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A COMPUTER PROGRAM FOR THE
KINETIC TREATMENT OF RADIATION-INDUCED
SIMULTANEOUS CHEMICAL REACTIONS

by

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1. ABSTRACT

WR16,* a program written in 3600-FORTRAN for a CDC-3600 digital computer, calculates, as a function of time, the concentrations of all the species taking part in the simultaneous first- and second-order chemical reactions occurring during and after exposure to ionizing radiation of any chemical system (for example, an aqueous solution). Homogeneous reaction kinetics is assumed for the computation. The variation of electrical conductivity and optical absorbance of the system can also be computed.

As data, the program requires the chemical reaction equations with rate constants, a list of the species involved with their radiation yields, rates of spontaneous formation (if any), initial concentrations, equivalent conductances and molar absorptivities, and the dose rate and duration of irradiation.

A simplified version of the program, adapted for an IBM-1620 computer system, is also included.

2. INTRODUCTION

The computer program presented in this report was developed to provide the radiation chemist with a tool to evaluate his experimental findings. Radiation chemistry experiments usually yield as results the amounts of one or several products formed, or the variation of some physical quantity (e.g., optical absorbance or electrical conductivity) during and/or after irradiation. In the latter case, irradiation is mostly applied in the form of short pulses ("pulse radiolysis").

A possible way to evaluate the results is to construct a model system including all the reactions known or assumed to be significant, using

*"WR" stands for "Water Radiolysis," the mathematical treatment of which necessitated the development of this program.

for rate constants, yields, etc., known values as far as available, and assumed or estimated values for the yet unknown quantities, and to compare the measured values with the corresponding quantities calculated for the model system.

Program WR16 makes it possible to set up, and investigate the properties of, such model systems of even considerable complexity in a simple way, since the chemical reaction equations themselves are entered as data, thus eliminating the necessity of setting up a new system of differential equations for every model. Apart from radiation chemistry, the program can be used for the treatment of other reaction-kinetic systems including radioactive decay schemes.

For users who have no access to a CDC-3600 computer but have available an IBM-1620 computer system, a somewhat less versatile version of this program, written in FORTRAN II-D for a system consisting of an IBM-1620 computer with a 40-k memory in connection with an IBM-1620 Monitor-II system,* is described in an appendix.

3. MATHEMATICAL METHOD

3.1 Setting Up Differential Equations

Let the chemical reaction scheme consist of n_r reactions of the following type:

where the species A_{mi} , $m = 1, \dots, 6$, need not all be different from each other, and where there may be less than four species on the right side of the equation, and k_i is the second-order rate constant for the reaction of A_{1i} with A_{2i} . Let, furthermore, $A'_1, A'_2, \dots, A'_{n_c}$ denote all the species involved in the reaction scheme. Then the following set of differential equations can be derived:

$$\frac{dc_j}{dt} = \frac{1}{100 N_a} G_j I + s'_j + \sum_{i=1}^{n_r} \alpha_{ji} k_i c'_{1i} c'_{2i}; \quad j = 1, \dots, n_c,$$

where c_j is the concentration of A'_j , c'_{mi} that of A_{mi} , N_a is Avogadro's number ($N_a = 6.0231 \times 10^{23}$), G_j is the radiation yield in particles per 100 eV, I is the dose rate in eV/l-sec, s'_j is the rate of spontaneous formation (e.g., in the case of H^+_{aq} and OH^-_{aq}), and the α_{ji} are integral constants.

*If only a Monitor-I system is available, a 60-k memory is required.

The program compares the species (Holerith words) A_{mi} with the A_j^i and calculates the matrix (α_{ji}) as follows.

$$\alpha_{ji} = -\delta_j^{1i} - \delta_j^{2i} + \delta_j^{3i} + \sum_{m=4}^6 \sigma_{mi} \delta_j^{mi}; \quad j = 1, \dots, n_c; \quad i = 1, \dots, n_r,$$

where σ_{mi} is the sign* of A_{mi} , and

$$\delta_j^{mi} = \begin{cases} 1 & \text{if } A_j^i = A_{mi} \\ 0 & \text{if } A_j^i \neq A_{mi} \end{cases}$$

3.2 Solving Differential Equations

The following abbreviations will be used:

$$\dot{c}_j = \frac{dc_j}{dt}; \quad g_j = \frac{1}{100 N_a} G_j I + s_j; \quad a_{ji} = \alpha_{ji} k_i;$$

$$f_j(\underline{c}) = f_j(c_1, c_2, \dots, c_{n_c}) = g_j + \sum_i a_{ji} c_i^1 c_i^1.$$

Thus, for the differential equations

$$\dot{c}_j = f_j(\underline{c}); \quad j = 1, \dots, n_c,$$

we have to find solutions $c_j(t)$ with $c_j(0) = \gamma_j$. This is accomplished by the program by applying a modification of Adam's extrapolation method.¹

If $t_1, t_2, \dots, t_n$ are equidistant points on the time axis with the increment τ , then approximate solutions $c_j^{(p)}(t)$ are computed as follows:

$$c_j^{(p)}(t_{n+1}) = c_j^{(p)} + \tau \sum_{m=1}^p \beta_{pm} f_j[c^{(p)}(t_{n-m+1})],$$

where p denotes the order of approximation and the β_{pm} are the constants listed in Table 1. For all t_n with $n \geq 5$, $p = 5$ is used; for $n < 5$, $p = n$. The time increments are determined automatically by the program (see Sect. 3.3).

If the dose rate is not constant, the total time range can be divided into n_t time intervals ($T_{k-1} \leq t < T_k$) with different values for I . In each time interval, the calculation restarts with $n = 1$. In the first time interval $t_1 = 0$ and $c_j^{(p)}(t_1) = \gamma_j$.

*The signs are usually plus (+), but in special cases (see Sect. 6.1.2) minus (-) signs may be formally used.

TABLE I. Values of β_{pm}

p	m				
	1	2	3	4	5
1	1				
2	$\frac{3}{2}$	$-\frac{1}{2}$			
3	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$		
4	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$	
5	$\frac{1901}{720}$	$-\frac{2774}{720}$	$\frac{2616}{720}$	$-\frac{1274}{720}$	$\frac{251}{720}$

3.3 Automatic Determination of Time Increments--Accuracy

Since the concentrations of the species involved in chemical reactions and the rate constants of such reactions may vary within a range of many orders of magnitude, it was desirable to find a suitable quantity from which to determine the time increments τ . Such a quantity can be found by the following considerations.

In Adam's extrapolation formula¹ the error term is

$$|\Delta \epsilon_j| \leq b_p \tau^{p+1} \left| \frac{d^p f_j(\underline{c})}{dt^p} \right|$$

where $\Delta \epsilon_j$ is the error increment of c_j for one step τ (error propagation not included), $b_p \leq 1/2$ for $p \leq 5$. At the same time, the increment of c_j is approximately

$$\Delta c_j \approx \tau f_j(\underline{c}).$$

Thus

$$\left| \frac{\Delta \epsilon_j}{\Delta c_j} \right| \leq b_p \tau^p \left| \frac{d^{p+1} c_j / dt^p}{f_j(\underline{c})} \right| = b_p \tau^p \left| \frac{d^{p+1} c_j / dt^p}{dc_j / dt} \right|$$

Therefore, the quantity

$$R_j^{(p)}(t) = \frac{1}{2} \tau^p \left| \frac{d^{p+1} c_j / dt^p}{dc_j / dt} \right|$$

can be regarded as a suitable measure for the accuracy of computation at a given time t . Now, for a differential equation of the form

$$\dot{c}_j = E_j - F_j c_j$$

it can easily be shown that

$$R_j^{(p)} = \frac{1}{2} F_j^p \tau^p = \frac{1}{2} \left(\frac{\tau}{T_j} \right)^p,$$

since $T_j = 1/F_j$ is the lifetime of the j -th species in this case, i.e., the accuracy depends on the ratio of time increment and lifetime. The actual differential equation

$$\dot{c}_j = f_j(\underline{c})$$

can be approximated within a small domain around any point $c^* = (c_1^*, \dots, c_n^*)$ by

$$\begin{aligned} \dot{c}_j &= f_j(\underline{c}^*) + \sum_{k=1}^{n_c} \frac{\partial f_j}{\partial c_k} (c_k - c_k^*) \\ &= \left\{ f_j(c^*) + \sum_{k=j} \frac{\partial f_j}{\partial c_k} (c_k - c_k^*) - \frac{\partial f_j}{\partial c_j} c_k^* \right\} + \frac{\partial f_j}{\partial c_j} c_j. \end{aligned}$$

If A_j is the species with the shortest lifetime, then in practically all cases the term in braces will be sufficiently constant and thus represent E . Since $\partial f_j / \partial c_j < 0$, we obtain the (time-dependent) "lifetime"

$$T_j = 1/F_j = -1/(\partial f_j / \partial c_j).$$

According to these considerations, the program determines the required time increment τ_r as follows.

$$\frac{\partial f_j}{\partial c_j} = \sum_{i=1}^{n_r} \alpha_{ji} k_i (c_{1i} \delta_j^{2i} + c_{2i} \delta_j^{1i}); \quad \tau_r = q / \max_j (|\partial f_j / \partial c_j|)$$

where q is an empirical "accuracy factor" which may be entered with the data. If no value is entered, the program will use $q = 0.05$, which value is appropriate in practically all cases.

After every 20 time increments the actual value of τ is compared with τ_r . If $\tau > 1.4 \tau_r$, it is decreased by a factor of 2; if $\tau < 0.7 \tau_r$, it is increased by the same factor.

Whenever τ has been decreased, the calculation restarts with $n = 1$ (i.e., $p = 1$), since the method used requires equidistant time values.

Fig. 1. "Link" Routine after Doubling of Time Increments

When τ has been increased, some of the previous points are skipped during the first 4 cycles ("link routine") so that only equidistant points enter the calculation. This is illustrated in Fig. 1.

For the first 20 cycles, the program uses as time increment a value $\tau_{\min}$ which may be entered with the data. Otherwise a suitable trial value is chosen by the program (see Sect. 5.1). $\tau_{\min}$ is the lower limit for τ . An upper limit $\tau_{\max}$ may also be predetermined.

Although the described procedure for the determination of τ is far from exact in the mathematical sense, it has proven quite satisfactory for a variety of widely different schemes of chemical reactions. In practice, an accuracy factor of 0.05 or even 0.1 is sufficient in many cases to yield values with all four printed digits exact. In general, the results are very accurate up to a certain size of the time increments, but a slight further increase will cause divergence, and therefore completely and obviously erroneous results. This observed behavior is consistent with the error-determining factor $(\tau/T)P$.

3.4 Options: Quasiequilibrium between Fast-reacting Species

3.4.1 Principle of the Method

In many reaction-kinetic systems, the fast-reacting species will soon reach a quasisteady state, i.e., in spite of high rates of formation and decay, the net rate of change of their concentrations will be very small and of the same order of magnitude as that of the slowly reacting species. Since the required time increments are determined by the rate of decay of the fastest-reacting species, the total (model) time range for the calculation will be very large compared to the time increments used, so that such calculations would require long computing times (often considerably more than the usual time limit of 10 min). For such cases, two options have been added to the program which allow treatment of the quasiequilibrium of the fast-reacting species separately. One option was especially designed for the equilibria of ionic species, whereas the other is of more general applicability. The common principle of both options is the following.

Let $\underline{c}^n = (c_1^n, c_2^n, \dots, c_{nn}^n)$ denote the concentrations of the species treated normally and $\underline{c}^e = (c_1^e, c_2^e, \dots, c_{ne}^e)$ those of the species treated by the equilibrium routine. Then we can set up the equation system

$$\begin{aligned} \dot{c}_j^n &= f_j(\underline{c}^n, \underline{c}^e), \quad j = 1, \dots, n_n \\ c_k^e &= \phi_k(\underline{c}^n), \quad k = 1, \dots, n_e, \end{aligned} \quad (n_n + n_e = n_c)$$

where the functions ϕ_k are derived from the steady-state conditions applied in either or both of the options. Let c^{n*} and c^{e*} be the concentrations at a time t^* . If τ_e is a time increment, approximate solutions $\tilde{c}_j$ for the time $t^* + \tau_e$ can be obtained by solving the set of equations

$$\dot{\tilde{c}}_j^n = f_j(\tilde{\underline{c}}^n, \underline{c}^{e*}) \text{ with } \tilde{c}_j^n(t^*) = c_j^n(t^*)$$

for the interval $t^* \leq t \leq t^* + \tau_e$ in the way described in Sects. 3.2 and 3.3, and then "adjusting" the concentrations c_k^e by means of the equations

$$c_k^e(t^* + \tau_e) = \phi_k[c^n(t^* + \tau_e)].$$

This procedure is repeated after every 20 time increments τ , i.e., $\tau_e = 20 \tau$. For the error introduced by this method one can derive the equation

$$\frac{\Delta \epsilon_j^e}{\tau_j} \approx - \tau_e \sum_{k,m} \frac{\partial f_j}{\partial c_k^e} \frac{\partial \phi_k}{\partial c_m^n} f_m,$$

where $\Delta \epsilon_j^e$ is the error increment for the concentration c_j^n per time increment τ_e (not including error propagation and the error produced by the normal routine).

This equation shows that the error at any given time is approximately proportional to the time increment τ_e . It can be used to check the feasibility of using one of the equilibrium options, especially since normally most of the terms of the sum are zero. Usually the trial method consisting of two runs with different time increments is more practical.

3.4.2 Ionic-equilibrium Routine

The calculations in this routine are based on a set of equilibrium equations of the type

where $i = 1, \dots, n_{eq}$ is a numbering index, K_{1i} and K_{2i} are the dissociation constants

$$K_{1i} = \frac{[H^+][HA_i^-]}{[H_2A_i]}; \quad K_{2i} = \frac{[H^+][A_i^-]}{[HA_i^-]}$$

The equilibrium equations with their dissociation constants are entered with the data in the form shown in Fig. 2. They are read in by a special subroutine (EQUIL1). The calculation is performed by another subroutine (EQUIL2). One can easily derive the equations

$$\left. \begin{aligned} [H_2A_i] &= \frac{C_{Ti}}{1 + \frac{K_{1i}}{[H^+]*} + \frac{K_{1i}K_{2i}}{[H^+]^2}} \\ [HA_i^-] &= K_{1i}[H_2A_i]/[H^+]* \\ [A_i^-] &= K_{2i}[HA_i^-]/[H^+]* \end{aligned} \right\} \quad i = 1, \dots, n_{eq}$$

$$[H^+] = [H^+]* + \sum_i (2[A_i^-] + [HA_i^-]) - \sum_k Q_k c_k^*$$

The term $\sum_k Q_k c_k^*$ represents the sum of the concentrations of all species except the HA_i^- and A_i^- , multiplied by their charges.

	1	2	3	4	5	6	7	8
	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
a	1127	1						
b	1 2 RAD1 H+	+ + RAD2 OH-	= = ATOM H2O	+ + (BLANK)	+ + (BLANK)	ION1 + ION2		2.000E+08 1.430E+11
c	1 2 3 4	RAD1 H+ ION1 MOLEC	1.55 3.605 5.0		1.439E-03 (BLANK)	1.003E-07 2.521E-05	349.82 55.6	2.565E+02
d	1 2 3		4.000E-06 1.000E-05 2.500E-02	1.200E+25	H+ OH- (BLANK)	2.000E-07 0.500E-07	0.500E-07	2 4 7 11 13 1
e	5.000E-03	150	2.000E-06	5.000E-09	1.000E-06	2.000E-04	1	
f	1 2 3	H+ H+ H+	* * *	OH- ION2 ION1	= = H2O ION1 ACIDX (BLANK)	* * *	1.833E-16 1.050E-07 3.225E-10	
	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
	1	2	3	4	5	6	7	8

Fig. 2. Format of Input Data. The data shown represent no actual calculation and are only correct in regard to format.

