

A CALCULATIONAL MODEL FOR CONDENSED STATE DIFFUSION
CONTROLLED FISSION PRODUCT ABSORPTION
DURING FALLOUT FORMATION
OCD Work Unit # 3111A -- GA

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GENERAL ATOMIC

DIVISION OF GENERAL DYNAMICS

GA-7598

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by

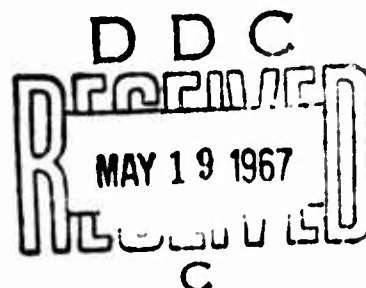
R. F. Korts and J. H. Norman

Performed for
Office of Civil Defense
Secretary of the Army
Department of Defense, 20301
under

Contract N0022866C0403

through the

**U.S. Naval Radiological Defense Laboratory
San Francisco, California 94135**



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The FORTRAN IV computer code for the UNIVAC 1108 described herein is as it existed on 12/1/66. The code has been in continuous development for 1 year and in its presented form has been applied successfully by General Atomic to the kind of problems discussed later in this report. However, the development and improvement of the code are being continued, so that duplication of results (or even close agreement) between problems run with the code as published and the code as it existed either before or after this time is not necessarily to be expected.

General Atomic has exercised due care in preparation, but does not warrant the merchantability, accuracy, and completeness of the code or of its description contained herein. The complexity of this kind of program precludes any guarantee to that effect. Therefore, any user must make his own determination of the suitability of the code for any specific use, and of the validity of the information produced by use of the code.

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ABSTRACT

A program is presented to compute fallout fission product absorption in an expanding, cooling, uniform field of gas and fallout particles where the rate of fission product absorption is controlled by fission product surface concentrations as given by Henry's law constants and diffusion of these fission products into the fallout particles. The calculations are made a nuclide chain at a time, employing nuclear device and fission product parameters. Program output includes average concentration versus particle size for each absorbed fission product at a preselected lower temperature and the amount of that fission product in the gas phase, with an option for the calculation of fission product radial profiles versus particle size. As a demonstration of this model, an initial computer study of fallout formation phenomenology is presented.

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SUMMARY

The computer code described in this report represents a model of fallout fission product absorption, the fallout particles being distributed uniformly in a cooling, expanding field of gas. Rates of fission product absorption are governed by fission product surface concentrations as given by Henry's law constants and by diffusion into the fallout particles. It is assumed that the particles neither agglomerate nor convect fission products during the time stepped calculational portion of the program. The absorption of fission products is considered for one decay chain at a time using detonation yields, initial fission product yields, half-lives, Henry's law constants, concentration independent diffusivities, and a fallout particle size versus quantity distribution. Output consists of surface concentration versus temperature for each absorbed fission product, average concentration versus particle size at a final lower temperature, and the amount of that fission product remaining in the gas phase. Optionally, radial profiles of fission product concentration versus particle size at this temperature are calculated.

Fission product distribution for mass chains 95 and 137 in fallout using this code are described. One of the important findings derived from these computer studies is an understanding of how this model considers fractionation to vary with fallout particle size distribution.

1. INTRODUCTION

Since the phenomenological discovery of fractionation of fission product elements in recovered fallout, the importance of the chemical properties of the fission products and fallout particles to the description of fallout formation has been recognized. In his treatise on fallout, Miller⁽¹⁾ has attempted to synthesize fractionation effects by allowing fission products to equilibrate with fallout until they have cooled to 1400°C and, thereafter, to surface condense on the fallout. This scheme has been considered an oversimplification and phenomenologically unsatisfactory. General Atomic has taken the position that condensed state diffusion of fission products in glassy silicate fallout particles can be considered to control the rate of fission product absorption. This report is a description of a calculational program written in FORTRAN IV for the UNIVAC 1108 in which the surface of fallout is considered to be in equilibrium with the gas phase, but bulk fallout phase absorption of fission products is diffusion controlled. In addition, fallout formation information derived from some computer experiments employing this model is presented in Appendix B.

