE RRCRT (TG)
C
C     ****************************************************************
C
C        PRCRT
C                STORES DESTRUCTION RATES OF SPECIES FOR WORRY
C                CALCULATES VIBRATIONAL LEVEL FORMATION RATES OF SPECIES
C                (NOT CURRENT WORRY VERSION)
C
C     ****************************************************************
C
      COMMON /BANDS/ MSTATE(20),NSTATE(20)
      COMMON /FU/ Y(90),P(90),S(90),R(90),CHT,TGEV,QQ,TNUM,NFLAG,NTG
      COMMON /KEN/ CONV,DT,N
      COMMON /XUX/ RR(200),CMD(90),RCRT(90),NSPEC
      REAL LFR(30)
      EQUIVALENCE (CMD(1),CH), (CMD(2),CLI), (CMD(3),CBE), (CMD(4),CMG),
     1 (CMD(5),CAL), (CMD(6),CSI), (CMD(7),CTI), (CMD(8),CFE), (CMD(9),C
     2CU), (CMD(10),CU), (CMD(11),COH), (CMD(12),CLIO), (CMD(13),CBEO),
     3(CMD(14),CMGO), (CMD(15),CALO), (CMD(16),CSIO), (CMD(17),CTIO), (C
     4MD(18),CFEO), (CMD(19),CCUO), (CMD(20),CUOPL), (CMD(21),CNOPL), (C
     5MD(22),CNO), (CMD(23),CNO2), (CMD(24),CN2O), (CMD(25),CCO), (CMD(2
     66),CCO2), (CMD(27),CO3), (CMD(28),CH2O), (CMD(30),CEL), (CMD(31),C
     7N2), (CMD(32),CN2A), (CMD(33),CN2B), (CMD(34),CNS), (CMD(35),CND),
     8 (CMD(36),CNP), (CMD(38),COP), (CMD(39),COD), (CMD(40),COS), (CMD(
     941),CN2PL), (CMD(42),CO2PL), (CMD(43),CNPL), (CMD(44),COPL), (CMD(
     $45),CN2APL), (CMD(46),CN2BPL), (CMD(50),CEN), (CMD(51),CO2), (CMD(
     $52),CO2D), (CMD(53),CO2B), (CMD(54),CO2SG)
      EQUIVALENCE (P(1),FH), (P(2),FLI), (P(3),FBE), (P(4),FMG), (P(5),F
     1AL), (P(6),FSI), (P(7),FTI), (P(8),FFE), (P(9),FCU), (P(10),FU), (
     2P(11),FOH), (P(12),FLIO), (P(13),FBEO), (P(14),FMGO), (P(15),FALO)
     3, (P(16),FSIO), (P(17),FTIO), (P(18),FFEO), (P(19),FCUO), (P(20),F
     4UOPL), (P(21),FNOPL), (P(22),FNO), (P(23),FNO2), (P(24),FN2O), (P(
     525),FCO), (P(26),FCO2), (P(27),FO3), (P(28),FH2O), (P(30),FEL), (P
     6(31),FN2), (P(32),FN2A), (P(33),FN2B), (P(34),FNS), (P(35),FND), (
     7P(36),FNP), (P(38),FO), (P(39),FOD), (P(40),FOS), (P(41),FN2PL), (
     8P(42),FO2PL), (P(43),FNPL), (P(44),FOPL), (P(45),FN2APL), (P(46),F
     9N2BPL), (P(50),FEN), (P(51),FO2), (P(52),FO2D), (P(53),FO2B), (P(5
     $4),FO2SG)
      EQUIVALENCE (S(1),DH), (S(2),DLI), (S(3),DBE), (S(4),DMG), (S(5),D
     1AL), (S(6),DSI), (S(7),DTI), (S(8),DFE), (S(9),DCU), (S(10),DU), (
     2S(11),DOH), (S(12),DLIO), (S(13),DBEO), (S(14),DMGO), (S(15),DALO)
     3, (S(16),DSIO), (S(17),DTIO), (S(18),DFEO), (S(19),DCUO), (S(20),D
     4UOPL), (S(21),DNOPL), (S(22),DNO), (S(23),DNO2), (S(24),DN2O), (S(
     525),DCO), (S(26),DCO2), (S(27),DO3), (S(28),DH2O), (S(30),DEL), (S
     6(31),DN2), (S(32),DN2A), (S(33),DN2B), (S(34),DNS), (S(35),DND), (
     7S(36),DNP), (S(38),DO), (S(39),DOD), (S(40),DOS), (S(41),DN2PL), (
     8S(42),DO2PL), (S(43),DNPL), (S(44),DOPL), (S(45),DN2APL), (S(46),D
     9N2BPL), (S(50),DEN), (S(51),DO2), (S(52),DO2D), (S(53),DO2B), (S(5
     $4),DO2SG)
      EQUIVALENCE (P(70),FLIO2), (P(71),FLIO3), (P(72),FBEO2), (P(73),FB
     1EO3), (P(74),FMGO2). (P(75),FMGO3), (P(76),FALO2), (P(77),FALO3),
     2(P(78),FSIO2), (P(79),FSIO3)  (P(80),FTIO2), (P(81),FTIO3), (P(82)
     3,FFEO2), (P(83),FFEO3), (P(84),FCUO2), (P(85),FCUO3), (P(86),FNOG)
     4, (P(87),FNOX), (P(88),FO3X), (P(89),FO3S), (S(70),DMTLO)
      EQUIVALENCE (R(1),RNSO2), (R(2),RNDO2), (R(3),RNSNO), (R(4),RNDNO)
     1, (R(5),TO2O), (R(6),RO3O), (R(7),RN2PEL), (R(8),XN2PO2), (R(9),RN
     22PLO), (R(10),RO2PEL), (R(11),XOPLO2), (R(12),RNOPEL), (R(13),XO2N
     3PL), (R(14),RO2NPL), (R(15),RN2OPL), (R(16),XOPLNO), (R(17),XO2PNO
     44), (R(18),XN2PNO), (R(19),XNPLNO), (R(20),RO2PLN), (R(21),RHO3), (