The concentrations marked by asterisks (*) are the values obtained by the computer at the time $t^* + \tau_e$ before the new equilibrium is calculated, and

$$C_{Ti} = [A_i^-]* + [HA_i^-]* + [H_2A_i]*$$

denotes the total amount of the acid H_2A_i regardless of its state of dissociation. C_{Ti} is one of the "species" named c_j^n in Sect. 3.4.1.

If only one state of dissociation exists, K_{2i} is set equal to zero.

The new equilibrium is now computed by using these equations in a fast-converging iteration procedure which consists in solving an equation of the form

$$[H^+] = F([H^+])$$

by calculating the sequence

$$x_0 = [H^+]^*$$

.....

$$x_{3n+1} = F(x_{3n})$$

$$x_{3n+2} = F(x_{3n+1})$$

$$x_{3(n+1)} = \frac{x_{3n+1}^2 - x_{3n} x_{3n+2}}{2 x_{3n+1} - x_{3n} - x_{3n+2}}$$

.....

$$[H^+] = \lim_{n \rightarrow \infty} x_{3n}.$$

It can be shown that this sequence is convergent if the expression

$$\frac{F'(x)F''(x)}{F'(x) - 1}$$

is bounded in a region around the point $x = [H^+]^*$ and if this point lies close enough to the correct value of $[H^+]$. This condition, however, is always fulfilled for our particular function $F(x)$ if the time increments are small enough.

It is also possible with this option to calculate equilibria of the form

In this case, the dissociation constants must be defined as

$$K'_{1i} = \frac{[\text{OH}^-][\text{B}_i\text{OH}^+]}{[\text{B}_i(\text{OH})_2]}; \quad K'_{2i} = \frac{[\text{OH}^-][\text{B}_i^{++}]}{[\text{B}_i\text{OH}^+]}$$

However, it is not possible to treat both types of equilibrium in the same run.

3.4.3 Steady-state Routine

The second option is independent of the nature of the particular species, and therefore more versatile and more convenient to use. It is, however, less economical in regard to computer time. The calculations are performed in a subroutine called EQUIL3, by means of the following procedure.

For a species A_j which has reached a quasisteady state, we have the equation

$$\frac{dc_j}{dt} = g_j + \sum_i \alpha_{ji} c'_{i1} c'_{i2} = 0.$$

This is a quadratic equation of the form

$$A_0 + A_1 c_j + A_2 c_j^2 = 0.$$

For the coefficients, one can obtain the expressions

$$A_0 = g_j + \sum_i \delta_j^{1i} \delta_j^{2i} c'_{i1} c'_{i2} \alpha_{ji};$$

$$A_1 = \sum_i \left(\delta_j^{1i} \delta_j^{2i} c'_{i2} + \delta_j^{1i} \delta_j^{2i} c'_{i1} \right) \alpha_{ji};$$

$$A_2 = \sum_i \delta_j^{1i} \delta_j^{2i} \alpha_{ji},$$

where $\delta_j^{ik} = 1 - \delta_j^{jk}$. The other denotations are the same as in Sect. 3.1. From the three coefficients the computer calculates

$$c_j = \begin{cases} -A_0/A_1 & \text{for } A_2 = 0 \\ \left(-A_1 - \sqrt{A_1^2 - 4A_0A_2} \right) / 2A_2 & \text{for } A_2 \neq 0. \end{cases}$$

If more than one species is to be processed by the Steady-state Routine, the program goes through the described procedure for each species separately, regarding the concentrations of the other species as constant. The entire sequence is repeated in an iteration procedure until all values remain sufficiently constant. No attempt was made to establish convergence conditions for this sequence, but as yet no case of divergence has been encountered.

4. OTHER OPTIONS OF THE PROGRAM

4.1 Skipping of Species

It occurs very often that the concentrations of one or more species drop to negligible values after some time, so that they have no more influence on the kinetic system. In this and other cases it is possible to "skip" this species starting in a desired time interval, i.e., to take it out of the calculation routine and assign to it a fixed concentration (for example 0) which will then be used for all further calculations. The skipping routine is also useful for species with large and practically constant concentrations, such as H_2O or dummy species with the concentration 1 (see Sect. 6.1.1).

The skipping option must be used furthermore for the species processed by the Ionic Equilibrium Routine as far as their concentrations are in a steady state (normally H^+ and OH^-), and all the species treated by the Steady-state Routine (see the example in Sect. 6.4.3). The concentrations of skipped species are in this case periodically adjusted by the equilibrium routines, but not effected by the main program.

A skipping instruction cannot be canceled. It stays in effect through all succeeding time intervals.

4.2 Skipping of Reactions

It is also possible to "skip" reactions in a way similar to the skipping of species, if, for example, a reaction becomes insignificant after some (model) time. A skipped reaction will be disregarded in the calculation process. This skipping instruction also cannot be revoked.

Even if all the species involved in a particular reaction have been skipped, it is still advisable to skip the reaction too in order to reduce computing time. The results will of course not be affected by the latter instruction.

4.3 "Freezing" of Time Increments

In some cases, for example if a chemical solution is irradiated continuously at a constant dose rate, the automatic time-increment routine may cause the time increments to decrease after some maximum has been reached. This decrease is often unnecessary from the standpoint of accuracy, since all concentrations are close to a steady state or are increasing at a linear rate. In such cases it is possible to "freeze" the time increments in the last time interval. They can then only increase but not decrease.

5. INPUT AND OUTPUT

5.1 General Requirements and Format of Input

Figure 2 shows the format of all the input data described in this paragraph. The required data are

- (a) A number (up to 4 digits) assigned to the particular run and a punch control digit. If this digit is different from zero, the results will be punched on cards (additionally to the printed output) for use with a plotting program.
- (b) A list of chemical reactions with their second-order rate constants in liter mole⁻¹ sec⁻¹. In case of reactions of the type $A + A \rightarrow B + \dots$, which contribute to the differential equation for the species A a term $-2kA^2$, the value k , not $2k$, must be entered. There must be two species on the left side of each equation, and there may be up to four species on the right side. Minus signs on the right side will be arithmetically treated as such; a minus sign on the left side will be treated as plus. No numerical factors are allowed; e.g., instead of "2 H₂O" one has to enter "H₂O + H₂O." Up to 30 reactions are allowed. The end of the list must be indicated by a blank card. A card with zero as rate constant will be treated as blank.
- (c) A list of species with G-values in particles per 100 eV, rates of spontaneous formation in moles liter⁻¹ sec⁻¹, equivalent conductances in mho cm² gram-equivalent⁻¹, and molar absorptivities in liter cm⁻¹ mole⁻¹. As species, any Holerith word with up to 5 characters, but with no leading blanks, may be used. Plus and minus signs in this Holerith word, except such in the place of the first character, are counted by a special subroutine ("SCAN") for determining the charge of the species.

In columns 7 and 8 a value for the charge other than zero may be entered, which will then override the value determined by the subroutine.

All of the species on the left side of the reaction equations must be included in the list, those on the right side only if their concentrations are to be calculated. The species may be numbered in columns 1-5

for convenience; these numbers will be ignored. The maximum number of species is 27. The end of the list must be indicated by a blank card.

(d) A list of time intervals with dose rates and instructions concerning the application of the equilibrium and skipping routines. Characters in columns 1-5 are again ignored so that these columns can be used for numbering. The values in columns 11-20 denote the end of each time interval (in sec); columns 21-30 contain the dose rates in $\text{eV liter}^{-1} \text{sec}^{-1}$. In columns 31-35 and 36-40, respectively, the Holerith names of two species to be skipped may be listed. For each of these species, a concentration value must be assigned and punched in columns 41-50 or 51-60, respectively, except if subroutine EQUIL3 is called in this time interval. Up to 5 reactions to be skipped may be listed in columns 61-63, 64-66, 67-69, 70-72, and 73-75, respectively, by the numbers of their position in the list of reactions.

Column 80 is used for instructions regarding the use of the equilibrium routines with the following code.

- 0 or blank: equilibrium routines not used
- 1: EQUIL2 (ionic equilibrium) is used
- 2: EQUIL3 (steady state) is used
- 3: both routines are used

The instruction to call either or both of the routines cannot be revoked in succeeding time intervals.

If the digit 2 or 3 is punched in column 80, any values in columns 41 through 60 are ignored. Species marked for skipping on such a card are in this case automatically treated by the Steady-state Subroutine (EQUIL3), and they will be assigned the value which they had at the end of the preceding time interval. Likewise, reactions which are marked for skipping on such cards will only be skipped in the main routine, but not in subroutine EQUIL3, whereas reactions marked for skipping on cards with a 1, 0, or blank in column 80 will be disregarded in the entire process of calculation.

(e) A single card which lists the accuracy factor q (see Sect. 3.3), the number n_p of cycles (time increments) between consecutive printouts of results, the minimum print interval $\Delta t_{p,\min}$ (which is the minimum time distance in sec between two printouts), the minimum time increment $\tau_{\min}$ in sec, the maximum time increment $\tau_{\max}$ in such time intervals where no equilibrium routine is used, the maximum time increment $\tau_{\max,\text{eq}}$ in such time intervals where at least one of the routines is used, and a "time increment freeze index" i_t . If the latter is different from zero, the time increments will be "frozen" during the last time interval.

If the said card is blank, the following values will be assumed by the computer:

$$\begin{aligned} q &= 0.05; \\ n_p &= 250; \\ \Delta t_{p,\min} &= 0; \\ \tau_{\min} &= T_{nt1}/10^6; \\ \tau_{\max} &= T_{nt1}/200; \\ \tau_{\max,eq} &= T_{nt}/10000; \\ i_t &= 0. \end{aligned}$$

Here T_{nt} is the end of the last time interval and T_{nt1} the end of the last time interval for which no equilibrium routine is used. Any values other than zero punched into this card will override the corresponding values given above. Of the two values $\Delta t_{p,\min}$ and n_p , the one resulting in a larger print interval overrides the other one.

(f) A list of equilibrium equations, followed by a blank card. If the Ionic Equilibrium Routine is not used, this list, but not the blank card, is omitted. The equilibrium equations must be entered in the sequence shown in Sect. 3.4.2, i.e., the second stage of dissociation must succeed the first one. If this sequence is reversed, an error message will be printed out. If there is no second dissociation stage, the corresponding equation must be omitted. No blank cards are allowed between equations. Figure 2 shows the required form of the equations. Dissociation constants must be given as defined in Sect. 3.4.2. There may be up to 10 pairs of equilibrium equations ($n_{eq} \leq 10$).

Any number of runs [complete sets of data as described under (a) through (f)] may be stacked in one computing sequence.

5.2 Output

Figure 3 shows an example of the printed output normally obtained. This figure is essentially self-explanatory.* The meaning of the abbreviations can be found in Sect. 7. The concentrations are printed out in groups of 6. Conductivity change, absorbance change, and time increment are printed in the same table after the concentrations. The maximum number of printed lines per group is 250. If this number is reached, the run will be terminated.

*In some cases, rows of asterisks are printed instead of the value 0. This does not affect the calculations.

Fig. 4. Calculation of the β Emission of Radon and Its Decay Products

RUN NUMBER 95

02/24/68

RN	+	DUMMY	=	RAA
RAA	+	DUMMY	=	RAB
RAA	+	DUMMY	=	AT
RAB	+	DUMMY	=	RAC
AT	+	DUMMY	=	RAC
RAC	+	DUMMY	=	RAC**
RAC**	+	DUMMY	=	RAD
RAC	+	DUMMY	=	RAD

K(1)	=	2.10-006
K(2)	=	3.78-004
K(3)	=	2.70-006
K(4)	=	4.31-004
K(5)	=	4.62-001
K(6)	=	4.75-003
K(7)	=	8.75-003
K(8)	=	1.11-003

NO	CHARGE	NAME	G	S	CI	EQCO	EXT
1	0	RN	-0.000	*****	1.000+000	-0.000	-0.000+000
2	0	RAA	-0.000	*****	*****	-0.000	2.700-000
3	0	RAB	-0.000	*****	*****	-0.000	4.311-004
4	0	AT	-0.000	*****	*****	-0.000	-0.000+000
5	0	RAC	-0.000	*****	*****	-0.000	1.114-003
6	0	RAC**	-0.000	*****	*****	-0.000	8.751-003
7	0	RAD	-0.000	*****	*****	-0.000	1.133-008
8	0	DUMMY	-0.000	*****	1.000+000	-0.000	-0.000+000

INITIAL CONDUCTIVITY = 0.000+000 MHO/CM
INITIAL ABSORBANCE = 0.000+000 /CM

NO	TIME	DOS- RATE	SPECIES	CSK1	CSK2	REACTIONS
	SEC	EV/L-SEC	SKIPPED	MOLES/L	MOLES/L	SKIPPED
1.	1.00+001	*****	DUMMY	1.000+000	*****	
2	2.00+001	*****		*****	*****	
3	5.00+001	*****		*****	*****	
4	1.00+002	*****		*****	*****	
5	1.50+002	*****		*****	*****	
6	2.00+002	*****		*****	*****	
7	3.00+002	*****		*****	*****	
8	5.00+002	*****		*****	*****	
9	7.00+002	*****		*****	*****	
10	1.00+003	*****		*****	*****	
11	1.00+004	*****		*****	*****	

```

ACCURACY FACTOR 2.00-001
VALUES PRINTED OUT EVERY -0 CYCLES
MINIMUM PRINT INTERVAL 4.000+002 SEC
MINIMUM TIME INCREMENT 1.000-002 SEC
MAXIMUM TIME INCREMENT 1.000+002 SEC
SAME IF EQUILIBRIUM IS
COMPUTED 1.000+000 SEC

```

TIME	RN	RAA	RAB	AT	RAC	RAC**
SECONDS	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L
0.000+000	1.000+000	-0.000+000	-0.000+000	-0.000+000	-0.000+000	-0.000+000
1.000+001	1.000+000	2.093+000	3.956+008	9.613+011	3.393+010	3.127+012
2.000+001	1.000+000	4.178+005	1.578+007	2.178+010	1.321+009	3.486+011
3.000+001	9.999+001	1.039+004	9.787+007	5.808+010	1.245+008	7.769+010
4.000+002	9.998+001	2.057+004	3.862+006	1.177+009	7.083+008	7.975+009
5.000+002	9.997+001	3.057+004	8.574+006	1.761+009	1.981+007	3.066+008
6.000+002	9.996+001	4.037+004	1.504+005	2.334+009	4.099+007	7.830+008
7.000+002	9.994+001	5.943+004	3.294+005	3.449+009	1.125+006	2.812+007
8.000+002	9.990+001	9.541+004	8.672+005	5.553+009	3.810+006	1.263+006
9.000+002	9.985+001	1.257+003	1.612+004	7.502+009	8.121+006	3.108+006
1.000+003	9.979+001	1.742+003	3.039+004	1.016+008	1.721+005	7.397+006
1.400+003	9.971+001	2.271+003	5.368+004	1.326+008	3.305+005	1.537+005
1.800+003	9.962+001	2.726+003	8.010+004	1.591+008	5.174+005	2.512+005
2.200+003	9.954+001	3.115+003	1.082+003	1.819+008	7.208+005	3.593+005
2.600+003	9.946+001	3.448+003	1.368+003	2.014+008	9.313+005	4.728+005
3.000+003	9.937+001	3.734+003	1.652+003	2.181+008	1.142+004	5.874+005
3.400+003	9.929+001	3.979+003	1.927+003	2.324+008	1.349+004	7.003+005
3.800+003	9.921+001	4.188+003	2.191+003	2.446+008	1.547+004	8.094+005
4.200+003	9.912+001	4.367+003	2.439+003	2.551+008	1.736+004	9.132+005
4.600+003	9.904+001	4.521+003	2.672+003	2.641+008	1.912+004	1.011+004
5.000+003	9.896+001	4.651+003	2.887+003	2.717+003	2.076+004	1.102+004
5.400+003	9.887+001	4.763+003	3.084+003	2.783+008	2.228+004	1.186+004
5.800+003	9.879+001	4.858+003	3.265+003	2.838+008	2.366+004	1.263+004
6.200+003	9.871+001	4.940+003	3.430+003	2.886+003	2.493+004	1.334+004
6.600+003	9.863+001	5.009+003	3.578+003	2.926+003	2.607+004	1.398+004
7.000+003	9.854+001	5.067+003	3.712+003	2.961+008	2.711+004	1.456+004
7.400+003	9.846+001	5.117+003	3.833+003	2.990+008	2.804+004	1.508+004
7.800+003	9.838+001	5.159+003	3.940+003	3.014+008	2.887+004	1.554+004
8.200+003	9.830+001	5.194+003	4.036+003	3.035+008	2.961+004	1.596+004
8.600+003	9.821+001	5.224+003	4.122+003	3.052+008	3.027+004	1.633+004
9.000+003	9.813+001	5.249+003	4.197+003	3.067+008	3.086+004	1.666+004
9.400+003	9.805+001	5.270+003	4.264+003	3.079+008	3.138+004	1.695+004
9.800+003	9.797+001	5.287+003	4.323+003	3.089+008	3.184+004	1.721+004
1.000+004	9.792+001	5.294+003	4.349+003	3.093+008	3.205+004	1.733+004