2. GENERAL DESCRIPTION

The problem consists of determining concentrations of radioactive isotopes in fallout particles. Absorption of fission products is considered a decay chain at a time where a chain consists of a number of isotopes generally of the same mass. The last isotope in the chain is assumed to be stable for the time periods being considered. The fallout particles are assumed to be non-agglomerating, internally non-convecting, refractory, spherical glassy silicate bodies of various sizes uniformly distributed throughout a uniform temperature-concentration cloud of particles, air, and fission products. Immediately after the detonation takes place, temperatures are very high and chemistry in the cloud is unimportant. However, at a time when the cloud has cooled sufficiently to consider chemistry, this program can be applied. From this point, as time progresses (and the temperature of the cloud further decreases) the isotopes are assumed to surface condense according to Henry's law and subsequently to be diffused into the particles. Concurrently, the isotopes decay from one to another at rates dependent upon their respective half-lives. At a sufficiently low temperature, the diffusion process is considered to terminate leaving the isotopes distributed among and within the particles in some manner. The purpose of the program is to describe that distribution in terms of surface concentrations, average concentrations, and concentrations throughout the particles (profiles). To find these various concentrations, it suffices to calculate gas and condensed phase mass balances in which surface concentrations of each isotope are determined as a function of time.

Time-temperature stepping is employed in the program, and mass balances are determined at each time step. In order to determine the mass

balances, it is necessary to use input nuclear cloud parameters and chemical information. Time scaling functions for temperature and for cloud volume and a fallout mass representation are employed according to Miller⁽¹⁾ but can be changed to fit other circumstances. Fission product yields can be taken from Crocker,⁽²⁾ and fission product decay rates can be taken from Crocker, Scheidt, and Connors.⁽³⁾ Henry's law constants for this program have been presented by Norman.⁽⁴⁾ A similar report on diffusion coefficients for this program is planned.

Surface concentrations are obtained directly from the mass balance calculations. Other output parameters are calculated from the surface concentration values and the degree of diffusion that has been calculated. The computation of concentration profiles of the various sized particles at a final temperature is optional. Another option allows calculation of late distributions at such a time that all remaining gaseous short-lived isotopes have decayed and condensed. In this option, it is assumed that the isotopes are deposited on the particles according to surface area.

Surface concentrations are calculated at a finite number of points assuming that an actual time-temperature distribution can be closely approximated by a step function as shown in Fig. 1. The exact nature of this step function depends on the starting, final, and incremental temperatures (see Section 4.1, item 4). Thus, all temperature (and time) dependent quantities are assumed to be step functions as well; in particular, volumes and diffusion constants and Henry's law constants for each isotope remain constant for each temperature interval. Fission product surface concentrations are also assumed constant during any time interval.