     5R(22),ROHO), (R(23),RO2SO2), (R(24),RO3NO), (R(25),TONO), (R(26),R
     6ONO2), (R(27),RNO2NA), (R(28),TNON), (R(29),RNO2NB), (R(30),RO2N2O
     77), (R(31),RNSO3), (R(32),RNPHV), (R(33),ROSHV), (R(34),RODHV), (R(
     835),RNPLO)
      EQUIVALENCE (R(50),RLIO2), (R(51),TLIO), (R(52),ROLIO), (R(53),RBE
     1O2), (R(54),TBEO), (R(55),ROBEO), (R(56),RMGO2), (R(57),TMGO), (R(
     258),ROMGO), (R(59),RALO2), (R(60),TALO), (R(61),ROALO), (R(62),RSI
     3O2), (R(63),TSIO), (R(64),ROSIO), (R(65),RTIO2), (R(66),TTIO), (R(
     467),ROTIO), (R(68),RFEO2), (R(69),TFEO), (R(70),ROFEO), (R(71),RCU
     5O2), (R(72),TCUO), (R(73),ROCUO), (R(74),RUO)
      EQUIVALENCE (R(75),RMTLO3), (R(76),RO3LIO), (R(77),RO3BEO), (R(78)
     1,RO3MGO), (R(79),RO3ALO), (R(80),RO3SIO), (R(81),RO3TIO), (R(82),R
     2O3FEO), (R(83),RO3CUO)
      EQUIVALENCE (R(90),POISO3)
      DATA LFR/0.1,0.25,0.25,0.25,0.25,0.25,0.25,0.25,0.25,0.25,.333333,
```

```
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     10.111111,0.25,0.25,0.25,0.1666666,0.050824,0.125,0.25,0.0,0.0,0.14
     22857,0.0,0.0,0.0,0.0,0.142857/
      DATA ELI/10000./
      DATA VLI/.0944/,VBE/0.1515/,VMG/0.0960/,VAL/0.0395/,VFE/0.108/,VCU
     1/0.377/
C
      TGEVIN=CONV/TG
      DO 35 MOL=1,20
      M=MSTATE(MOL)
      N=NSTATE(MOL)
      IF (N.EQ.0) GO TO 35
      GO TO (1,3,4,5,6,7,9,11,12,13,15,16,19,21,23,25,27,30,32,34), MOL
C     OH
    1 DO 2 L=1,N
      I=M+L
    2 RR(I)=FOH*LFR(1)
      GO TO 35
C     LIO
    3 EXL=EXP(-VLI*TGEVIN)
C     GROUND STATE
      RR(M+1)=FLIO3*LFR(2)+FLIO2*(1-EXL)
      RR(M+2)=FLIO3*LFR(2)+FLIO2*EXL
      RR(M+3)=FLIO3*LFR(2)
      RR(M+4)=FLIO3*LFR(2)
      GO TO 35
C     BEO
    4 EXL=EXP(-VBE*TGEVIN)
      RR(M+1)=FBEO3*LFR(3)+FBEO2*(1-EXL)
      RR(M+2)=FBEO3*LFR(3)+FBEO2*EXL
      RR(M+3)=FBEO3*LFR(3)
      RR(M+4)=FBEO3*LFR(3)
      GO TO 35
C     MGO
    5 EXL=EXP(-VMG*TGEVIN)
      RR(M+1)=FMGO3*LFR(4)+FMGO2*(1-EXL)
      RR(M+2)=FMGO3*LFR(4)+FMGO2*EXL
      RR(M+3)=FMGO3*LFR(4)
      RR(M+4)=FMGO3*LFR(4)
      GO TO 35
C     ALO
    6 EXL=EXP(-VAL*TGEVIN)
      RR(M+1)=FALO3*LFR(5)+FALO2*(1-EXL)
      RR(M+2)=FALO3*LFR(5)+FALO2*EXL
      RR(M+3)=FALO3*LFR(5)
      RR(M+4)=FALO3*LFR(5)
      GO TO 35
C     SIO
    7 DO 8 L=1,N
      I=M+L
    8 RR(I)=(FSIO3+FSIO2)*LFR(6)
      GO TO 35
C     TIO
    9 DO 10 L=1,N
      I=M+L
   10 RR(I)=(FTIO3+FTIO2)*LFR(7)
      GO TO 35
C     FEO
   11 EXL=EXP(-VFE*TGEVIN)
      RR(M+1)=FFEO3*LFR(8)+FFEO2*(1-EXL)
      RR(M+2)=FFEO3*LFR(8)+FFEO2*EXL
      RR(M+3)=FFEO3*LFR(8)
      RR(M+4)=FFEO3*LFR(8)
      GO TO 35
C     CUO
   12 EXL=EXP(-VCU*TGEVIN)
      RR(M+1)=FCUO3*LFR(9)+FCUO2*(1-EXL)
      RR(M+2)=FCUO3*LFR(9)+FCUO2*EXL
      RR(M+3)=FCUO3*LFR(9)
      RR(M+4)=FCUO3*LFR(9)
      GO TO 35
C     UO
   13 DO 14 L=1,N
      I=M+L
   14 RR(I)=FUOPL*LFR(10)
      GO TO 35
```

```
C         NO+                                                            N 150
15        RR(M+1)=FNOPL*LFR(11)                                          N 151
          RR(M+2)=FNOPL*LFR(11)                                          N 152
          RR(M+3)=FNOPL*LFR(11)                                          N 153
          RR(M+4)=FNOPL*LFR(21)                                          N 154
          GO TO 35                                                       N 155
C         NO                                                             N 156
16        DO 17 L=1,7                                                    N 157
          I=M+L                                                          N 158
17        RR(I)=FNOX*LFR(12)+FNOG*LFR(22)                                N 159