TIME	RAD	DUMMY	CONDC	ABSC	DT
SECONDS	MOLES/L	MOLES/L	MHO/CM	/CM	SEC
0.000+000	-0.000+000	1.000+000	0.000+000	0.000+000	1.000-002
1.000+001	8.069-013	1.000+000	0.000+000	7.386-011	0.200-001
2.000+001	9.864-012	1.000+000	0.000+000	1.826-010	0.200-001
5.000+001	2.781-010	1.000+000	0.000+000	7.230-010	0.200-001
1.000+002	3.848-009	1.000+000	0.000+000	2.369-009	0.200-001
1.500+002	1.869-008	1.000+000	0.000+000	5.010-009	0.200-001
2.000+002	5.796-008	1.000+000	0.000+000	8.715-009	0.200-001
3.000+002	2.851-007	1.000+000	0.000+000	1.952-008	0.200-001
5.000+002	2.032-006	1.000+000	0.000+000	5.525-008	0.200-001
7.000+002	7.031-006	1.000+000	0.000+000	1.022-007	0.200-001
1.000+003	2.460-005	1.000+000	0.000+000	2.195-007	0.200-001
1.400+003	7.487-005	1.000+000	0.000+000	4.089-007	0.200-001
1.800+003	1.141-004	1.000+000	0.000+000	8.001-007	0.200-001
2.200+003	2.883-003	1.000+000	0.000+000	8.695-007	0.200-001
2.600+003	4.807-004	1.000+000	0.000+000	1.116-006	0.200-001
3.000+003	7.224-004	1.000+000	0.000+000	1.363-006	0.200-001
3.400+003	9.334-004	1.000+000	0.000+000	1.605-006	0.200-001
3.800+003	1.322-003	1.000+000	0.000+000	1.836-006	0.200-001
4.200+003	1.697-003	1.000+000	0.000+000	2.056-006	0.200-001
4.600+003	2.115-003	1.000+000	0.000+000	2.262-006	0.200-001
5.000+003	2.574-003	1.000+000	0.000+000	2.453-006	0.200-001
5.400+003	3.071-003	1.000+000	0.000+000	2.629-006	0.200-001
5.800+003	3.602-003	1.000+000	0.000+000	2.790-006	0.200-001
6.200+003	4.165-003	1.000+000	0.000+000	2.937-006	0.200-001
6.600+003	4.757-003	1.000+000	0.000+000	3.070-006	0.200-001
7.000+003	5.375-003	1.000+000	0.000+000	3.190-006	0.200-001
7.400+003	6.017-003	1.000+000	0.000+000	3.298-006	0.200-001
7.800+003	6.680-003	1.000+000	0.000+000	3.395-006	0.200-001
8.200+003	7.362-003	1.000+000	0.000+000	3.481-006	0.200-001
8.600+003	8.061-003	1.000+000	0.000+000	3.558-006	0.200-001
9.000+003	8.775-003	1.000+000	0.000+000	3.626-006	0.200-001
9.400+003	9.502-003	1.000+000	0.000+000	3.686-006	0.200-001
9.800+003	1.024-002	1.000+000	0.000+000	3.739-006	0.200-001
1.000+004	1.061-002	1.000+000	0.000+000	3.763-006	0.200-001

The interval between successive printouts is determined by the values of n_p or $\Delta t_{p,\min}$. Furthermore, printouts are always given at $t = 0$ and $t = T_n (n = 1, \dots, n_t)$, i.e., for the time values punched in columns 11-20 of the cards in group d (Sect. 5.1 and Fig. 2).

If the punch index [see Sect. 5.1, (a)] is not zero, the results, but not the data, are also punched on cards for use with a plotting program.* Figure 4 shows an example of the punched output. The line 95*1 34 1.000+004 means: Run No. 95, Group No. 1, 34 lines of results per group, maximum time (T_{nt}) 10^4 sec. In the lines marked (MAX) and (MIN), the minimum and maximum value of each column is given.** The last card of each group is a blank card with a minus sign in the 80th column.

*A plotting program for use with an IBM-1620 (40k) computer, provided with an IBM-1627 plotter, may be obtained from the author.

**If the two values have the same sign, the value closer to 0 will be replaced by 0.

6. SUGGESTIONS FOR THE USE OF THE PROGRAM

6.1 Application of the Program in Some Special Cases

6.1.1 First-order Reactions

A first-order reaction of the type $A \rightarrow B + \dots$ with λ as the first-order rate constant (decay constant) can be entered in the form

"DUMMY" is a dummy species to which is assigned the concentration 1. In order to keep this concentration constant, the species DUMMY must be "skipped" (with CSK = 1).

6.1.2 Third- and Fourth-order, Pseudo Second-order Reactions

A reaction of the type $A + B + C + D \rightarrow E + F$ whose rate is determined by the concentrations of A and B only, can be entered in the form

with k as second-order rate constant.*

6.1.3 Labeling of Species

For some studies, for example if the contribution of one particular reaction to the yield of a certain product is to be determined, species can be "labeled" in a way analogous to the radioactive tracer method. Thus, in the reaction scheme

*An example for such a reaction is

This can be regarded as the net reaction of the sequence

in which the first reaction is rate-determining.

the relative contributions of the three different ways in which the product F is formed, can be studied by writing the reaction system as

It may be pointed out that all labeled and unlabeled species must appear in the list of species.

6.1.4 Photochemical Reactions

Under certain restrictions, photochemical reactions can be studied with the program in a way similar to reactions induced by ionizing radiations. One possibility is to replace G-values by quantum yields, and to enter the radiation intensity with the dimension "(quanta per 100 liters) per second." This application of the program is possible if the absorption of the effective wavelength by the irradiated substance does not change appreciably during the reaction.

6.1.5 Calculation of Other Linear Combinations of Concentrations

Instead of the optical absorbance, other linear combinations of concentrations,

$$L = \sum x_j c_j$$

can be calculated by entering the factors x_j in the EXT column. L is then obtained as $L_0 + \Delta L$, where L_0 is printed under INITIAL ABSORBANCE and ΔL appears in the ABSC column. With certain restrictions, the EQCO and CONDC columns may also be used for this purpose by entering the values (1000 x_j) under EQCO and assigning to all the species involved the charge $Q_j = +1$. In this case, subroutine EQUIL2 cannot be used. Furthermore,

the printout of the values (1000.xj), but not that of the results, may be incorrect due to the output format specification (F 10.3) for the EQCO column.

6.1.6 Reactions with More Than Four Products

Reactions of the type

can be entered as a combination of two reactions as follows:

The concentrations of A and B are not affected by the second reaction.

6.2 Special Error Messages and Countermeasures

A number of error messages are provided by the program and its subroutines:

(1) "ERROR IN EQUILIBRIUM EQUATIONS, RUN ABANDONED"

This message is printed if (a) the first species in all equilibrium equations is not the same or (b) if the equilibrium equation for the second stage of dissociation precedes the equation for the first stage. The program then proceeds to the next run.

(2) "DIVERGENCE IN EQUIL2, EQUILIBRIUM NOT COMPUTED, RUN ABANDONED"

This message appears if the iteration procedure for computing the equilibrium of ionic species has not sufficiently converged after 20 steps. This can only occur if the main program produces erroneous concentration values, e.g., if the time increments are too great. After printing this message, the program proceeds to the next run.

Possible remedies: Check data, especially time increments, for the main program. Check equilibrium equations for errors.

(3) "DIVERGENCE IN EQUIL3, RUN ABANDONED"

This message is printed if the iteration process in the Steady-state Routine has not sufficiently converged after 20 steps. The program then proceeds to the next run.

Possible remedies: Check data for errors. Check time increments; reduce them if feasible. Change sequence of the species treated in this subroutine in such a way that they are arranged in the order of decreasing rate of change. (The subroutine treats the species in the order in which they are listed in the list of species.)

(4) "LESS THAN 20 SEC LEFT, SEQUENCE TERMINATED"

If only 20 sec of the computing time assigned to the computing sequence are left, all the values calculated up to that point are printed out. The entire sequence is then terminated.

Possible remedies: Increase accuracy factor as far as possible. Use freezing option where applicable. Simplify reaction system. Use equilibrium routines as far as possible.

(5) "PRINT LIMIT REACHED, RUN TERMINATED"

If the limit of 250 lines of results per group is reached, these results are printed out. The program then proceeds to the next run.

Possible remedies: Increase minimum print interval ($\Delta t_{p,min}$) or number of cycles between printouts (n_p).

6.3 First Trial Run

If one wants to study a new reaction system, it is often difficult to make reliable quantitative estimates about the behavior of the system, which are necessary to determine parameters such as the maximum (model) time range, minimum time increments, etc., and the necessity and feasibility of using the equilibrium options. In such cases it has proven useful to start with a trial run without the equilibrium and freezing options, with a maximum time range (T_{nt}) that is large compared to the estimated reaction time, and with a parameter card e that is blank except for the minimum time increment τ_{min} . As τ_{min} one may choose $1/1000$ of the estimated lifetime of the (supposedly) fastest reacting species. For the other parameters to be entered on card e, the computer will then use the values listed in Sect. 5.1, (e). The computer time limit should be set at 10 min.

It is very likely that in this trial run one of the error messages listed in Sect. 6.2 will appear, but even so the results obtained will permit suitable adjustments of the data. Completely erroneous concentration values such as -4.718×10^{172} often indicate that the time increments are too large. This, however, is very unlikely with an accuracy factor of 0.05.

6.4 Examples of Computer Runs

In the following paragraphs, three computations carried out with program WR16 are presented for illustrative purposes. The data are shown

in the format in which they were printed out by the computer. They were entered in the format shown in Fig. 2. The data used in the third example are suitable as test data since they require all the main features of the program and subroutines.

6.4.1 Example 1: Pulse Radiolysis of Pure Degassed Water

In this example, the behavior of pure degassed water during and after irradiation with a 4- μ sec electron pulse from a 15-MeV linear accelerator was studied. All important chemical reactions presently known or supposed to take place between the radiation-produced intermediates and products have been taken into account.² As rate constants, yields, etc., experimental values were used in most cases; some values were estimated. An initial O_2 concentration of $10^{-6}M$ was assumed, since "degassed" water without special treatment still contains approximately this amount of oxygen. The dose-rate values assumed were those measured in an actual experiment; the nonrectangular pulse shape was taken into account by approximating it by a stair function. The equilibrium routines were not used, so that the value for $\Delta t_{max,eq}$ ("SAME IF EQUILIBRIUM IS COMPUTED") has no significance. The complete computer printout is shown in Fig. 3. The required computer time for this run was 43 sec.

6.4.2 Example 2: Decay Products of Radon

This computer run illustrated the possibility of studying first-order reactions. The columns EXT and ABSC were used to calculate the total β emission (in particles/sec per radon atom). In the branch RaC-RaC'-RaD, the very short-lived (1.5×10^{-5} sec) intermediate RaC' was omitted.

As an accuracy factor, the relatively large value of 0.2 was chosen, since mathematical considerations indicate that for first-order reactions larger time increments may be used for obtaining a given accuracy than for second-order reactions.

The printout for this run is shown in Fig. 4. The results are presented in the form in which they were punched out for plotting purposes. The required computer time was 4 min 16 sec. This time could have been considerably shortened by applying the Steady-state Routine EQUIL3 for the species At, the lifetime of which (1.5 sec) is very short compared to the overall time range.

6.4.3 Example 3: Removal of Traces of Oxygen from Hydrogen-saturated Water by Preirradiation with a Co^{60} Source

For this study essentially the same reaction scheme was assumed as in example 1. The printout of the data and results is shown in Fig. 5. Reactions 1, 4, 10, 12, 21, and 22 of example 1 (Run No. 92) were omitted as supposedly unimportant. Two new reactions (18 and 19 in Run No. 93),

Fig. 5. (Contd.)