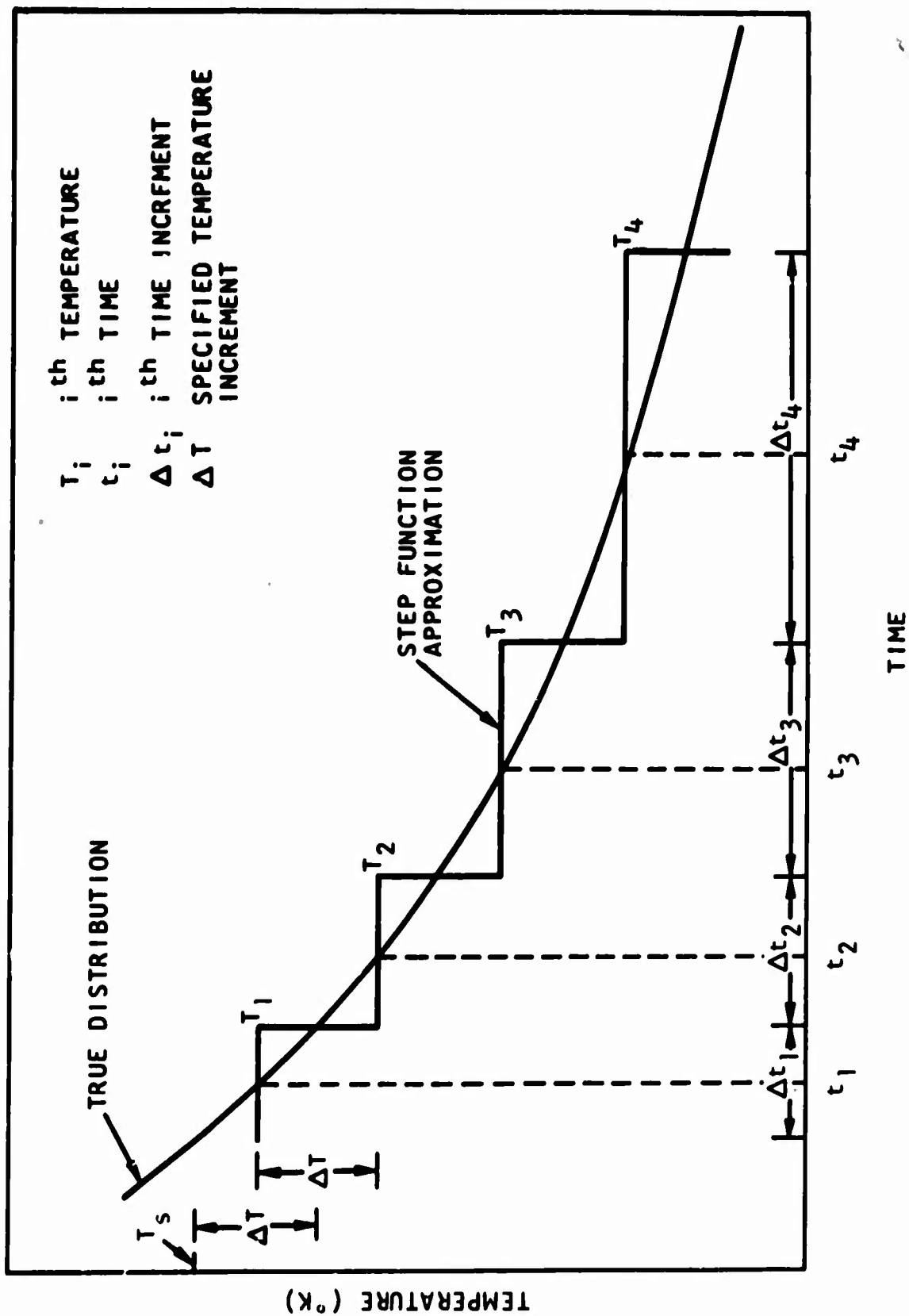


Fig. 1 -- Step function approximation to time-temperature distribution

3. METHOD

To determine the surface concentration of a given isotope at some temperature, the surface concentrations of that isotope and all its precursors at all preceding temperatures must be employed, since some fraction of each precursor will decay into the next isotope and previous surface concentrations will affect the total surface concentration at the specified temperature. We start by assuming that all of the fission products are uniformly distributed throughout the cloud at some sufficiently high temperature. To find surface concentrations at the first temperature, the following expression is used:

$$\frac{C_{i1} V_1 M_i H_{i1}}{RT_1} + C_{i1} \sum_{s=1}^P D_{i11}^{(s)} w_s = Y_{i1} \quad (1)$$