          DO 18 L=8,N                                                    N 160
          I=M+L                                                          N 161
18        RR(I)=FNOX*LFR(12)                                             N 162
          GO TO 35                                                       N 163
C         NO2                                                            N 164
19        DO 20 L=1,N                                                    N 165
          I=M+L                                                          N 166
20        RR(I)=FNO2*LFR(13)                                             N 167
          GO TO 35                                                       N 168
C         N2O                                                            N 169
21        DO 22 L=1,N                                                    N 170
          I=M+L                                                          N 171
22        RR(I)=FN2O*LFR(14)                                             N 172
          GO TO 35                                                       N 173
C         CO                                                             N 174
23        DO 24 L=1,N                                                    N 175
          I=M+L                                                          N 176
24        RR(I)=0.0*LFR(15)                                              N 177
          GO TO 35                                                       N 178
C         CO2                                                            N 179
25        DO 26 L=1,N                                                    N 180
          I=M+L                                                          N 181
26        RR(I)=0.0*LFR(16)                                              N 182
          GO TO 35                                                       N 183
C         O3                                                             N 184
27        DO 28 L=1,7                                                    N 185
          I=M+L                                                          N 186
28        RR(I)=FO3X*LFR(17)+FO3S*LFR(27)                                N 187
          DO 29 L=8,N                                                    N 188
          I=M+L                                                          N 189
29        RR(I)=FO3X*LFR(17)                                             N 190
          GO TO 35                                                       N 191
C         H2O                                                            N 192
30        DO 31 L=1,N                                                    N 193
          I=M+L                                                          N 194
31        RR(I)=0.0*LFR(18)                                              N 195
          GO TO 35                                                       N 196
C         CN                                                             N 197
32        DO 33 L=1,N                                                    N 198
          I=M+L                                                          N 199
33        RR(I)=0.0*LFR(19)                                              N 200
          GO TO 35                                                       N 201
C         E-                                                             N 202
34        CONTINUE                                                       N 203
35        CONTINUE                                                       N 204
C         O                                                              N 205