TIME	E-	H+	OH-	OH	H	H2O2	H2	HO2	O2-	O2	H2O	DUMMY	CONDC	ABSC	DT			
SECONDS	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MOLES/L	MHO/CM	/CM	SEC			
0.000+000	-0.000+000	1.003-007	1.003-007	-0.000+000	-0.000+000	-0.000+000	1.000-003	-0.000+000	-0.000+000	1.000-006	5.490+001	1.000+000	0.000+000	0.000+000	1.000-008	0.000+000	0.000+000	0.000+000
2.900-005	4.566-012	1.003-007	1.003-007	3.496-012	3.354-012	1.685-012	1.000-003	3.156-014	2.323-012	1.000-006	5.490+001	1.000+000	8.128-012	0.000+000	4.000-008	0.000+000	0.000+000	0.000+000
5.900-005	6.963-012	1.003-007	1.003-007	4.459-012	7.380-012	3.428-012	1.000-003	7.743-014	9.136-012	1.000-006	5.490+001	1.000+000	1.313-011	0.000+000	4.000-008	0.000+000	0.000+000	0.000+000
8.900-005	8.165-012	1.003-007	1.003-007	4.709-012	1.021-011	5.172-012	1.000-003	1.200-013	1.906-011	1.000-006	5.490+001	1.000+000	1.672-011	0.000+000	4.000-008	0.000+000	0.000+000	0.000+000
1.000-004	8.435-012	1.003-007	1.003-007	4.743-012	1.095-011	5.811-012	1.000-003	1.343-013	2.322-011	1.000-006	5.490+001	1.000+000	1.785-011	0.000+000	4.000-008	0.000+000	0.000+000	0.000+000
5.000-004	9.372-012	1.004-007	1.002-007	4.796-012	1.429-011	2.907-011	1.000-003	4.186-013	2.085-010	9.998-007	5.490+001	1.000+000	2.930-011	0.000+000	2.560-006	0.000+000	0.000+000	0.000+000
1.000-003	9.373-012	1.005-007	1.001-007	4.796-012	1.429-011	5.817-011	1.000-003	8.953-013	4.454-010	9.996-007	5.490+001	1.000+000	6.387-011	0.000+000	5.120-006	0.000+000	0.000+000	0.000+000
1.000-002	9.386-012	1.027-007	9.796-008	4.798-012	1.432-011	5.885-010	1.000-003	9.638-012	4.694-009	9.953-007	5.490+001	1.000+000	7.202-010	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
2.558-001	9.598-012	1.523-007	6.603-008	4.878-012	1.531-011	3.188-008	1.000-003	2.623-010	8.629-008	8.965-007	5.490+001	1.000+000	1.790-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
5.048-001	9.736-012	1.664-007	6.046-008	5.041-012	1.669-011	9.380-008	9.999-004	3.523-010	1.059-007	8.280-007	5.490+001	1.000+000	2.318-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
7.538-001	9.886-012	1.680-007	5.987-008	5.227-012	1.832-011	1.624-007	9.999-004	3.632-010	1.081-007	7.682-007	5.490+001	1.000+000	2.380-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
1.003+000	1.005-011	1.676-007	6.001-008	5.418-012	2.020-011	2.303-007	9.998-004	3.606-010	1.076-007	7.098-007	5.490+001	1.000+000	2.365-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
1.252+000	1.024-011	1.668-007	6.028-008	5.611-012	2.239-011	2.963-007	9.998-004	3.556-010	1.066-007	6.517-007	5.490+001	1.000+000	2.337-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
1.501+000	1.044-011	1.659-007	6.061-008	5.807-012	2.496-011	3.602-007	9.997-004	3.495-010	1.053-007	5.937-007	5.490+001	1.000+000	2.302-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
1.750+000	1.067-011	1.649-007	6.100-008	6.007-012	2.802-011	4.220-007	9.996-004	3.425-010	1.039-007	5.358-007	5.490+001	1.000+000	2.262-003	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
1.999+000	1.092-011	1.636-007	6.147-008	6.212-012	3.174-011	4.817-007	9.996-004	3.342-010	1.021-007	4.781-007	5.490+001	1.000+000	2.214-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
2.248+000	1.120-011	1.621-007	6.204-008	6.423-012	3.635-011	5.391-007	9.995-004	3.244-010	1.001-007	4.206-007	5.490+001	1.000+000	2.157-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
2.497+000	1.151-011	1.603-007	6.275-008	6.643-012	4.221-011	5.944-007	9.995-004	3.126-010	9.752-008	3.633-007	5.490+001	1.000+000	2.088-003	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
2.746+000	1.186-011	1.560-007	6.366-008	6.873-012	4.991-011	6.475-007	9.994-004	2.981-010	9.433-008	3.063-007	5.490+001	1.000+000	2.002-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
2.995+000	1.225-011	1.551-007	6.485-008	7.115-012	6.046-011	6.983-007	9.993-004	2.799-010	9.023-008	2.499-007	5.490+001	1.000+000	1.893-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
3.244+000	1.270-011	1.513-007	6.649-008	7.375-012	7.585-011	7.470-007	9.993-004	2.564-010	8.477-008	1.941-007	5.490+001	1.000+000	1.751-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
3.493+000	1.320-011	1.460-007	6.888-008	7.660-012	1.005-010	7.937-007	9.992-004	2.252-010	7.713-008	1.396-007	5.490+001	1.000+000	1.557-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
3.742+000	1.377-011	1.384-007	7.268-008	7.984-012	1.467-010	8.388-007	9.991-004	1.818-010	6.569-008	8.697-008	5.490+001	1.000+000	1.279-008	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
3.991+000	1.441-011	1.263-007	7.966-008	8.399-012	2.699-010	8.834-007	9.990-004	1.176-010	4.657-008	3.851-008	5.490+001	1.000+000	8.496-003	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
4.240+000	1.505-011	1.044-007	9.635-008	9.906-012	1.905-009	9.279-007	9.989-004	1.673-011	8.016-009	2.196-009	5.490+001	1.000+000	1.252-003	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
4.489+000	1.586-011	1.003-007	1.003-007	1.223-011	4.831-009	8.715-007	9.989-004	4.439-014	2.213-011	6.181-017	5.490+001	1.000+000	7.811-013	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
4.738+000	1.685-011	1.003-007	1.003-007	1.187-011	4.830-009	8.051-007	9.988-004	4.337-014	2.162-011	5.850-017	5.490+001	1.000+000	9.539-013	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
4.987+000	1.789-011	1.003-007	1.003-007	1.153-011	4.829-009	7.427-007	9.987-004	4.245-014	2.116-011	5.602-017	5.490+001	1.000+000	1.149-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
5.236+000	1.900-011	1.003-007	1.003-007	1.121-011	4.828-009	6.840-007	9.987-004	4.161-014	2.074-011	5.383-017	5.490+001	1.000+000	1.367-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
5.486+000	2.017-011	1.003-007	1.003-007	1.089-011	4.827-009	6.290-007	9.986-004	4.085-014	2.036-011	5.188-017	5.490+001	1.000+000	1.607-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
5.735+000	2.141-011	1.003-007	1.003-007	1.058-011	4.826-009	5.775-007	9.986-004	4.017-014	2.002-011	5.016-017	5.490+001	1.000+000	1.869-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
5.984+000	2.271-011	1.003-007	1.003-007	1.028-011	4.825-009	5.294-007	9.985-004	3.956-014	1.972-011	4.864-017	5.490+001	1.000+000	2.152-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
6.233+000	2.407-011	1.003-007	1.003-007	9.995-012	4.823-009	4.845-007	9.985-004	3.901-014	1.944-011	4.729-017	5.490+001	1.000+000	2.456-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
6.482+000	2.550-011	1.003-007	1.003-007	9.717-012	4.822-009	4.429-007	9.984-004	3.851-014	1.920-011	4.609-017	5.490+001	1.000+000	2.779-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
6.731+000	2.697-011	1.003-007	1.003-007	9.448-012	4.820-009	4.043-007	9.984-004	3.807-014	1.898-011	4.504-017	5.490+001	1.000+000	3.119-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
6.980+000	2.849-011	1.003-007	1.003-007	9.189-012	4.818-009	3.687-007	9.983-004	3.768-014	1.878-011	4.412-017	5.490+001	1.000+000	3.475-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
7.229+000	3.005-011	1.003-007	1.003-007	8.939-012	4.817-009	3.359-007	9.983-004	3.733-014	1.861-011	4.331-017	5.490+001	1.000+000	3.844-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
7.478+000	3.164-011	1.003-007	1.003-007	8.699-012	4.815-009	3.059-007	9.983-004	3.702-014	1.845-011	4.260-017	5.490+001	1.000+000	4.223-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
7.727+000	3.324-011	1.003-007	1.003-007	8.469-012	4.813-009	2.785-007	9.982-004	3.675-014	1.832-011	4.199-017	5.490+001	1.000+000	4.608-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
7.976+000	3.485-011	1.003-007	1.003-007	8.250-012	4.811-009	2.536-007	9.982-004	3.652-014	1.820-011	4.145-017	5.490+001	1.000+000	4.996-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
8.225+000	3.643-011	1.003-007	1.003-007	8.042-012	4.809-009	2.311-007	9.982-004	3.631-014	1.810-011	4.099-017	5.490+001	1.000+000	5.382-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
8.474+000	3.799-011	1.003-007	1.003-007	7.847-012	4.807-009	2.109-007	9.982-004	3.613-014	1.801-011	4.059-017	5.490+001	1.000+000	5.763-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
8.723+000	3.950-011	1.003-007	1.003-007	7.663-012	4.806-009	1.928-007	9.982-004	3.598-014	1.793-011	4.025-017	5.490+001	1.000+000	6.134-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
8.972+000	4.095-011	1.003-007	1.003-007	7.493-012	4.804-009	1.767-007	9.981-004	3.585-014	1.787-011	3.996-017	5.490+001	1.000+000	6.491-012	0.000+000	3.277-004	0.000+000	0.000+000	0.000+000
9.221+000	4.233-011	1.003-007	1.003-007	7.335-012	4.802-009	1.624-007	9.981-004	3.573-014	1.781-011	3.97								

Fig. 5. Mathematical Model for the Deoxygenation of Water by Irradiation

RUN NUMBER 93

03/11/66

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E- + H+ = H
E- + H2O2 = OH- + H2
E- + H2O = H+ + OH-
H+ + OH- = H2O
H+ + H2 = H2O
OH + H2O2 = H2O + H
OH + H2O2 = H2O + HO2
E- + O2 = O2-
HO2 + DUMMY = H+ + O2-
H+ + O2- = H2O2
O2- + H2O2 = O2 + H+ - H+
H+ + H2O2 = H2O2 - H+