- where C_{i1} = surface concentration (g/g)* of isotope i at time t_1 (sec)
 V_1 = volume of nuclear cloud at time t_1 (liters)
 M_i = molecular weight of isotope i (g/mole)
 H_{i1} = Henry's law constant for isotope i at time t_1 (atm/g/g)
 R = ideal gas constant (liter atm/°K mole)
 T_1 = temperature at time t_1 (°K)
 Y_{i1} = yield, or total amount of isotope i , available at time t_1 (g)
 w_s = weight of soil (g) contained in particle size fraction s of radius r_s (cm)
 $D_{i11}^{(s)}$ = solution of the diffusion equation as if diffusion had taken place at a constant surface concentration C_{i1} (see Section 4.3) for particle of s^{th} radius, with the $\delta_{i1}\Delta t_1$ term for isotope i assumed constant during Δt_1 (δ_{i1} is the pertinent diffusion coefficient (δ in cm^2/sec)). The diffusion coefficients are assumed to be concentration independent.

*Suggested self-consistent units.

The Y_{i1} value is computed by considering the decay of isotopes and the H_{i1} value is computed from characteristics of the isotope and temperature (see Section 4. 1).

The first term on the left of Eq. (1) represents the amount of isotope i in the gas phase at time 1. The second term is the amount in the solid, or condensed, phase. For each s ,

$$D_{i11}^{(s)} = \frac{\bar{C}_{i1}^{(s)}}{C_{i1}}$$

for the s^{th} particle size, where $\bar{C}_{i1}^{(s)}$ is the average concentration during time t_1 . Thus

$$\begin{aligned} C_{i1} \sum_{s=1}^p D_{i11}^{(s)} w_s &= C_{i1} \sum_{s=1}^p \frac{\bar{C}_{i1}^{(s)} w_s}{C_{i1}} \\ &= \sum_{s=1}^p \bar{C}_{i1}^{(s)} w_s \end{aligned}$$

It should be noted that in this program an approximation system is used in representing the decay of fission products. During the time intervals used, a fission product is assumed to decay to one and only one product. Thus, decay is not treated as a dynamic process but as a discrete process occurring only at the end of a time step period. A nearly correct fission-product distribution is obtained at the initiation of the program by stepping the time in many small increments to this initial time after detonation. The time increments then become governed by the temperature increments. This system will cause some deviation from an exact decay solution but, generally, will only alter the final answers in a negligible fashion. Of course, as the temperature increment approaches zero, the decay system will approach the theoretical limit.

To find surface concentrations at the second temperature, the expression is

$$\begin{aligned}
& \frac{C_{i2} V_2 M_i H_{i2}}{RT_2} + C_{i1} \exp(-k_i \Delta t_1) \sum_{s=1}^P D_{i,1,2}^{(s)} w_s \\
& + C_{(i-1)1} [1 - \exp(-k_{i-1} \Delta t_1)] \sum_{s=1}^P D_{(i-1),1,1;i,2,2}^{(s)} w_s \\
& + \{C_{i2} - C_{i1} \exp(-k_i \Delta t_1) - C_{(i-1)1} [1 - \exp(-k_{i-1} \Delta t_1)]\} \sum_{s=1}^P D_{i,2,2}^{(s)} w_s = Y_{i2}
\end{aligned} \tag{2}$$

The terms on the left side of Eq. (2) can be explained as follows:

1. The first term is due to the amount of isotope i still in the gas phase.
2. The second term is due to the amount of i surface condensed associated with time t_1 decaying for Δt_1 and being diffused for $\delta_{i1} \Delta t_1 + \delta_{i2} \Delta t_2$.
3. The third term is due to the amount of isotope $i-1$ (the immediate precursor at t_1 of i) surface condensed at time t_1 decaying into i and being diffused as $i-1$ during time Δt_1 and as i during time Δt_2 .
4. The fourth term represents the amount of i being diffused within the particles as the result of the surface concentration increment caused by the temperature-time-volume increment.

The D 's are further defined in Appendix A.

It is apparent that as time is increased, the number of terms in the expression for C_{iN} becomes quite large. In fact, it can be shown (Appendix A) that if there are $n-1$ predecessors to an isotope, the number of terms required to find C_{iN} is

$$2^N - 1 \quad \text{if } N \leq n$$

and

$$\sum_{k=0}^{n-1} \left(\sum_{j=n}^{N-1} \binom{j}{k} \right) + 2^n - 1 \quad \text{if } N > n \quad (3)$$

plus additional terms for the gas phase contribution and yields.