          RR(199)=ROOHV*COD                                              N 206
          RR(200)=ROSHV*COS                                              N 207
          RCRT(11)=DOH                                                   N 208
          RCRT(12)=DLIO                                                  N 209
          RCRT(13)=DBEO                                                  N 210
          RCRT(14)=DMGO                                                  N 211
          RCRT(15)=DALO                                                  N 212
          RCRT(16)=DSIO                                                  N 213
          RCRT(17)=DTIO                                                  N 214
          RCRT(18)=DFEO                                                  N 215
          RCRT(19)=DCOO                                                  N 216
          RCRT(20)=0.0                                                   N 217
          RCRT(21)=DNOPL                                                 N 218
          RCRT(22)=DNO                                                   N 219
          RCRT(23)=DNO2                                                  N 220
          RCRT(24)=DN2O                                                  N 221
          RCRT(27)=DO3                                                   N 222
          RCRT(39)=DOD                                                   N 223
          RCRT(40)=DOS                                                   N 224
```

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 2401           RETURN                                                       N 225      2401
 2402           END                                                          N 226-     2402
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      SUBROUTINE RATE (TG,CON)
C**********************************************************************
C
C     RATE
C            CALCULATES AND STORES REACTION RATE CONSTANTS IN R ARRAY
C**********************************************************************
C
C
      COMMON /BURST/ DAY
      COMMON /FJ/ Y(90),P(90),S(90),R(90),CHT,TGEV,QQ,TNUM,NFLAG,NTG
      COMMON /KEN/ CONV,DT,N
      EQUIVALENCE (Y(50),CMTL), (Y(61),CMTLO)
      EQUIVALENCE (R(1),RNSO2), (R(2),RNDO2), (R(3),RNSNO), (R(4),RNDNO)
     1, (R(5),TO2O), (R(6),RO3O), (R(7),RN2PEL), (R(8),XN2PO2), (R(9),RN
     22PLO), (R(10),RO2PEL), (R(11),XOPLO2), (R(12),RNOPEL), (R(13),XO2N
     3PL), (R(14),RO2NPL), (R(15),RN2OPL), (R(16),XOPLNO), (R(17),XO2PNO
     4), (R(18),XN2PNO), (R(19),XNPLNO), (R(20),RO2PLN), (R(21),RHO3), (
     5R(22),ROHO), (R(23),RO2SO2), (R(24),RO3NO), (R(25),TONO), (R(26),X
     6ONO2), (R(27),RNO2NA), (R(28),TNON), (R(29),RNO2NB), (R(30),RO2N2O
     7), (R(31),RNSO3), (R(32),RNPHV), (R(33),ROSHV), (R(34),RODHV), (R(
     835),RNPLO)
      EQUIVALENCE (R(50),RLIO2), (R(51),TLIO), (R(52),ROLIO), (R(53),RBE
     1O2), (R(54),TBEO), (R(55),ROBEO), (R(56),RMGO2), (R(57),TMGO), (R(
     258),ROMGO), (R(59),RALO2), (R(60),TALO), (R(61),ROALO), (R(62),RSI
     3O2), (R(63),TSIO), (R(64),ROSIO), (R(65),RTIO2), (R(66),TTIO), (R(
     467),ROTIO), (R(68),RFEO2), (R(69),TFEO), (R(70),ROFEO), (R(71),RCU
     5O2), (R(72),TCUO), (R(73),ROCUO), (R(74),RUO)
      EQUIVALENCE (R(75),RMTLO3), (R(76),RO3LIO), (R(77),RO3BEO), (R(78)
     1,RO3MGO), (R(79),RO3ALO), (R(80),RO3SIO), (R(81),RO3TIO), (R(82),R
     2O3FEO), (R(83),RO3CUO)
      EQUIVALENCE (R(90),POISO3)
      DATA CON1/0.0/
      DATA TG1,TG2,TG3/3*0.0/
      DATA XI1,XI2,XI3/1.E-6,1.E-5,1.E-4/
      DATA RCLI/1.72/,RCBE/0.52/,RCMG/1.62/,RCAL/0.08/,RCSI/2.62/,RCTI/2