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```

KK( 1) = 2.20+010
KK( 2) = 2.50+010
KK( 3) = 1.20+010
KK( 4) = 1.50+001
KK( 5) = 1.43+011
KK( 6) = 1.00+010
KK( 7) = 2.50+010
KK( 8) = 4.50+007
KK( 9) = 4.50+007
KK(10) = 4.00+007
KK(11) = 2.00+010
KK(12) = 2.00+010
KK(13) = 2.50+006
KK(14) = 5.00+010
KK(15) = 2.70+006
KK(16) = 1.70+007
KK(17) = 1.50+007
KK(18) = 2.00+010
KK(19) = 2.00+010

```

NO	CHARGE	NAME	G	S	CI	EQCO	EXT
1	-1	E-	2.600	*****	*****	177.000	-0.000+000
2	-1	H+	3.620	1.439-003	1.003-007	349.820	-0.000+000
3	-1	OH-	1.000	1.439-003	1.003-007	197.600	-0.000+000
4	0	OH	2.600	*****	*****	-0.000	-0.000+000
5	0	H	0.500	*****	*****	-0.000	-0.000+000
6	0	H2O2	0.700	*****	*****	-0.000	-0.000+000
7	0	H2	0.450	*****	1.000-003	-0.000	-0.000+000
8	0	HO2	0.020	*****	*****	-0.000	-0.000+000
9	-1	O2-	-0.000	*****	*****	75.000	-0.000+000
10	0	O2	-0.000	*****	1.000-006	-0.000	-0.000+000
11	0	H2O	-0.000	*****	5.490+001	-0.000	-0.000+000
12	0	DUMMY	-0.000	*****	1.000+000	-0.000	-0.000+000

INITIAL CONDUCTIVITY = 5.491-008 MHO/CM
INITIAL ABSORBANCE = 0.000+000 /CM

NO	TIME	DOSE RATE	SPECIES	CSK1	CSK2	REACTIONS	I
	SEC	EV/L-SEC	SKIPPED	MOLES/L	MOLES/L	SKIPPED	EQ
1	1.00-004	5.00+018	DUMMY H2O	1.000+000	5.490+001	-0 -0 -0 -0 -0 0	0
2	5.00-004	5.00+018	H+ OH-	1.003-007	1.003-007	5 13 14 -0 -0 1	1
3	1.00-003	5.00+018	H OH	*****	*****	7 -0 -0 -0 -0 3	3
4	1.00-002	5.00+018	E-	*****	*****	1 2 4 -0 -0 3	3
5	1.00+001	5.00+018		*****	*****	-0 -0 -0 -0 -0 3	3

ACCURACY FACTOR 1.00-001
VALUES PRINTED OUT EVERY 750 CYCLES
MINIMUM PRINT INTERVAL -0.000+000 SEC
MINIMUM TIME INCREMENT 1.000-008 SEC
MAXIMUM TIME INCREMENT 5.000-007 SEC
SAME IF EQUILIBRIUM IS
COMPUTED 5.000-004 SEC

H+ * OH- = H2O * 1.832-016
H+ * O2- = HO2 * 5.000-005

which might have some influence on the rate of removal of oxygen, were added. An initial concentration of $10^{-3}M$ was assumed for H_2 . The supposed effect of such an H_2 concentration is the conversion of most of the oxidizing OH radicals into reducing H atoms via reaction 8. Although there is a net formation of oxygen in H_2 -free water, the addition of hydrogen effects a net decay by causing a considerable decrease in the rate of formation of oxygen via the reactions 9, 13, 15, 16, and 17, so that, as this calculation and also experiments³ show, traces of oxygen can be practically completely removed within a few seconds of irradiation.

For the first 10^{-4} sec none of the equilibrium routines were used, in order to give the charged species time to reach a quasisteady state. After that, the ionic equilibria as determined by the two equilibrium equations printed at the end of the data were computed. For this purpose, the fast-reacting species H^+ and OH^- had to be skipped. At the same time it was possible and desirable to skip reactions 5, 13, and 14 since these affected only the species adjusted by the equilibrium routine. The species H, E^- , and OH have reached a quasisteady state after about 5×10^{-4} sec. Therefore, the Steady-state Subroutine EQUIL3 could have been introduced at that time for adjusting these species, which implied skipping reactions 1, 2, 4, and 7. As already mentioned in Sect. 5.1, the latter instruction causes these reactions to be disregarded by the main program, but not by EQUIL3.

The reason why E^- was skipped after 10^{-3} rather than 5×10^{-4} sec is simply that skipping instructions for only 2 species can be given in each time interval; further, it was also desired to force printouts at 10^{-3} and 10^{-2} sec. The value 0.1 was chosen as an accuracy factor because this value had previously yielded results of good accuracy in most cases. Trial runs had shown that a minimum time increment of 10^{-8} sec was sufficiently small; this value is smaller by a factor of 4 than the one later chosen by the computer. The space reserved for T_{max} on data card e was left blank; the printed value is therefore that determined by the computer. For $T_{max,eq}$ a value smaller than usual was chosen since in this particular case a considerable increase in accuracy could be accomplished at the expense of a relatively small amount of additional computer time (more than half of the total computer time was needed for the first 10^{-3} sec of model time).

7. FORTRAN NOTATION

Table II includes the names of all variable and constant numbers and arrays used in the main program and/or subroutines except for those whose definition is evident from the source deck listings. Arrays are given without their dimensions.

TABLE II. FORTRAN Notation in WR16 and Subroutines

FORTRAN Name	Notation in Text	Explanation
A	A_{mi}	species (Holerith name) in reaction equations
AO, A1, A2	A_0, A_1, A_2	coefficients of quadratic equation
AAC		same as AC, rearranged
AAN		same as AN, rearranged
ABSC	ΔA	absorbance change
ABSI	A_0	initial absorbance
AC	A_j	species (Holerith name) in list of species
ACCFAC	q	accuracy factor
AE	$H^+, HA_i^-, \text{etc.}$	species (Holerith name) in equilibrium equations
AM	β_{pm}	coefficients of Adam's extrapolation formula
AN		Holerith headings
B		+ or - sign (Holerith)
BLANK		5 blank spaces (Holerith)
C	c_j	concentration
CC		same as C, rearranged
CCMAX		maximum concentration
CCMIN		minimum concentration
CH	Q_j	charge of species (TYPE REAL)
CHARGE	Q_j	same, TYPE INTEGER
CHEM		species (Holerith name) in SCAN subroutine
CI	γ_j	initial concentration
CONDC	$\Delta \kappa$	conductivity change
CONDI	κ_0	initial conductivity
CP		concentrations, rearranged for output
CSK		concentration assigned to skipped species
DCDT	$\dot{c}_j$	dc_j/dt

TABLE II (Contd.)

FORTTRAN Name	Notation in Text	Explanation
DELTA		accuracy limit for iteration procedure
DFDC	$\partial f_i / \partial c_j$	(see text)
DFDCAB		absolute value of DFDC
DFDCMA		maximum value of DFDCAB
DR	I	dose rate
DT	τ	time increment
DTMAX	$\tau_{\max}$	upper limit for time increments
DTMIN	$\tau_{\min}$	minimum time increment
DTMXEQ	$\tau_{\max,eq}$	maximum time increment if equilibrium routines are used
DTP		model time elapsed since last printout
DTPMIN	$\Delta t_{p,min}$	minimum interval between printed lines
DTREQ	τ_r	required time increment
EQ	K_1, K_2	equilibrium constants
EQ2	K_2	same for second stage of dissociation only
EQCO	Λ_j	equivalent conductance
EXT	ϵ_j	molar absorptivity
G	G_j	radiation yield
HPLUS	$[H^+], [OH^-]$	concentration of first species in equilib- rium equations
IDATE		date (Holerith)
IEQ		index controlling use of equilibrium routines
IFAIL		error index for equilibrium subroutines
IFR		"freeze" index
ILINK		index controlling "link" routine
IPUNCH		punch control index
ISHIFT		index controlling rearrangement of equilibrium equations
ISK		skip index for reactions

TABLE II (Contd.)

FORTTRAN Name	Notation in Text	Explanation
ISK3		same for reactions not to be disregarded by EQUIL3
ISKIP		similar to ISHIFT
JSK		skip index for species
JSK3		same for species processed by EQUIL3
KOEFF	α_{ji}	coefficients of differential equations
KOEFL	$-\delta_j^{li} - \delta_j^{zi}$	contribution to KOEFF by left side of reaction equation
LAND		octal representation of + or - sign extracted from CHEM
LCYCL	p	order of approximation in Adam's formula
LEQ		identifying number for species in EQUIL1 and EQUIL2
LT		count of lines printed
M1	li	identifying number for reacting species
M2	2i	similar to M1
MIN		octal representation of - sign at different places of 5-character Holerith word
MINLOG		index which equals 1 if SCAN finds - sign
MINUS		- sign (Holerith)
MEQ		index controlling use of equilibrium routines
NC	n_c	number of species
NEQ	n_{eq}	number of equilibrium equations
NORUN		number of run
NP	n_p	number of time increments between printed lines
NR	n_r	number of reactions
NRS		number of a reaction to be skipped
NT	n_t	number of time intervals

TABLE II (Contd.)

FORTTRAN Name	Notation in Text	Explanation
NTI	n_{ti}	number of time intervals in which equilibrium routines are not used
OCT		octal numbers 007700 ..., 00007700 ... etc.
P	p	order of approximation (maximum value of NCYCL)
PLU		octal representation of + sign at different places of 5-character Holerith word
PLULOG		index which equals 1 if SCAN finds + sign
RF	g_j	rate of formation (without decay)
RK	k_i	rate constant
S	s_j	rate of spontaneous formation
SLOPE	$\Delta c_j / \tau$	slope of line connecting successive points of $c_j(t)$
SPSK		species skipped
T	T_n	end of each time interval
TIME	t	model time
TLFT		real computing time left (in msec)
TOTAL	C_{Ti}	total amount of i-th acid (or base)
TT		model time (stored for output)
XMAX		same as CCMAX (rearranged)
XMIN		same as CCMIN (rearranged)

8. LISTING OF FORTRAN SOURCE DECKS

In the succeeding pages of this section, the FORTRAN source decks of the main program and all required subroutines are listed, with the exception of the ANL library subroutine TIMEF³ which makes available to the FORTRAN program the date (IDATE) and the computer time in milliseconds remaining in the current computing sequence (TIMELEFT).

The following subroutines are required for the main program WR16:

SCAN (Determines the charge of a species from the number of minus or plus signs in its Holerith notation)

STORE (stores model time and concentration values selected for output. Calculates and stores the change in conductivity ($\Delta\kappa$) and optical absorbance (ΔA) by means of the expressions

$$\Delta\kappa = -\kappa_0 + \left(\sum_j Q_j \Lambda_j c_j \right) / 1000;$$

$$\Delta A = -A_0 + \sum_j \epsilon_j c_j,$$

(where κ_0 and A_0 are the initial values for conductivity and absorbance, Λ_j is the equivalent conductance, ϵ_j is the molar absorptivity)

EQUIL1 (Reads and prints equilibrium equations. Checks for second stage of dissociation and rennumbers equations)

EQUIL2 (Computes equilibrium of ionic species)

EQUIL3 (Computes steady-state concentrations of fast-reacting species)

TIMEF (See above)

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C      PROGRAM WR16
      WATER RADIOLYSIS, WITH EQUILIBRIUM, FOR CDC 3600, K. SCHMIDT.
      TYPE INTEGER AC,BLANK,AAC,A,B,AN,AAN,SPSK,AE,CHARGE,P
      DATA (BLANK=5H ),(MINUS=1H-),(DELTA=2.5E-06),(P=5),
1      (AM=1.5,1.916666667,2.291666667,2.640277778,-0.5,-1.333333333,
2      -2.458333333,-3.852777778,0.,0.416666667,1.541666667,
3      3.633333333,0.,0.,-0.375,-1.769444444,3(0.),0.348611111)
      COMMON/BLOCK1/AC(30),C(30),CHARGE(28),NC,IFAIL
      COMMON/BLOCK2/AE(3,11),LEQ(4,11),EQ(11),NEQ,EQ2(11)
      COMMON/BLOCK3/DELTA
      COMMON/BLOCK4/TIME,TT(250),CC(30,250),CONDI,ABSI,DT,EQCO(28),
1      EXT(28),LT,NPR,DTP,NC1,NC2,NC3
      COMMON/BLOCK5/RF(27),RK(31),M1(30),M2(30),KOEFL(27,30),
1      KOEFF(27,30),JSK(30),JSK3(30),ISK(30),ISK3(30),NR
      DIMENSION A(31,6),DR(31),G(28),S(28),CI(30),T(31),PROD(30),
1      B(31,6),DCDT(30,20),IEQ(31),NRS(5,31),CCMAX(30),CCMIN(30),CP(6)
2      ,AAC(6),IND(4),XMAX(6),XMIN(6),AN(30),AAN(6),SPSK(2,31),
3      CSK(2,31),AM(4,5)
1      READ 200,NORUN,IPUNCH
      I=IDATE1(0.)
      IF(EQF,60) 600,2
2      PRINT 300,NORUN,I
      READ, COUNT AND PRINT CHEMICAL REACTIONS
3      DO 5 I = 1,31
      READ 201,(A(I,K),K=1,3),(B(I,K),A(I,K),K=4,6),RK(I)
      IF(RK(I))5,6,5
5      PRINT 301,(A(I,K),K=1,3),(B(I,K),A(I,K),K=4,6),I,RK(I)
6      NR=I-1
C      READ, COUNT AND PRINT SPECIES ETC.
      PRINT 302
      DO 10 J=1,28
      READ 203,CHARGE(J),AC(J),G(J),S(J),CI(J),EQCO(J),EXT(J)
      IF(CHARGE(J).EQ.0)CALL SCAN(CHARGE(J),AC(J))
9      IF(AC(J)-BLANK)10,11,10
10     PRINT 303,J,CHARGE(J),AC(J),G(J),S(J),CI(J),EQCO(J),EXT(J)
11     NC=J-1
C      DEFINE SOME VALUES
      NC1=NC+1 $ NC2=NC+2 $ NC3=NC+3
      DO 12 J=NC1,30
      CI(J)=0.
C      COMPUTE AND PRINT INITIAL CONDUCTIVITY AND OPTICAL DENSITY
      CONDI=0. $ ABSI=0.
      DO 100 M=1,NC
      CONDI=CONDI+CI(M)*EQCO(M)*ABSF(FLOATF(CHARGE(M)))*0.001
100     ABSI=ABSI+CI(M)*EXT(M)
      PRINT 400,CONDI,ABSI
C      READ, COUNT AND PRINT DOSE RATE VALUES
      PRINT 304
      DO 15 K=1,31
      READ 205,T(K),DR(K),SPSK(1,K),SPSK(2,K),CSK(1,K),CSK(2,K)

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1      , (NRS(M,K),M=1,5),IEQ(K)
      IF (IEQ(K).EQ.0.AND.T(K).GT.0.)NT1=XMAXOF(1,K)
14     IF (T(K))15,19,15
15     PRINT 305,K,T(K),DR(K),SPSK(1,K),SPSK(2,K),CSK(1,K),CSK(2,K)
1      , (NRS(M,K),M=1,5),IEQ(K)
19     NT=K-1
C      READ OR DEFINE, AND PRINT, SOME PARAMETERS FOR COMPUTATION
      READ 206,ACCFAC,NP,DTPMIN,DTMIN,DTMAX,DTMXEQ,IFR
      IF (ACCFAC.LE.0.)ACCFAC=0.05
      IF (DTPMIN.LE.0..AND.NP.LE.1)NP=250
      IF (DTMIN.LE.0.)DTMIN=T(NT1)/1000000.
      IF (DTMAX.LE.0.)DTMAX=T(NT1)/200
      IF (DTMXEQ.LE.0.)DTMXEQ=T(NT1)/10000.
      PRINT 306,ACCFAC,NP,DTPMIN,DTMIN,DTMAX,DTMXEQ
      IF (IFR.NE.0)PRINT 307
      PRINT 308
C      READ AND PRINT EQUILIBRIUM EQUATIONS
      IFAIL=0
      CALL EQUIL1
      IF (IFAIL)425,425,535
535     PRINT 666
      GO TO 1
425     PRINT 999
C      CALCULATE COEFFICIENTS OF DIFFERENTIAL EQUATIONS
      DO 30 I=1,NR
      ISK(I)=0
      ISK3(I)=0
      DO 30 J=1,NC
      KOEFF(J,I)=0
      KOEFFL(J,I)=0
      IF (AC(J)-A(I,1)) 23,22,23
22     KOEFF(J,I)=KOEFF(J,I)-1
      M1(I)=J
23     IF (AC(J)-A(I,2))25,24,25
24     KOEFF(J,I)=KOEFF(J,I)-1
      M2(I)=J
25     KOEFFL(J,I)=KOEFF(J,I)
      DO 30 K=3,6
      IF (AC(J)-A(I,K))30,26,30
26     KOEFF(J,I)=KOEFF(J,I)+1
      IF (B(I,K)-MINUS)30,27,30
27     KOEFF(J,I)=KOEFF(J,I)-2
30     CONTINUE
C      INITIALIZE
      DO 50 J=1,30
      C(J)=CI(J)
      JSK(J)=0
      JSK3(J)=0
50     CC(J,1)=CI(J)
      TIME = 0.
      DT=DTMIN
      LT=0
      CALL STORE
      MEQ=0
C      START SOLVING DIFFERENTIAL EQUATIONS
      DO 120 IT=1,NT
C      SKIPPING PROCEDURE
      DO 450 M=1,2
      IF (SPSK(M,IT)-BLANK)431,450,431
431     DO 435 J=1,NC
      IF (SPSK(M,IT)-AC(J))435,432,435
432     JSK(J)=JSK(J)+1
      IF (IEQ(IT).GE.2)JSK3(J)=JSK(J)
      IF (IEQ(IT).LT.2)C(J)=CSK(M,IT)
      GO TO 450
435     CONTINUE
450     CONTINUE
      DO 470 M=1,5
      IF (NRS(M,IT))470,470,455
455     I=NRS(M,IT)
      ISK(I)=ISK(I)+1
      IF (MEQ.GE.2)ISK3(I)=ISK(I)
470     CONTINUE
      MEQ=XMAXOF(MEQ,IEQ(IT))
      IF (TIME-T(IT)) 34,120,120
C      END OF SKIPPING ROUTINE
34     DO 35 L=1,NC
35     RF(L)=S(L)+(DR(IT)*G(L))/6.0231E+25
      LCYCL=0
      ILINK=0
      IF (DT.GE.(2.*DTMIN))DT=DT*0.5
36     DO 65 NCYCL=1,20
      LCYCL=XMINOF(LCYCL+1,P)
C      START CYCLE OF COMPUTATION
      TIME=TIME+DT
      DO 51 I=1,NR
      IF (ISK(I))52,52,51
52     N1=M1(I)
      N2=M2(I)
      PROD(I)=C(N1)*C(N2)*RK(I)
51     CONTINUE
      DO 60 L=1,NC
      IF (JSK(L))43,43,60
43     DCDT(L,NCYCL)=RF(L)
      DO 42 I=1,NR
      IF (ISK(I))44,44,42
44     IF (KOEFF(L,I)) 41,42,41
41     DCDT(L,NCYCL)=DCDT(L,NCYCL)+PROD(I)*FLOAT(KOEFF(L,I))
42     CONTINUE
      SLOPE=0.

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C      IF(ILINK)54,54,58
C      STANDARD ROUTINE FOR COMPUTING SLOPE
54      IF(LCYCL-1)55,55,36
55      SLOPE=DCDT(L,NCYCL)
      GO TO 59
56      DO 57 K=1,LCYCL
      INDK=NCYCL+20+1-K-20*((NCYCL+20-K)/20)
57      SLOPE=SLOPE+AM(LCYCL-1,K)*DCDT(L,INDK)
      GO TO 59
C      *LINK* ROUTINE FOR COMPUTING SLOPE
58      IDIF=-1
      DO 158 K=1,P
      ISTEP=1
      IF((K+ILINK).GT.(P+1))ISTEP=2
      IDIF=IDIF+ISTEP
      INDK=NCYCL+20-IDIF-20*((NCYCL+20-IDIF-1)/20)
158     SLOPE=SLOPE+AM(P-1,K)*DCDT(L,INDK)
C      CALCULATE AND STORE NEW CONCENTRATIONS
59     IF(TIME.LT.T(IT))159,258
258     C(L)=C(L)+SLOPE*(DT+T(IT)-TIME)
      GO TO 60
159     C(L)=C(L)+DT*SLOPE
60     CONTINUE
      IF(TIME.GE.T(IT))259,160
259     TIME=T(IT)
      LCYCL=0
      GO TO 73
160     ILINK=XMAXOF(0,ILINK-1)
      NPR=NPR+1 $ DTP=DTP+DT
      IF(NPR.GE.NP.AND.DTP.GE.DTPMIN.AND.MEQ.EQ.0)62,65
62     CALL STORE $ IF(LT.GE.250)GO TO 130
65     CONTINUE
C      CHECK TIME LIMIT
      TLFT=TIMELEFT(0.)
      IF(TLFT.LE.20000.)GO TO 130
C      BRANCH TO EQUILIBRIUM ROUTINES
73     IF((MEQ.EQ.1.OR.MEQ.EQ.3).AND.NEQ.GT.0)CALL EQUIL2
      IF(MEQ.GE.2)CALL EQUIL3
      IF(MEQ.NE.0)75,273
75     IF(IFAIL)174,174,575
575     PRINT 666
      GO TO 130
174     LCYCL=0
273     IF((NPR.GE.NP.AND.DTP.GE.DTPMIN).OR.TIME.EQ.T(IT))274,175
274     CALL STORE $ IF(LT.GE.250)GO TO 130
      IF(TIME.EQ.T(IT))120,175
C      REDETERMINE TIME INCREMENTS
175     DFDCMA=0.
      DO 360 L=1,NC
      IF(JSK(L).GE.1)GO TO 360
      DFDC=0.
      DO 350 I=1,NR
      IF(ISK(I).GE.1)GO TO 350
      M1I=M1(I) $ M2I=M2(I)
      IF(M1I.EQ.L)DFDC=DFDC+FLOATF(KOEFF(L,I))*RK(I)*C(M2I)
      IF(M2I.EQ.L)DFDC=DFDC+FLOATF(KOEFF(L,I))*RK(I)*C(M1I)
350     CONTINUE
      DFDCAB=ABSF(DFDC)
      IF(DFDCAB.GT.DFDCMA)DFDCMA=DFDCAB
360     CONTINUE
      DTREQ=ACCFAC/DFDCMA
      DTMX=DTMAX
      IF(MEQ.GT.0)DTMX=DTMXEQ
      IF(DT.GT.(1.4*DTREQ).AND.DT.GE.(2.*DTMIN).AND.(IT.NE.NT.OR.
      1 IFR.EQ.0))365,370
365     DT=DT*.5
      LCYCL=0
      GO TO 36
370     IF(DT.LT.(0.7*DTREQ).AND.DT.LE.(0.5*DTMX))375,36
375     DT=2.*DT
      ILINK=P-1
      GO TO 36
120     CONTINUE
C      DIFFERENTIAL EQUATIONS SOLVED.
C      DETERMINE MINIMA AND MAXIMA OF FUNCTIONS (FOR PLOTTING)
130     DO 121 M=1,30
121     CCMIN(M)=0. $ CCMAX(M)=0.
      DO 125 M=1,NC3
      DO 125 LL=1,LT
      IF(CC(M,LL).GT.CCMAX(M))CCMAX(M)=CC(M,LL)
      IF(CC(M,LL).LT.CCMIN(M))CCMIN(M)=CC(M,LL)
125     CONTINUE
C      DEFINE COLUMN HEADINGS
      DO 220 J=1,NC
220     AN(J)=7HMOLES/L
      DO 225 J=NC1,30
      AC(J)=5H
225     AN(J)=7H
      AC(NC1)=5HCOND
      AC(NC2)=5HABSC
      AC(NC3)=5HCT
      AN(NC1)=7H MHO/CM
      AN(NC2)=7H /CM
      AN(NC3)=7H SEC
C      ARRANGE RESULTS FOR OUTPUT.
      IGROUP=(NC3+5)/6
      DO 150 IG=1,IGROUP
      IF(IPUNCH.GT.0)PUNCH 315,NORUN,IG,LT,T(NT)
      DO 140 L=1,6
      IGL=(IG-1)*6+L
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AAC(L)=AC(IGL)
AAN(L)=AN(IGL)
XMAX(L)=CCMAX(IGL)
140 XMIN(L)=CCMIN(IGL)
PRINT 310,(AAC(L),L=1,6),(AAN(L),L=1,6)
IF(IPUNCH)142,142,141
141 PUNCH 310,(AAC(L),L=1,6),(AAN(L),L=1,6)
PUNCH 311,(XMAX(L),L=1,6)
PUNCH 312,(XMIN(L),L=1,6)
142 DO 144 LL=1,LT
DO 145 L=1,6
IGL=(IG-1)*6+L
145 CP(L)=CC(IGL,LL)
PUNCH AND/OR PRINT RESULTS
IF(IPUNCH.GT.0)PUNCH 313,TT(LL),(CP(L),L=1,6)
IF((LL.EQ.56.OR.LL.EQ.115.OR.LL.EQ.174.OR.LL.EQ.233).AND.
1 (LT.GT.57))PRINT 999
144 PRINT 313, TT(LL),(CP(L),L=1,6)
PRINT 999
IF(IPUNCH.GT.0)PUNCH 998
150 CONTINUE
IF(TLFT.LE.20000.)PRINT 667
IF(LT.GE.250)PRINT 668
IF(TLFT.LE.20000.)600,1
600 CALL EXIT
200 FORMAT(1X,I4,I5)
201 FORMAT(3(5X,A5),3(1X,A1,3X,A5),5X,E15,2)
203 FORMAT(6X,12,2X,A5,E10,3,3E15,3,E10,3)
205 FORMAT(5X,E15,3,E10,3,2A5,2E10,3,5I3,4X,I1)
206 FORMAT(E10,3,15,4E10,3,15)
300 FORMAT(1X,10HRUN NUMBER,15,56X,A8//)
301 FORMAT(6X,A5,5H + ,A5,5H = ,A5,3(1X,A4,A5),2X,2HK(,
1 12,3H) =,E10,2)
302 FORMAT(//6X,2HNO,2X,6HCHARGE,3X,4HNAME,5X,1HG, 9X,1HS,11X,2HCI,
1 10X,4HEQCO,7X,3HEXT//)
303 FORMAT(18,4X,12,5X,A5,F7,3,2(3X,E9,3,1X),F10,3,2X,E10,3)
304 FORMAT(6X,2HNO,4X,4HTIME,4X,9HDOSE RATE,3X,7HSPECIES,6X,4HCSK1,7X,
1 4HCSK2,7X,9HREACTIONS,3X,1H1/79X,1HE/12X,3HSEC,5X,8HEV/L-SEC,4XWR16
2 ,7HSKIPPED,5X,7HMOLES/L,4X,7HMOLES/L,3X,7HSKIPPED,4X,1HQ//)
305 FORMAT(18,2(2X,E8,2),2X,A5,1X,A5,2(2X,E9,3),5I3,1X,I1)
306 FORMAT(1H1/6X,15HACCURACY FACTOR,E10,2/
1 6X,24HVALUES PRINTED OUT EVERY,16,7H CYCLES/
2 6X,23HMINIMUM PRINT INTERVAL ,E10,3,4H SEC/
36X,23HMINIMUM TIME INCREMENT ,E10,3,4H SEC/
4 6X,23HMAXIMUM TIME INCREMENT ,E10,3,4H SEC/
5 6X,22HSAME IF EQUILIBRIUM IS,76X,8HCOMPUTED,15X,E10,3,4H SEC)
307 FORMAT(6X,*TIME INCREMENTS FROZEN IN LAST TIME INTERVAL*)
308 FORMAT(///)
310 FORMAT (6X,4HTIME,3X,6(5X,A5,1X)//
15X,7HSECONDS,6(4X,A7)//)
311 FORMAT(6X,5H(MAX),2X,6E11,3)
312 FORMAT(6X,5H(MIN),2X,6E11,3/)
313 FORMAT(2X,7E11,3)
315 FORMAT(14,1H*,11,1H*,13,E10,3/)
400 FORMAT(//6X,*INITIAL CONDUCTIVITY =*,E11,3,1X,*MHO/CM*/
1 6X,*INITIAL ABSORBANCE =*,E11,3,1X,*CM*//)
666 FORMAT(1X,*RUN ABANDONED*)
667 FORMAT(1X,*LESS THAN 20 SEC LEFT, SEQUENCE TERMINATED*)
668 FORMAT(1X,*PRINT LIMIT REACHED, RUN TERMINATED*)
998 FORMAT(79X,1H-)
999 FORMAT(1H1)
END PROGRAM WR16
SUBROUTINE SCAN(CHARGE,CHEM)
TYPE INTEGER OCT,PLU,CHEM,CHARGE
TYPE LOGICAL MINLOG,PLULOG
DIMENSION OCT(4),MIN(4),PLU(4),LAND(4),MINLOG(4),PLULOG(4)
CHARGE=0
DO 10 I=3,6
OCT(7-I)=63*64**I
MIN(7-I)=32*64**I
10 PLU(7-I)=MIN(7-I)/2
DO 50 I=1,4
LAND(I)=CHEM.AND.OCT(I)
MINLOG(I)=MIN(I)-LAND(I)
PLULOG(I)=PLU(I)-LAND(I)
IF(MINLOG(I).EQ.0) CHARGE=CHARGE-1
IF(PLULOG(I).EQ.0) CHARGE=CHARGE+1
50 CONTINUE
RETURN
END SUBROUTINE SCAN
SUBROUTINE STORE
C CALCULATE CONDUCTIVITY AND ABSORBANCE. STORE SET OF OUTPUT VALUES
TYPE INTEGER CHARGE
COMMON/BLOCK1/NN(30),C(30),CHARGE(28),NC,NNN
COMMON/BLOCK4/TIME,TT(250),CC(30,250),CONDI,ABSI,DT,EQCO(28),
1 EXT(28),LT,NPR,DTP,NC1,NC2,NC3
CONDC=-CONDI $ ABSC=-ABSI
LT=LT+1
DO 20 L=1,NC
CC(L,LT)=C(L)
TT(LT)=TIME
CONDC=CONDC+C(L)*EQCO(L)*ABSF(FLOATF(CHARGE(L)))*0.001
20 ABSC=ABSC+C(L)*EXT(L)
CC(NC1,LT)=CONDC
CC(NC2,LT)=ABSC
CC(NC3,LT)=DT
IF(NC3-30)25,40,40
25 NC4=NC3+1
DO 30 L=NC4,30
CC(L,LT)=0.
30 NPR=0 $ DTP=0.
40 RETURN
END SUBROUTINE STORE

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WR16 300
WR16 301
WR16 302
WR16 303
WR16 304
WR16 305
WR16 306
WR16 307
WR16 308
WR16 309
WR16 310
WR16 311
SCAN0000
SCAN0001
SCAN0002
SCAN0003
SCAN0004
SCAN0005
SCAN0006
SCAN0007
SCAN0008
SCAN0009
SCAN0010
SCAN0011
SCAN0012
SCAN0013
SCAN0014
SCAN0015
SCAN0016
SCAN0017
STORE 0
STORE 1
STORE 2
STORE 3
STORE 4
STORE 5
STORE 6
STORE 7
STORE 8
STORE 9
STORE 10
STORE 11
STORE 12
STORE 13
STORE 14
STORE 15
STORE 16
STORE 17
STORE 18
STORE 19
STORE 20
STORE 21
STORE 22