The general expression for surface concentration can be written as

$$C_{iN} \frac{M_i V_N H_{iN}}{RT_N} + A_{iN} = Y_{iN} \quad (4)$$

where A_{iN} consists of the number of terms described by Eq. (3). Each term of A_{iN} is of the form

$$C_{(i-r)(N-j)} (\text{decay term}) \sum_{s=1}^P (D_{(1)} - D_{(2)})^w_s \quad (5)$$

where $0 \leq r \leq i-n+1$

$0 \leq j \leq N-1$

The decay term depends on the position of the isotope $i-r$ in the chain and on the time. $D_{(1)}$ and $D_{(2)}$ are diffusion terms which also depend on the position and time. (See Appendix A for details.)

Once surface concentrations have been found for all times, it remains to compute average concentrations and concentrations at various radii within the particles. Average concentrations can be obtained by mathematically combining concentration increments according to an additivity rule, as explained in Appendix A. Concentrations at any point within a particle can be found in an analogous way using relationships given by Crank. ⁽⁵⁾

4. SUBPROGRAM DESCRIPTIONS

This section describes each of the FORTRAN IV subroutines used by this code. Most of the variables used are stored in one of the common blocks described in Table 1.

4.1. SUBROUTINE INITAL

This routine reads the data cards for each calculation and prepares the input data for the main program. The flow is in approximately the order described below.

1. Read input cards. The following information is read for each calculation with the internal variable name indicated in each case. (See Appendix C for card formats.)
 - a. Length of the chain, LC (≤ 6)
 - b. Yield of device used for calculating fission product yields (in kilotons TNT), YKT
 - c. Yield of device used for calculating the time-temperature distribution and the cloud volume (in kilotons TNT), BKT
 - d. For each isotope in the chain:
 - (1) Chemical symbol, NAME
 - (2) Molecular weight (in g/mole), WMOL
 - (3) Initial yield (in atoms/ 10^4 fissions), YI
 - (4) Half-life (in seconds), HL
 - (5) Constants used in calculating Henry's law constants and diffusion coefficients (see item 8), DC1, DC2, HC1, and HC2
 - e. Starting temperature, final temperature and incremental temperature (in $^{\circ}\text{K}$), HTMP, ETMP, and TEMPV (also referred to as T_s , T_f , and ΔT)

TABLE I
VARIABLES IN COMMON BLOCKS

Variable	Dimensions	Description
BLANK Common: Contained in NORMAN, BCALC, INITIAL		
YLD	(6, 40)	Yield of each isotope at each time step
NAME	(6)	Chemical symbol of each isotope
WMOL	(6)	Molecular weight of each isotope
DFC	(6, 40)	Diffusion coefficients of each isotope at each time step
HEN	(6, 40)	Henry's law constants for each isotope at each time step
AK	(6)	Exponential constant associated with each half-life
R	(30)	Radius of each particle size
WT	(30)	Weight of soil in each particle size
VOL	(40)	Volume of the cloud at each time step
T	(40)	Time increments
TEMP	(40)	Temperatures at each time step
ATM	(40)	Times at each step
SING: Contained in NORMAN, FINAL, BCALC, INITIAL		
LC	(1)	Length of chain
IR	(1)	Number of particle sizes
NTOT	(1)	Number of time steps
NCS1	(1)	Case identification
NCS2	(1)	Case identification
TWT	(1)	Total mass of soil
ILG	(1)	Flag: if = 0, do not do FINAL calculation if $\neq$ 0, do FINAL calculation
IDPTH	(1)	Number of radii used for profile calculations
Q	(11)	Relative radii for profile calculations
B1: Contained in NORMAN, BCALC, DELTA		
DCY	(6, 40, 40)	Array of decay constants for each isotope from each time step to each other
WN	(6, 40)	Array of concentration ratios times weights for each isotope at each time step
INLOOP: Contained in NORMAN, BCALC, DELTA		
L	(1)	Subscript of isotope presently under consideration