     1.08/,RCFE/0.92/,RCCU/1.04/
      DATA RALO2,RSIO2,RTIO2,RUO/4*2.E-10/
      DATA ROLIO,ROBEO,ROMGO,ROFEO,ROCUO/5*2.E-10/
      DATA THLIO,THBEO,THMGO,THALO,THSIO,THTIO,THFEO,THCUO/8*1.E-31/
      DATA XN2PO2/2.E-10/,RN2PLO/1.25E-10/,XOPLO2/2.E-11/,XO2NPL/2.5E-10
     1/,RO2NPL/5.E-10/,XOPLNO/2.4E-11/,XO2PNO/8.E-10/,XN2PNO/5.E-10/,XNP
     2LNO/8.E-10/,RO2PLN/1.8E-10/,RHO3/2.6E-11/,ROHO/5.E-11/,RO2SO2/1.E-
     312/
      DATA RN2OPL/1.3E-12/
      DATA RNO2NA/1.5E-11/,RNO2NB/1.5E-11/,RO2N2O/1.E-13/,RNPHV/7.87402E
     1-2/
      DATA RMTLO3,RO3LIO,RO3MGO,RNPLO/3*1.E-11,1.E-12/
      DATA ROSHV/0.6993006993/,RODHV/0.00625/
      DATA O3BE,O3AL,O3SI,O3TI,O3FE,O3CU/0.535,1.135,3.865,2.135,0.135,0
     1.015/
C
      C=ABS((CON-CON1)/CON)
      IF (C.LE.0.01) GO TO 1
      TLIO=THLIO*CON
      TBEO=TLIO
      TMGO=TLIO
      TALO=TLIO
      TSIO=TLIO
      TTIO=TLIO
      TFEO=TLIO
      TCUO=TLIO
      T1=2.8E-35*CON
      T2=1.3E-31*CON
      T3=1.E-34*CON
      TG1=0.0
      TG2=0.0
      TG3=0.0
      CON1=CON
      CONTINUE
      TGEV=TG/CONV
      TGIN=1./TGEV
      TGSQ=TG*TG
      IF (CMTL.LE.0.0) GO TO 2
      DELTG=ABS(TG-TG1)
```

```
           IF  (DELTG.LT.XI1*TGSQ)  GO  TO  2               0   75
           RLIO2=2.E-10*EXP(-RCLI*TGIN)                      0   76
           RBEO2=2.E-10*EXP(-RCBE*TGIN)                      0   77
           RMGO2=2.E-10*EXP(-RCMG*TGIN)                      0   78
           ROSIO=2.E-10*EXP(-RCSI*TGIN)                      0   79
           ROTIO=2.E-10*EXP(-RCTI*TGIN)                      0   80
           RFEO2=2.E-10*EXP(-RCFE*TGIN)                      0   81
           RCUO2=2.E-10*EXP(-RCCU*TGIN)                      0   82
           RO3BEO=1.E-11*EXP(-O3BE*TGIN)                     0   83
           RO3ALO=1.E-11*EXP(-O3AL*TGIN)                     0   84
           RO3SIO=1.E-11*EXP(-O3SI*TGIN)                     0   85
           RO3TIO=1.E-11*EXP(-O3TI*TGIN)                     0   86
           TG1=TG                                            0   87
 2         CONTINUE                                          0   88
           DELTG=ABS(TG-TG2)                                 0   89
           IF  (DELTG.LT.XI2*TGSQ)  GO  TO  3               0   90
           TEIN3=0.026*TGIN                                  0   91
           TOV3=TG/300.                                      0   92
           SQ=SQRT(TOV3)                                     0   93
           RNSO2=6.68E-12*EXP(-3590./TG)                     0   94
           TO2O=T1*EXP(900./TG)                              0   95
           RO3O=2.0E-11*EXP(-2400./TG)                       0   96
           RO3NO=9.5E-13*EXP(-1300./TG)                      0   97
           TNCN=T3*EXP(-1000./TG)                            0   98
           RNSO3=3.4E-11*SQ*EXP(-1200./TG)                   0   99
           ROALO=2.E-10*EXP(-RCAL*TGIN)                      0  100
           RO3FEO=1.E-11*EXP(-O3FE*TGIN)                     0  101
           TG2=TG                                            0  102
 3         CONTINUE                                          0  103
           DELTG=ABS(TG-TG3)                                 0  104
           IF  (DELTG.LT.XI3*TGSQ)  GO  TO  4               0  105
           RNSNO=5.1E-11*EXP(-166./TG)                       0  106
           RONO2=2.8E-11*EXP(-550./TG)                       0  107
           RNDO2=6.0E-12*SQ                                  0  108
           RNDNO=6.E-11*SQ                                   0  109
           RN2PEL=2.8E-7*TEIN3**0.2                          0  110