```

SUBROUTINE EQUIL1
C   READ AND PRINT EQUILIBRIUM EQUATIONS
TYPE INTEGER AC,AE,BLANK,CHARGE
COMMON/BLOCK1/AC(30),C(30),CHARGE(28),NC,IFAIL
COMMON/BLOCK2/AE(3,11),LEQ(4,11),EQ(11),NEG,EQ2(11)
DIMENSION ISHIFT(10),ISKIP(10)
DATA (BLANK=5H
DO 510 K=1,10
READ 211,(AE(M,K),M=1,3),EQ(K)
IF(AE(1,K)-BLANK)510,511,510
510 PRINT 311,(AE(M,K),M=1,3),EQ(K)
511 NEQ=K-1
C   IDENTIFY SPECIES IN EQUILIBRIUM
DO 520 K=1,NEQ
DO 520 M=1,3
DO 515 L=1,NC
IF(AC(L)-AE(M,K))515,512,515
512 LEQ(M,K)=L
GO TO 520
515 CONTINUE
IF(L-NC)520,520,526
520 CONTINUE
C   ERROR CHECK
DO 525 K=1,NEQ
IF(AE(1,K)-AE(1,1))526,525,526
525 CONTINUE
C   CHECK FOR 2ND DISSOCIATION STAGE. RENUMBER
ISKIP(1)=0
ISHIFT(1)=0
DO 630 K=1,NEQ
ISKIP(K+1)=0
ISHIFT(K+1)=ISHIFT(K)
LEQ(4,K)=NC+1
EQ2(K)=0
IF(ISKIP(K))630,605,630
605 IF(LEQ(2,K)-LEQ(3,K+1))630,610,630
610 IF(LEQ(3,K)-LEQ(2,K+1))615,526,615
615 EQ2(K)=EQ(K+1)
LEQ(4,K)=LEQ(2,K+1)
ISHIFT(K+1)=ISHIFT(K)+1
ISKIP(K+1)=1
630 CONTINUE
DO 650 K=1,NEQ
IF(ISKIP(K))650,635,650
635 EQ(K-ISHIFT(K))=E(K)
EQ2(K-ISHIFT(K))=EQ2(K)
DO 640 M=1,4
640 LEQ(M,K-ISHIFT(K))=LEQ(M,K)
650 CONTINUE
NEQ=NEQ-ISHIFT(NEQ)
GO TO 530
526 PRINT 777
IFAIL=1
530 RETURN
211 FORMAT(3(5X,A5),5X,E10.3)
311 FORMAT(6X,A5,5H * ,A5,5H = ,A5,4H * ,E10.3)
777 FORMAT(1X,*ERROR IN EQUILIBRIUM EQUATIONS*)
END SUBROUTINE EQUIL1

SUBROUTINE EQUIL2
C   COMPUTE EQUILIBRIUM OF IONIC SPECIES
TYPE INTEGER AC,AE,CHARGE
COMMON/BLOCK1/AC(30),C(30),CHARGE(28),NC,IFAIL
COMMON/BLOCK2/AE(3,11),LEQ(4,11),EQ(11),NEG,EQ2(11)
COMMON/BLOCK3/DELTA
DIMENSION HPLUS(3),TOTAL(10)
LEQ1=LEQ(1,1)$CH=FLOATF(CHARGE(LEQ1))
HPLUS(1)=C(LEQ1)
DO 540 K=1,NEQ
LEQ2K=LEQ(2,K)
LEQ3K=LEQ(3,K)
LEQ4K=LEQ(4,K)
540 TOTAL(K)=C(LEQ2K)+C(LEQ3K)+C(LEQ4K)
DO 560 NSTEP=1,20
DO 555 I=2,3
DO 545 K=1,NEQ
LEQ2K=LEQ(2,K)
LEQ3K=LEQ(3,K)
LEQ4K=LEQ(4,K)
C(LEQ3K)=TOTAL(K)/(1.+EQ(K)/HPLUS(I-1)+EQ(K)*EQ2(K)/HPLUS(I-1)**2)
C(LEQ2K)=EQ(K)*C(LEQ3K)/HPLUS(I-1)
545 C(LEQ4K)=EQ2(K)*C(LEQ2K)/HPLUS(I-1)
HPLUS(I)=HPLUS(I-1)
DO 551 L=1,NC
IF(CHARGE(L))550,551,550
550 HPLUS(I)=HPLUS(I)-CH*FLOATF(CHARGE(L))*C(L)
551 CONTINUE
CHECK=ABSF((HPLUS(I)-HPLUS(1))/(HPLUS(I)+HPLUS(1)))
IF(CHECK-DELTA*0.1)553,553,555
553 C(LEQ1)=(HPLUS(I)+HPLUS(1))/2.
GO TO 562
555 C(LEQ1)=HPLUS(1)
HPLUS0=HPLUS(1)
HPLUS(1)=(HPLUS(2)**2-HPLUS(1)*HPLUS(3))/(2.*HPLUS(2)-HPLUS(1)
1 -HPLUS(3))
C(LEQ1)=HPLUS(1)
CHECK=ABSF((HPLUS(1)-HPLUS0)/(HPLUS(1)+HPLUS0))
IF(CHECK-DELTA)562,562,560
560 CONTINUE
IFAIL=1
PRINT 777
GO TO 570

```