           RO2PEL=2.2E-7*TEIN3**0.7                          0  111
           RNOPEL=5.E-7*TEIN3**1.2                           0  112
           TONO=T2*TOV3**-2.5                                0  113
           RO3CUO=1.E-11*EXP(-O3CU*TGIN)                     0  114
           TG3=TG                                            0  115
 4         CONTINUE                                          0  116
           PDISO3=0.                                         0  117
           IF  (DAY)  6,6,5                                  0  118
 5         RHO=CON/4.E22                                     0  119
           PDISO3=1.E-3*EXP(-RHO/2.E-5)                      0  120
 6         CONTINUE                                          0  121
           RETURN                                            0  122
           END                                               0  123-
```

```
      SUBROUTINE PLOTPK (START,END,NPROB)
      COMMON PSKL,XSKL,IXN,IPX
      COMMON /PLTS/ XPLOTS(7,54),NPPL(54),IPL,NO(7)
      COMMON /SWR/ SWTCH(90)
      DIMENSION X(900), P(900,7), PA(900,7), XA(900)
      DIMENSION XP(54)
      DIMENSION SPEC(54)
      DATA (SPEC(I),I=1,54)/5H    H,5H   LI,5H   BE,5H   MG,5H   AL,5H
     1 SI,5H   TI,5H   FE,5H   CU,5H    U,5H   OH,5H  LIO,5H  BEO,5H  MG
     20,5H  ALO,5H  SIO,5H  TIO,5H  FEO,5H  CUO,5H UOPL,5H NOPL,5H   NO,
     35H  NO2,5H  N2O,5H   CO,5H  CO2,5H   O3,5H  H2O,5H     ,5H   EL,5H
     4   N2,5H  N2A,5H  N2B,5H   NS,5H   NO,5H   NP,5H     ,5H   OP,5H
     5 OD,5H   OS,5H N2PL,5H O2PL,5H  NPL,5H  OPL,5HN2APL,5HN2BPL,5H
     6 ,5H     ,5H     ,5H   EN,5H   O2,5H  O2D,5H  O2B,5H O2SG/
C     NOTE THAT TIMES HAVE TO BE IN INCREASING ORDER
      CALL MAP (0.,10.,0.,10.,0.,1.,0.,1.)
      CALL PMODE (3)
      CALL PLOTS (150.,0,5)
      CALL ROTATE (90.)
      REWIND 4
      REWIND 1
      REWIND 8
      NXX=0
      INFL=4
      IF (SWTCH(59).NE.1HF) INFL=1
      IF (SWTCH(61).EQ.1HC) INFL=4
      IF (SWTCH(14).EQ.1HR.AND.SWTCH(15).NE.1HS) INFL=8
      N=NPPL(NPROB)
      GO TO 2
    1 INFL=8
      NXX=1
    2 CONTINUE
      DO 5 I=1,N
      DO 3 IJ=1,54
      IF (XPLOTS(I,NPROB).EQ.SPEC(IJ)) GO TO 4
    3 CONTINUE
    4 NO(I)=IJ
    5 CONTINUE
    6 J=1
    7 CONTINUE
      READ (INFL,30) X(J),(XP(K),K=1,54)
      IF (ENDFILE INFL) 10,8
    8 CONTINUE
      DO 9 I=1,N
      IX=NO(I)
      P(J,I)=XP(IX)
    9 CONTINUE
      IF (X(J).GT.END) GO TO 10
      IF (X(J).LT.START) GO TO 6
      J=J+1
      IF (J.LT.900) GO TO 7
   10 CONTINUE
      IF (SWTCH(61).NE.1HC) GO TO 16
   11 JA=1
   12 CONTINUE
      READ (1,30) XA(JA),(XP(K),K=1,54)
      IF (ENDFILE 1) 15,13
   13 CONTINUE
      DO 14 I=1,N
      IX=NO(I)
      PA(JA,I)=XP(IX)
   14 CONTINUE
      IF (XA(JA).GT.END) GO TO 15
      IF (XA(JA).LT.START) GO TO 11
      JA=JA+1
      IF (JA.LT.900) GO TO 12
   15 CONTINUE
   16 CONTINUE
      KATIME=JA-1
      KTIME=J-1
      PRINT 31, KTIME,KATIME
      PMAX=-5.
      XMAX=-5.
      PMIN=10.
      XMIN=10.
```

```
      DO 17 I=1,KTIME
      X(I)=ALOG10(X(I))
      XMAX=AMAX1(X(I),XMAX)
      XMIN=AMIN1(X(I),XMIN)
17    CONTINUE
      DO 19 I=1,KTIME
      DO 19 NT=1,N
      IF (P(I,NT).GT.0.) GO TO 18
      P(I,NT)=-1.23456789
      GO TO 19
18    P(I,NT)=ALOG10(P(I,NT))
      PMAX=AMAX1(P(I,NT),PMAX)
      PMIN=AMIN1(P(I,NT),PMIN)
      PMIN=AMAX1(1.0,PMIN)
19    CONTINUE
      IF (SWTCH(61).NE.1HO) GO TO 22
      DO 21 I=1,KATIME
      XA(I)=ALOG10(XA(I))
      DO 21 NT=1,N
      IF (PA(I,NT).GT.0.) GO TO 20
      PA(I,NT)=-1.23456789
      GO TO 21
20    PA(I,NT)=ALOG10(PA(I,NT))
21    CONTINUE
22    CONTINUE
      IF (NXX.EQ.1) GO TO 23
      IPX=PMAX+1.
      IXX=XMAX+1.
      IXN=XMIN-1.
      IPN=PMIN-1.
C     SCALE TO UNITS PER INCH
      PSKL=(IPX-IPN)/8.
      XSKL=(IXX-IXN)/8.
      IF (SWTCH(15).EQ.1HS) GO TO 1
23    CONTINUE
      CALL GRID (NPROB)
      NT=1
      IT=1
      I=1
24    XP=(X(I)-IXN)/XSKL+1.
      YP=(P(I,NT)-IPN)/PSKL+1.
      IF (I.GE.KTIME) GO TO 29
      I=I+1
      IF (YP.GT.9..OR.YP.LT.1.) GO TO 24
      CALL PLOT (XP,YP,3)
      CALL NUMBER (XP,YP,.1,IT,0.,2HI2)
      CALL PLOT (XP,YP,3)
      II=I-1
      DO 26 I=II,KTIME
      YP=(P(I,NT)-IPN)/PSKL+1.
      XP=(X(I)-IXN)/XSKL+1.
      IF (YP.GT.9..OR.YP.LT.1.) GO TO 26
      CALL PLOT (XP,YP,2)
      IF (MOD(I,175)) 26,25,26
25    CALL NUMBER (XP,YP,.1,IT,0.,2HI2)
      CALL PLOT (XP,YP,3)
26    CONTINUE
      IF (YP.GT.9..OR.YP.LT.1.) GO TO 27
      CALL NUMBER (XP-.25,YP,.1,IT,0.,2HI2)
27    IF (SWTCH(51).NE.1HO) GO TO 29
      DO 28 I=1,KATIME
      YP=(PA(I,NT)-IPN)/PSKL+1.
      XP=(XA(I)-IXN)/XSKL+1.
      IF (YP.GT.9..OR.YP.LT.1.) GO TO 28
      CALL SYMBOL (XP,YP,.12,NT,0.,-1)
28    CONTINUE
29    CONTINUE
      NT=NT+1
      IT=IT+1
      I=1
      IF (NT.LT.N+1) GO TO 24
      CALL PLOT (13.,0.,-3)
      IF (NPROB.LT.IPL) RETURN
      CALL SYMBOL (2.,2.,2.,3HOWG,0.,3)
      CALL PLOT (13.,0.,-3)
```

```
      C                                                         Q 151
             RETURN                                             Q 152
      C                                                         Q 153
      C                                                         Q 154
      30     FORMAT (E13.6,(6E13.6,/))                          Q 155
      31     FORMAT (1X,6HKTIME=,I5,9H  KATIME=,I5)             Q 156
             END                                                Q 157-
```

```
      SUBROUTINE GRID (NPROB)
      COMMON PSKL,XSKL,IXN,IPX
      COMMON /PLTS/ XPLOTS(7,54),NPPL(54),IPL,NO(7)
      COMMON /TITLE/ TITL(7)
      DIMENSION SPEC(54)
      DIMENSION SPEC2(1)
      DATA (SPEC(I),I=1,54)/5H     H,5H    LI,5H    BE,5H    MG,5H    AL,5H
     1 SI,5H    TI,5H    FE,5H    CU,5H     U,5H    OH,5H   LIO,5H   BEO,5H   MG
     20,5H   ALO,5H   SIO,5H   TIO,5H   FEO,5H   CUO,5H UOPL,5H NOPL,5H    NO,
     35H   NO2,5H   N2O,5H    CO,5H   CO2,5H    O3,5H   H2O,5H     ,5H    EL,5H
     4    N2,5H   N2A,5H   N2B,5H    NS,5H    NO,5H    NP,5H     ,5H    OP,5H
     5 OD,5H    OS,5H N2PL,5H O2PL,5H  NPL,5H  OPL,5HN2APL,5HN2BPL,5H
     6 ,5H     ,5H     ,5H    EN,5H    O2,5H   O2D,5H   O2B,5H O2SG/
      NP=NPPL(NPROB)
      IP=PSKL*8.
      IX=XSKL*8.