```

EQU1 1
EQU1 2
EQU1 3
EQU1 4
EQU1 5
EQU1 6
EQU1 7
EQU1 8
EQU1 9
EQU1 10
EQU1 11
EQU1 12
EQU1 13
EQU1 14
EQU1 15
EQU1 16
EQU1 17
EQU1 18
EQU1 19
EQU1 20
EQU1 21
EQU1 22
EQU1 23
EQU1 24
EQU1 25
EQU1 26
EQU1 27
EQU1 28
EQU1 29
EQU1 30
EQU1 31
EQU1 32
EQU1 33
EQU1 34
EQU1 35
EQU1 36
EQU1 37
EQU1 38
EQU1 39
EQU1 40
EQU1 41
EQU1 42
EQU1 43
EQU1 44
EQU1 45
EQU1 46
EQU1 47
EQU1 48
EQU1 49
EQU1 50
EQU1 51
EQU1 52
EQU1 53
EQU1 54
EQU1 55
EQU1 56
EQU1 57
EQU1 58
EQU2 1
EQU2 2
EQU2 3
EQU2 4
EQU2 5
EQU2 6
EQU2 7
EQU2 8
EQU2 9
EQU2 10
EQU2 11
EQU2 12
EQU2 13
EQU2 14
EQU2 15
EQU2 16
EQU2 17
EQU2 18
EQU2 19
EQU2 20
EQU2 21
EQU2 22
EQU2 23
EQU2 24
EQU2 25
EQU2 26
EQU2 27
EQU2 28
EQU2 29
EQU2 30
EQU2 31
EQU2 32
EQU2 33
EQU2 34
EQU2 35
EQU2 36
EQU2 37
EQU2 38
EQU2 39
EQU2 40
EQU2 41
EQU2 42
EQU2 43

```


562	DO 565 K=1,NEQ	EQU2	44
	LEQ2K=LEQ(2,K)	EQU2	45
	LEQ3K=LEQ(3,K)	EQU2	46
	LEQ4K=LEQ(4,K)	EQU2	47
	C(LEQ3K)=TOTAL(K)/(1.+EQ(K)/HPLUS(1)+EQ(K)*EQ2(K)/HPLUS(1)**2)	EQU2	48
	C(LEQ2K)=EQ(K)*C(LEQ3K)/HPLUS(1)	EQU2	49
565	C(LEQ4K)=EQ2(K)*C(LEQ2K)/HPLUS(1)	EQU2	50
570	RETURN	EQU2	51
777	FORMAT(1X,*DIVERGENCE IN EQUIL2*)	EQU2	52
	END SUBROUTINE EQUIL2	EQU2	53
	SUBROUTINE EQUIL3	EQU30000	
	COMMON/BLOCK1/NN(30),C(30),NNN(28),NC,IFAIL	EQU30001	
	COMMON/BLOCK3/DELTA	EQU30002	
	COMMON/BLOCK5/RF(27),RK(31),M1(30),M2(30),KOEFL(27,30),	EQU30003	
1	KOEFF(27,30),JSK(30),JSK3(30),ISK(30),ISK3(30),NR	EQU30004	
	DO 150 N=1,20	EQU30006	
	TEST=0.	EQU30007	
	DO 100 J=1,NC	EQU30008	
	IF(JSK3(J).NE.0)5,100	EQU30009	
5	C0=C(J)	EQU30010	
	A0=RF(J)	EQU30011	
	A1=0.	EQU30012	
	A2=0.	EQU30013	
	DO 50 I=1,NR	EQU30014	
	IF(ISK(I).NE.0.AND.ISK3(I).EQ.0)50,7	EQU30015	
7	M1I=M1(I) \$ M2I=M2(I)	EQU30016	
	IF(KOEFL(J,I).EQ.-2)A2=A2+RK(I)*FLOATF(KOEFL(J,I))	EQU30017	
	IF(KOEFL(J,I).EQ.-1)10,30	EQU30018	
10	IF(M1I.EQ.J)15,20	EQU30019	
15	A1=A1+RK(I)*FLOATF(KOEFL(J,I))*C(M2I)	EQU30020	
20	IF(M2I.EQ.J)25,30	EQU30021	
25	A1=A1+RK(I)*FLOATF(KOEFL(J,I))*C(M1I)	EQU30022	
30	IF(KOEFL(J,I).EQ.0.AND.KOEFL(J,I).NE.0)A0=A0+RK(I)*FLOATF(KOEFL	EQU30023	
1	(J,I))*C(M1I)*C(M2I)	EQU30024	
50	CONTINUE	EQU30025	
	IF(A2.EQ.0.)C(J)=-A0/A1	EQU30026	
	IF(A2.NE.0.)C(J)=(-A1-SQRTF(A1*A1-4.*A0*A2))/(2.*A2)	EQU30027	
	TEST=TEST+ABSF(C(J)-C0)	EQU30029	
100	CONTINUE	EQU30030	
	IF(TEST.LE.2.*DELTA)GO TO 160	EQU30031	
150	CONTINUE	EQU30032	
	IFAIL=1	EQU30033	
	PRINT 666	EQU30034	
160	RETURN	EQU30035	
666	FORMAT(1X,*DIVERGENCE IN EQUIL3*)	EQU30036	
	END SUBROUTINE EQUIL3	EQU30037	

9. APPENDIX

Modification of the Program for Use with an
IBM-1620 Computer System

Since computers of the type IBM-1620 are more commonly available than the much larger and more expensive CDC-3600, it was attempted to adapt program WR16 for a computer system of the former type. This was only possible with certain restrictions because of the storage requirements of the program. The adapted program can now be used with an IBM-1620 computer equipped with either a 60-k memory and an IBM-1620 Monitor-I system, or a 40-k memory and an IBM-1620 Monitor-II system.

In order to reduce storage requirements, the arithmetic portion of the program had to be separated and converted into a subroutine. Also, Ionic Equilibrium Option had to be eliminated altogether.

9.1 Required Programs and Subroutines

- WR17 (Main program, which performs essentially the same operations as program WR16, except that the arithmetic portion has been separated.)
- CYCL17 (Performs most of the arithmetic operations.)
- STORE (Essentially the same as the STORE subroutine used with WR16.)*
- EQUIL3 (Essentially the same as the EQUIL3 subroutine used with WR16.)*

9.2 Suggested Operating Procedure

Load main program and subroutines on disk in the usual way described in the IBM reference manual. For execution enter data together with the control cards shown in Fig. 6. These control cards include some storage-saving options:

(1) The Floating-point Arithmetic and the Input-Output subroutines are loaded in core alternatively when they are called (digit 3 on XEQS control card).

1	2	3	4	5	6	7	8
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
##JOB 5	04800						
##XEQSWR17		301					
*LOCALWR17	CYCL17,EQUIL3,STORE						
----	----	----	(INSERT DATA HERE)	----	----	----	----

1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
1	2	3	4	5	6	7	8

Fig. 6. Control Cards for Executing Program WR17

*Note that the source deck of this subroutine is somewhat different from the subroutine with the same name used with WR16.

(2) The subroutines CYCL17, STORE, and EQUIL3 are loaded in core one at a time when required. They occupy the same storage area (LOCAL control card).

Two features of the program controlled by program switches are described in Sect. 9.3.

9.3 Restrictions and Additional Features of Program WR17 as Compared to WR16

- (1) Only 25, rather than 30, chemical reactions may be entered.
- (2) Only 21, rather than 27, species may be used.
- (3) The maximum number of characters in the Holerith notations of the species is 4, rather than 5.
- (4) The maximum number of time intervals is 20, rather than 30.
- (5) Since there is no SCAN subroutine, the charges of the species are not determined. Also, charge values entered with the data are ignored. Instead of the equivalent conductance (EQCO), the atomic conductance (ATCO = EQCO times the valence of the species) must be entered.
- (6) There is no Ionic Equilibrium Option. Any digit greater than 0 for IEQ (in column 80 of the d-cards) will put the Steady-state Option (EQUIL3) into effect, i.e., it conveys the same instruction as the digit 2 in program WR16. No equilibrium equations must be entered with the data.
- (7) The entire output is punched on cards. The results appear in the way in which they are punched by WR16 with a punch index different from 0. A punch index will be ignored by WR17. The heading IEQ in WR16 is replaced by IE, the heading CONDC by CNDC.
- (8) No date is punched and no time check performed.
- (9) Since calculations with an IBM-1620 system require considerably more (approximately 100 times as much) time than those with a CDC-3600, two additional options controlled by program switches on the console have been added which permit the user to follow the computation and terminate it at any desired time. These are the switch settings and their effects:

Program Switch 2 On:

Each time when a set of concentrations, etc., is stored for output, the console typewriter prints the current number of this set, the (model) time, and all concentrations including CNDC, ABSC, and DT. [As an example, the printout for $t = 2.790 \times 10^{-7}$ sec in Run No. 92 (see Sect. 6.4.1) is reproduced in Fig. 7.]

Program Switches 2 and 3 On:

This has the same effect as if the print limit were reached. All results stored up to that point are punched out, and the run is terminated.

3 2.790E-07

```

3.949E-08  1.554E-07  1.154E-07  7.618E-09  3.962E-08  1.067E-08
6.895E-09  2.366E-10  1.996E-10  9.999E-07  5.490E+01  1.000E+00
2.926E-08  6.318E-04  1.000E-08  0.000E-99  0.000E-99  0.000E-99

```

Fig. 7. Example of a Typewriter Printout Obtained by Turning on Program Switch 2.

9.4 FORTRAN Notation and Listing of Source Decks

Table III includes those notations used in program WR17 and its subroutines that are not used or have a different meaning in program WR16 and its subroutines.

TABLE III. FORTRAN Notation for WR17 and Subroutines as Far as Not Listed in Table II

FORTRAN Name	Notation in Text	Explanation
A	(A_{ji})	same as in WR16, except that part of the A matrix is used for the quantities forming the B matrix of WR16
AAN		see NAA1
AN		see NA1
ATCO	$\Lambda_j Q_j $	atomic conductance
COEFF	α_{ji}	same as KOEFF, but in floating-point mode
NA1, AN, NA2		Holerith headings, same as AN1 and AN2 in WR16
NAA1, AAN, NAA2		Holerith headings, same as AAN1 and AAN2 in WR16
IIT		current number of time interval
IPRINT		index controlling the premature termination of a run

In the remaining pages of this section, the FORTRAN source decks of program WR17 and all necessary subroutines are listed.

```

*FANDK0804
C WATER RADIOLYSIS, WITH STEADY STATE, FOR IBM-1620. K. SCHMIDT
  DIMENSION AC(24),C(24),ATCO(22),EXT(22),RF(21),RK(26),M1(25),M2(25)
  1 ,KOEFF(21,25),JSK(24),ISK(25),CCMIN(24),CCMAX(24),AM(4,5),
    DCDT(24,10),T(21)
  DIMENSION CSK(2,21),A(26,9),DR(21),G(22),S(22),CI(24),
    1 IEQ(21),NRS(5,21),CP(6),AAC(6),XMAX(6),XMIN(6),NA1(24),NA2(24),
    2 NAA1(6),NAA2(6),SPSK(2,21),AN(24),AAN(6)
  COMMON AC,C,ATCO,EXT,RF,RK,M1,M2,KOEFF,JSK,ISK,CCMIN,CCMAX,AM,DCDT
  1 ,T,NC,NR,IFAIL,CONDI,ABSI,DT,LT,NPR,DTP,NC1,NC2,NC3,LCYCL,ILINK,
    2 IGROUP,IPRINT,TIME,IIT
  EQUIVALENCE(AAN1,AN1),(AAN2,AN2),(XMAX,CCMAX),(XMIN,CCMIN),(C,CI)
  1 ,(CP,ATCO),(DCDT,A)
  DEFINE DISK(7,1000)
  DO 610 I=1,4
  DO 610 K=1,3
610 AM(I,K)=0.
  AM(1,1)=SQRTF(2.25)
  AM(2,1)=1.9166667
  AM(3,1)=2.2916667
  AM(4,1)=2.6402778
  AM(1,2)=1.-AM(1,1)
  AM(2,2)=-1.3333333
  AM(3,2)=-2.4583333
  AM(4,2)=-3.8527773
  AM(2,3)=0.4166666
  AM(3,3)=1.5416666
  AM(4,3)=3.6333333
  AM(3,4)=-0.375
  AM(4,4)=-1.7694444
  AM(4,5)=0.3486111
  1 READ 200,NORUN
  IF(NORUN)600,600,2
  2 PUNCH 300,NORUN.
  C READ, COUNT AND PRINT CHEMICAL REACTIONS
  3 DO 5 I = 1,26
  READ 201,(A(I,K),K=1,3),A(I,7),A(I,4),A(I,8),A(I,5),A(I,9),
    1 A(I,6),RK(I)
  IF(RK(I))5,6,5
  5 PUNCH 301,(A(I,K),K=1,3),A(I,7),A(I,4),A(I,8),A(I,5),A(I,9),
    1 A(I,6),I,RK(I)
  6 NR=I-1
  C READ, COUNT AND PRINT SPECIES ETC.
  PUNCH 302
  DO 10 J=1,22
  READ 203,AC(J),G(J),S(J),CI(J),ATCO(J),EXT(J)
  9 IF(AC(J))10,11,10
  10 PUNCH 303,J,AC(J),G(J),S(J),CI(J),ATCO(J),EXT(J)
  11 NC=J-1
  C DEFINE SOME VALUES
  NC1=NC+1
  NC2=NC+2
  NC3=NC+3
  IGROUP=(NC3+5)/6
  DO 12 J=NC1,24
  12 CI(J)=0.
  C COMPUTE AND PRINT INITIAL CONDUCTIVITY AND OPTICAL DENSITY
  CONDI=0.
  ABSI=0.
  DO 100 M=1,NC
  CONDI=CONDI+CI(M)*ATCO(M)*0.001
  100 ABSI=ABSI+CI(M)*EXT(M)
  PUNCH 400,CONDI,ABSI
  C READ, COUNT AND PRINT DOSE RATE VALUES
  PUNCH 304
  DO 15 K=1,21
  READ 205,T(K),DR(K),SPSK(1,K),SPSK(2,K),CSK(1,K),CSK(2,K)
  1 ,(NRS(M,K),M=1,5),IEQ(K)
  IF(IEQ(K))14,615,14
  615 IF(T(K))14,14,616
  616 NT1=K
  IF(NT1)617,617,14
  617 NT1=1
  14 IF(T(K))15,19,15
  15 PUNCH 305,K,T(K),DR(K),SPSK(1,K),SPSK(2,K),CSK(1,K),CSK(2,K)
  1 ,(NRS(M,K),M=1,5),IEQ(K)
  19 NT=K-1
  C READ OR DEFINE, AND PRINT, SOME PARAMETERS FOR COMPUTATION
  READ 206,ACCFAC,NP,DTPMIN,DTMIN,DTMAX,DTMXEQ,IFR
  IF(ACCFAC)619,619,620
  619 ACCFAC=0.1
  620 IF(DTPMIN)621,621,623
  621 IF(NP-1)622,622,623
  622 NP=40
  623 IF(DTMIN)624,624,625
  624 DTMIN=T(NT1)/10000.
  625 IF(DTMAX)626,626,627
  626 DTMAX=T(NT1)/200.
  627 IF(DTMXEQ)628,628,629
  628 DTMXEQ=T(NT)/200.
  629 PUNCH 306,ACCFAC,NP,DTPMIN,DTMIN,DTMAX,DTMXEQ
  IF(IFR)630,631,630
  630 PUNCH 307
  631 PUNCH 999

```

C	CALCULATE COEFFICIENTS OF DIFFERENTIAL EQUATIONS	WR17	94
	DO 30 I=1,NR	WR17	95
	ISK(I)=0	WR17	96
	DO 30 J=1,NC	WR17	97
	KOEFF(J,I)=0	WR17	98
	IF(AC(J)-A(I,1)) 23,22,23	WR17	99
22	KOEFF(J,I)=KOEFF(J,I)-1	WR17	100
	M1(I)=J	WR17	101
23	IF(AC(J)-A(I,2))25,24,25	WR17	102
24	KOEFF(J,I)=KOEFF(J,I)-1	WR17	103
	M2(I)=J	WR17	104
25	DO 30 K=3,6	WR17	105
	IF(AC(J)-A(I,K))30,26,30	WR17	106
26	KOEFF(J,I)=KOEFF(J,I)+1	WR17	107
	IF(A(I,K+3)-0.20)30,27,30	WR17	108
27	KOEFF(J,I)=KOEFF(J,I)-2	WR17	109
30	CONTINUE	WR17	110
C	INITIALIZE	WR17	111
	DO 50 J=1,24	WR17	112
	C(J)=CI(J)	WR17	113
	CCMIN(J)=0.	WR17	114
	CCMAX(J)=0.	WR17	115
50	JSK(J)=0	WR17	116
	TIME = 0.	WR17	117
	DT=DTMIN	WR17	118
	LT=0	WR17	119
	CALL STORE	WR17	120
	MEQ=0	WR17	121
C	START SOLVING DIFFERENTIAL EQUATIONS	WR17	122
	DO 120 IT=1,NT	WR17	123
	IIT=IT	WR17	124
C	SKIPPING PROCEDURE	WR17	125
	DO 450 M=1,2	WR17	126
	IF(SPSK(M,IT)-BLANK)431,450,431	WR17	127
431	DO 435 J=1,NC	WR17	128
	IF(SPSK(M,IT)-AC(J))435,432,435	WR17	129
432	JSK(J)=JSK(J)+1	WR17	130
	IF(IEQ(IT))723,723,440	WR17	131
723	C(J)=CSK(M,IT)	WR17	132
	GO TO 450	WR17	133
440	JSK(J)=JSK(J)+50	WR17	134
	GO TO 450	WR17	135
435	CONTINUE	WR17	136
450	CONTINUE	WR17	137
	DO 470 M=1,5	WR17	138
	IF(NRS(M,IT))470,470,455	WR17	139
455	I=NRS(M,IT)	WR17	140
	ISK(I)=ISK(I)+1	WR17	141
	IF(IEQ(IT))470,470,633	WR17	142
633	ISK(I)=ISK(I)+50	WR17	143
470	CONTINUE	WR17	144
	MEQ=MEQ+IEQ(IT)	WR17	146
	IF(TIME-T(IT)) 34,120,120	WR17	147
C	END OF SKIPPING ROUTINE	WR17	148
34	DO 35 L=1,NC	WR17	149
35	RF(L)=S(L)+(DR(IT)*G(L))/6.0231E+25	WR17	150
	LCYCL=0	WR17	151
	ILINK=0	WR17	152
	IF(DT-2.*DTMIN)36,636,636	WR17	153
636	DT=DT*0.5	WR17	154
36	CALL CYCL17	WR17	155
C	CALL EQUILIBRIUM ROUTINE	WR17	156
	IF(MEQ)273,273,74	WR17	157
74	CALL EQUIL3	WR17	158
75	IF(IFAIL)174,174,575	WR17	159
575	PRINT 666	WR17	160
	GO TO 130	WR17	161
174	LCYCL=0	WR17	162
273	IF(NPR-NP)642,641,641	WR17	163
641	IF(DTP-DTPMIN)642,274,274	WR17	164
642	IF(TIME-T(IT))175,274,274	WR17	165
274	CALL STORE	WR17	166
	IF(LT+(IPRINT-1)*250)275,130,130	WR17	167
275	IF(TIME-T(IT))175,120,120	WR17	168
C	REDETERMINE TIME INCREMENTS	WR17	169
175	DFDCMA=0.	WR17	170
	DO 360 L=1,NC	WR17	171
	IF(JSK(L)-1)643,360,360	WR17	172
643	DFDC=0.	WR17	173
	DO 350 I=1,NR	WR17	174
	IF(ISK(I)-1)644,350,350	WR17	175
644	M1I=M1(I)	WR17	176
	M2I=M2(I)	WR17	177
	COEFF=KOEFF(L,I)	WR17	178
	IF(M1I-L)646,645,646	WR17	179
645	DFDC=DFDC+COEFF*RK(I)*C(M2I)	WR17	180
646	IF(M2I-L)350,647,350	WR17	181
647	DFDC=DFDC+COEFF*RK(I)*C(M1I)	WR17	182
350	CONTINUE	WR17	183
	DFDCAB=ABSF(DFDC)	WR17	184
	IF(DFDCAB-DFDCMA)360,360,355	WR17	185
355	DFDCMA=DFDCAB	WR17	186

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360 CONTINUE
   DTREQ=ACCFAC/DFDCMA
   DTMX=DTMAX
   IF(MEQ)362,362,361
361 DTMX=DTMREQ
362 IF(DT-1.4*DTREQ)370,370,745
745 IF(DT-2.*DTMIN)370,746,746
746 IF(IT-NT)365,363,363
363 IF(IFR)370,365,370
365 DT=DT*0.5
   LCYCL=0
   GO TO 36
370 IF(DT-0.7*DTREQ)747,36,36
747 IF(DT-0.5*DTMX)375,375,36
375 DT=2.*DT
   ILINK=4
   GO TO 36
C 120 CONTINUE
C DIFFERENTIAL EQUATIONS SOLVED.
C DEFINE COLUMN HEADINGS
130 DO 220 J=1,NC
   NA1(J)=5456
   AN(J)=0.534562
220 NA2(J)=2153
   DO 225 J=NC1,24
   AC(J)=0.
   NA1(J)=0
   AN(J)=0.
225 NA2(J)=0
   AC(NC1)=0.43554443
   AC(NC2)=0.41426243
   AC(NC3)=0.4463
   NA1(NC1)=5448
   AN(NC1)=0.562100
   NA2(NC1)=4354
   AN(NC2)=0.214354
   AN(NC3)=0.624543
C REARRANGE AND PUNCH HEADINGS
DO 150 IG=1,IGROUP
PUNCH 315,NORUN,IG,LT,T(NT)
DO 140 L=1,6
   IGL=(IG-1)*6+L
   AAC(L)=AC(IGL)
   NAA1(L)=NA1(IGL)
   AAN(L)=AN(IGL)
   NAA2(L)=NA2(IGL)
   XMAX(L)=CCMAX(IGL)
   XMIN(L)=CCMIN(IGL)
140 PUNCH 310,(AAC(L),L=1,6),(NAA1(L),AAN(L),NAA2(L),L=1,6)
   PUNCH 311,(XMAX(L),L=1,6)
   PUNCH 312,(XMIN(L),L=1,6)
C FETCH AND PUNCH RESULTS
DO 145 LL=1,LT
   IREC=(IG-1)*250+LL
   FETCH(IREC)TT,(CP(L),L=1,6)
145 PUNCH 313,TT,(CP(L),L=1,6)
   PUNCH 999
150 CONTINUE
   IF(LT-250)655,650,650
650 PRINT 668
655 IF(SENSE SWITCH 4)660,1
660 CALL LINK(PLWR17)
600 CALL EXIT
200 FORMAT(2X,I3)
201 FORMAT(3(5X,A4,1X),3(1X,A1,3X,A4,1X),5X,E15.3)
203 FORMAT(10X,A4,1X,E10.3,3E15.3,E10.3)
205 FORMAT(5X,E15.3,E10.3,2(A4,1X),2E10.3,5I3,4X,I1)
206 FORMAT(E10.3,15,4E10.3,15)
300 FORMAT(1X,10HRUN NUMBER,14,/)
301 FORMAT(6X,A4,6H + ,A4,6H = ,A4,3(2X,A4,A4,1X),2HK(,
1 12,3H) =,E10.3)
302 FORMAT(7/6X,2HNO,3X,4HNAME,5X,1HG,9X,1HS,11X,2HCI,
1 1CX,4HATCO,7X,3HEXT/)
303 FORMAT(18,5X,A4,F8.3,2(2X,E10.3,1X),F10.3,2X,E10.3)
304 FORMAT(6X,2HNO,4X,4HTIME,4X,9HDOSE RATE,3X,7HSPECIES,6X,4HCSK1,7X,
1 4HCSK2,7X,9HREACTIONS,3X,1HI/79X,1HE/12X,3HSEC,5X,8HEV/L-SEC,4X,
2 7HSKIPPED,5X,7HMOLES/L,4X,7HMOLES/L,6X,7HSKIPPED/)
305 FORMAT(18,2(1X,E9.2),2X,A4,2X,A4,1X,2(1X,E10.3),5I3,1X,I1)
306 FORMAT(79X,1H-/6X,15HACCURACY FACTOR,1X,E9.2/6X,24HVALUES PUNCHED
1OUT EVERY,16,7H CYCLES/6X,23HMINIMUM PUNCH INTERVAL ,E10.3,4H SEC/
26X,23HMINIMUM TIME INCREMENT ,E10.3,4H SEC/6X,23HMAXIMUM TIME INCRW/
3EMENT ,E10.3,4H SEC/6X,22HSAME IF EQUILIBRIUM IS/6X,8HCOMPUTED,15X
4,E10.3,4H SEC)
307 FORMAT(6X,44HTIME INCREMENTS FROZEN IN LAST TIME INTERVAL)
310 FORMAT(6X,4HTIME,3X,6(5X,A4,2X)//
15X,7HSECONDS,6(4X,A2,A3,A2)/)
311 FORMAT(6X,5H(MAX),3X,6(E10.3,1X))
312 FORMAT(6X,5H(MIN),3X,6(E10.3,1X)/)
313 FORMAT(3X,7(E10.3,1X))
315 FORMAT(14,1H*,11,1H*,13,E10.3/)
400 FORMAT(/6X,22HINITIAL CONDUCTIVITY =,1X,E10.3,7H MHO/CM/
1 6X,22HINITIAL ABSORBANCE =,1X,E10.3,4H /CM//)
666 FORMAT(14H RUN ABANDONED)
668 FORMAT(36H PUNCH LIMIT REACHED, RUN TERMINATED)
999 FORMAT(79X,1H-)
END

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*FANDK0804
SUBROUTINE CYCL17
DIMENSION AC(24), C(24), ATCO(22), EXT(22), RF(21), RK(26), M1(25), M2(25)
1 ,KOEFF(21,25), JSK(24), ISK(25), CCMIN(24), CCMAX(24), AM(4,5),
2 DCDT(24,10), T(21)
DIMENSION PROD(25)
COMMON AC, C, ATCO, EXT, RF, RK, M1, M2, KOEFF, JSK, ISK, CCMIN, CCMAX, AM, DCDT
1 ,T, NC, NR, IFAIL, CONDI, ABSI, DT, LT, NPR, DTP, NC1, NC2, NC3, LCYCL, ILINK,
2 IGROUP, IPRINT, TIME, IT
DO 65 MCYCL=1,2
DO 65 NCYCL=1,10
LCYCL=LCYCL+1
IF(LCYCL-5)38,38,37
37 LCYCL=5
C START CYCLE OF COMPUTATION
38 TIME=TIME+DT
DO 51 I=1,NR
IF(ISK(I))52,52,51
52 N1=M1(I)
N2=M2(I)
PROD(I)=C(N1)*C(N2)*RK(I)
51 CONTINUE
DO 60 L=1,NC
IF(JSK(L))43,43,60
43 DCDT(L,NCYCL)=RF(L)
DO 42 I=1,NR
IF(ISK(I))44,44,42
44 IF (KOEFF(L,I)) 41,42,41
41 COEFF=KOEFF(L,I)
DCDT(L,NCYCL)=DCDT(L,NCYCL)+PROD(I)*COEFF
42 CONTINUE
SLOPE=0.
IF(ILINK)54,54,58
C STANDARD ROUTINE FOR COMPUTING SLOPE
54 IF(LCYCL-1)55,55,56
55 SLOPE=DCDT(L,NCYCL)
GO TO 59
56 DO 57 K=1,LCYCL
INDK=NCYCL+11-K-10*((NCYCL+10-K)/10)
57 SLOPE=SLOPE+AM(LCYCL-1,K)*DCDT(L,INDK)
GO TO 59
C *LINK* ROUTINE FOR COMPUTING SLOPE
58 IDIF=-1
DO 158 K=1,5
IDIF=IDIF+1+(K+ILINK)/7
INDK=NCYCL+10-IDIF-10*((NCYCL+10-IDIF-1)/10)
158 SLOPE=SLOPE+AM( 4,K)*DCDT(L,INDK)
C CALCULATE NEW CONCENTRATIONS
59 IF(TIME-T(IT))159,159,258
258 C(L)=C(L)+SLOPE*(DT+T(IT)-TIME)
GO TO 60
159 C(L)=C(L)+DT*SLOPE
60 CONTINUE
IF(TIME-T(IT))61,259,259
259 TIME=T(IT)
LCYCL=0
GO TO 70
61 IF(ILINK)63,63,64
64 ILINK=ILINK-1
63 NPR=NPR+1
DTP=DTP+DT
65 CONTINUE
70 RETURN
END

*FANDK0804
SUBROUTINE STORE
C CALCULATE CONDUCTIVITY AND ABSORBANCE. STORE SET OF OUTPUT VALUES
DIMENSION AC(24), C(24), ATCO(22), EXT(22), RF(21), RK(26), M1(25), M2(25)
1 ,KOEFF(21,25), JSK(24), ISK(25), CCMIN(24), CCMAX(24), AM(4,5),
2 DCDT(24,10), T(21)
COMMON AC, C, ATCO, EXT, RF, RK, M1, M2, KOEFF, JSK, ISK, CCMIN, CCMAX, AM, DCDT
1 ,T, NC, NR, IFAIL, CONDI, ABSI, DT, LT, NPR, DTP, NC1, NC2, NC3, LCYCL, ILINK,
2 IGROUP, IPRINT, TIME, IT
CONDC=-CONDI
ABSC=-ABSI
LT=LT+1
IPRINT=0
DO 5 L=1,NC
CONDC=CONDC+C(L)*ATCO(L)*0.001
5 ABSC=ABSC+C(L)*EXT(L)
C(NC1)=CONDC
C(NC2)=ABSC
C(NC3)=DT
DO 25 J=1,NC3
IF(CCMAX(J)-C(J))10,15,15
10 CCMAX(J)=C(J)
15 IF(CCMIN(J)-C(J))25,25,20
20 CCMIN(J)=C(J)
25 CONTINUE
DO 30 IG=1,IGROUP
IREC=(IG-1)*250+LT
FIND(IREC)

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K1=(IG-1)*6+1	STORE	28
K2=IG*6	STORE	29
30 RECORD(IREC)TIME,(C(K),K=K1,K2)	STORE	30
NPR=0	STORE	31
DTP=0.	STORE	32
IF(SENSE SWITCH 2)35,50	STORE	33
35 PRINT 101,LT,TIME	STORE	34
DO 40 IG=1,IGROUP	STORE	35
K1=(IG-1)*6+1	STORE	36
K2=IG*6	STORE	37
40 PRINT 102,(C(K),K=K1,K2)	STORE	38
IF(SENSE SWITCH 3)45,50	STORE	39
45 IPRINT=1	STORE	40
50 RETURN	STORE	41
101 FORMAT(/I3,2X,E10.3/)	STORE	42
102 FORMAT(10X,3(E10.3,1X))	STORE	43
END	STORE	44
*FANDK0804	EQU3	0
SUBROUTINE EQUIL3	EQU3	1
DIMENSIONAC(24),C(24),ATCO(22),EXT(22),RF(21),RK(26),M1(25),M2(25)	EQU3	2
1 ,KOEFF(21,25),JSK(24),ISK(25),CCMIN(24),CCMAX(24),AM(4,5),	EQU3	3
2 DCDT(24,10),T(21)	EQU3	4
COMMON AC,C,ATCO,EXT,RF,RK,M1,M2,KOEFF,JSK,ISK,CCMIN,CCMAX,AM,DCDTEQU3	EQU3	5
1 ,T,NC,NR,IFAIL,COND1,ABS1,DT,LT,NPR,DTP,NC1,NC2,NC3,LCYCL,ILINK,	EQU3	6
2 IGROUP,IPRINT,TIME,IT	EQU3	7
DO 150 N=1,20	EQU3	8
TEST=0.	EQU3	9
DO 100 J=1,NC	EQU3	10
IF(JSK(J)-50)100,100,5	EQU3	11
5 C0=C(J)	EQU3	12
A0=RF(J)	EQU3	13
A1=0.	EQU3	14
A2=0.	EQU3	15
DO 50 I=1,NR	EQU3	16
IF(ISK(I))7,7,6	EQU3	17
6 IF(ISK(I)-50)50,7,7	EQU3	18
7 M1I=M1(I)	EQU3	19
M2I=M2(I)	EQU3	20
COEFF=KOEFF(J,I)	EQU3	21
IF(M1I-J)10,108,10	EQU3	22
108 IF(M2I-J)10,110,10	EQU3	23
110 A2 =A2 +RK(I)*COEFF	EQU3	24
GO TO 50	EQU3	25
10 IF(M1I-J)20,15,20	EQU3	26
15 A1 =A1 +RK(I)*COEFF	EQU3	27
GO TO 50	EQU3	28
20 IF(M2I-J)30,25,30	EQU3	29
25 A1 =A1 +RK(I)*C(M1I)*COEFF	EQU3	30
30 IF(COEFF)40,50,40	EQU3	31
40 A0=A0+RK(I)*COEFF*C(M1I)*C(M2I)	EQU3	32
50 CONTINUE	EQU3	33
IF(A2)70,60,70	EQU3	34
60 C(J)=A0/A1	EQU3	35
GO TO 90	EQU3	36
70 C(J)=(-A1-SQRTF(A1*A1-4.*A0*A2))/(2.*A2)	EQU3	37
90 TEST=TEST+ABSF(C(J)-C0)	EQU3	38
100 CONTINUE	EQU3	39
IF(TEST-5.E-06)155,155,150	EQU3	40
150 CONTINUE	EQU3	41
PRINT 666	EQU3	42
IFAIL=1	EQU3	43
GO TO 160	EQU3	44
155 IFAIL=0	EQU3	45
160 RETURN	EQU3	46
666 FORMAT(21H DIVERGENCE IN EQUIL3)	EQU3	47
END	EQU3	48

10. ACKNOWLEDGMENTS

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11. REFERENCES

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