      CALL NUMBER (.80,.7,.21,10,0.,2HI2)
      CALL NUMBER (1.16,.81,.14,IXN,0.,2HI2)
      CALL PLOT (1.,1.,3)
      TIB1=8.0/IP
      TIB=8.0/IX
      DO 2 I=1,IX
      XX=I*8./IX+1.
      DO 1 LK=1,9
      PJ=ALOG10(LK+1.)
      DIST=1.+(I-1.+PJ)*TIB
      CALL PLOT (DIST,1.,2)
      CALL PLOT (DIST,1.1,2)
    1 CALL PLOT (DIST,1.,3)
      CALL NUMBER (XX-.2,.70,.21,10,0.,2HI2)
      CALL NUMBER (XX+.16,.81,.14,IXN+I,0.,2HI2)
    2 CALL PLOT (XX,1.,3)
      CALL PLOT (9.,9.,2)
      CALL PLOT (1.,9.,2)
      CALL NUMBER (.31,8.85,.21,10,0.,2HI2)
      CALL NUMBER (.67,9.09,.14,IPX,0.,2HI2)
      CALL PLOT (1.,9.,3)
      DO 4 II=1,IP
      I=IP-II
      YY=I*8./IP+1.
      DO 3 LK=1,9
      IK=10.-LK
      PJ=ALOG10(IK+1.)
      DIST=1.+(I+PJ)*TIB1
      CALL PLOT (1.,DIST,2)
      CALL PLOT (1.1,DIST,2)
    3 CALL PLOT (1.0,DIST,3)
      CALL PLOT (1.,YY,2)
      CALL NUMBER (.31,YY-.16,.21,10,0.,2HI2)
      CALL NUMBER (.67,YY+.09,.14,IPX-II,0.,2HI2)
    4 CALL PLOT (1.,YY,3)
      IXM=IX
      DO 5 I=1,IXM,2
      XX=(I*8.)/IX+1.
      CALL PLOT (XX,1.,3)
      CALL PLOT (XX,9.,2)
      IF (I+1.GE.IXM) GO TO 6
      XX=(I+1)*8./IX+1.
      CALL PLOT (XX,9.,3)
    5 CALL PLOT (XX,1.,2)
    6 IPM=IP
      DO 7 I=1,IPM,2
      YY=I*8./IP+1.
      CALL PLOT (9.,YY,3)
      CALL PLOT (1.,YY,2)
      IF (I+1.GE.IPM) GO TO 8
      YY=(I+1)*8./IP+1.
      CALL PLOT (1.,YY,3)
    7 CALL PLOT (9.,YY,2)
    8 CALL SYMBOL (2.5,9.2,.21,31HSPECIES NUMBER DENSITY VS. TIME,0.,31)
      CALL SYMBOL (.4,9.6,.21,TITL,0.0,50)
      CALL PLOT (1.,9.,3)
      DO 9 I=1,IX
      DO 9 LK=1,9
      PJ=ALOG10(LK+1.)
```

```
      DIST=1.+(I-1.+PJ)*TI8                                 R  76
      CALL PLOT (DIST,9.,3)                                 R  77
    9 CALL PLOT (DIST,8.9,2)                                R  78
      DO 10 II=1,IP                                         R  79
      I=IP-II                                               R  80
      DO 10 LK=1,9                                          R  81
      IK=10.-LK                                             R  82
      PJ=ALOG10(IK+1.)                                      R  83
      DIST=1.+(I+PJ)*TI81                                   R  84
      CALL PLOT (9.,DIST,3)                                 R  85
   10 CALL PLOT (8.9,DIST,2)                                R  86
      CALL SYMBOL (.22,3.1,.21,22HSPECIES NUMBER DENSITY,90.,22)  R  87
      CALL SYMBOL (3.5,.2,.21,10HTIME (SEC),0.,10)          R  88
      CALL PLOT (9.1,9.0,3)                                 R  89
      X=9.05                                                R  90
      Y=9.0                                                 R  91
      IF (PLOTNUM.EQ.2.) GO TO 12                           R  92
      DO 11 K=1,NP                                          R  93
      I=NO(K)                                               R  94
      CALL NUMBER (X,Y,.1,K,0.,2HI2)                        R  95
      CALL SYMBOL (X+.25,Y,.1,SPEC(I),0.,5)                 R  96
   11 Y=Y-.4                                                R  97
      GO TO 14                                              R  98
   12 Y=9.0                                                 R  99
      DO 13 I=1,11                                          R 100
      CALL NUMBER (X,Y,.1,I,0.,2HI2)                        R 101
      CALL SYMBOL (X+.25,Y,.1,SPEC2(I),0.,5)                R 102
   13 Y=Y-.4                                                R 103
   14 RETURN                                                R 104
      END                                                   R 105-
      NOLIST
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