- f. Number of particle sizes, IR (≤ 30)
 - g. For each particle size, its radius (in cm) and the fraction of soil contained in particles of that size, R, PW
 - h. The total mass of soil (in g/KT), TWGT
2. Check starting temperature. If the starting temperature is so high that all the fission products are uniformly distributed throughout each particle, that temperature is lowered by one increment and the procedure is repeated until a temperature is reached where this is not the case. Calculations are initiated after stepping back one temperature increment or to the starting temperature. To accomplish this, a D for the largest particle radius is found for each isotope at an initial time step. A D of 1 implies that an isotope is uniformly distributed throughout all particles. If $D = 1$ for all isotopes and particle sizes, the process is not yet diffusion controlled; thus, if

$$\sum_{i=1}^{LC} D_i = LC ,$$

all D's are unity. (Note that $D \leq 1$.) If this is satisfied, the temperature is reduced and the procedure is repeated.

3. Calculate w_s , the weight of soil in each particle size:
 $w_s = TWT \cdot PW_s$, where $TWT = TWGT \cdot BKT$.
4. Calculate the time-temperature distribution. Using the formula⁽²⁾

$$T = 4.66 \times 10^3 (BKT)^{-0.010} \exp(-0.546(BKT)^{-0.373} t) = f(t) , \quad (6)$$

times and incremental times are calculated to correspond to each specified temperature. The temperatures are calculated from

$$T_n = T_s - \left(\frac{2n - 1}{2} \right) \Delta T ,$$

and the times such that

$$T_n = f(t_n) .$$

Δt_n is defined by

$$\Delta t_n = f^{-1}\left(T_n + \frac{\Delta T}{2}\right) - f^{-1}\left(T_n - \frac{\Delta T}{2}\right) \text{ (see Fig. 1) } . \quad (7)$$

5. Convert initial yields, Y_i , to grams.

$$Y_i(g) = Y_i \cdot \text{WMOL} \cdot YKT \cdot 2.3410261 \times 10^{-5}$$

6. Find the quantities k_i . These quantities are used to calculate decay coefficients where

$$d_{inm} = \exp[-k_i(\Delta t_n + \Delta t_{n+1} + \dots + \Delta t_m)] \quad m > n$$

$$= \exp(k_i \Delta t_n) \quad m = n$$

$$= 1 \text{ (a computational aid)} \quad m < n$$

and

$$k_i = \frac{\ln(2)}{HL_i} .$$

7. Calculate yields at t_s where

$$t_s = f^{-1}(T_s) .$$

Yields at t_s are approximated by the following scheme:

Let $\Delta h = \min(HL)/10$ when $\min(HL)$ is the minimum half-life in the chain

Let $\tau_n = n(\Delta h)$, and let $i-1$ specify the precursor of isotope i . Then,

$$Y_i(\tau_1) = Y_i(0) \exp(-k_i \Delta h) + Y_{i-1}(0) [1 - \exp(-k_{i-1} \Delta h)] \quad (8)$$

$\vdots$

$$Y_i(\tau_n) = Y_i(\tau_{n-1}) \exp(-k_i \Delta h) + Y_{i-1}(\tau_{n-1}) [1 - \exp(-k_{i-1} \Delta h)] \quad (9)$$

Equation (9) is repeated for all n and i until n is such that $\tau_{n+1} > t_s$. For the last step, Δh is changed such that $\Delta h = t_s - \tau_n$ and Eq. (9) is repeated. If the original $\Delta h \geq t_s$, Δh is set equal to t_s and only Eq. (8) is used.

8. Calculate diffusion coefficients and Henry's law constants. The expressions⁽⁴⁾

$$\log(H_{in}) = HC1_i - HC2_i / T_n \quad (10)$$

and

$$\log(\delta_{in}) = DC1_i - DC2_i / T_n \quad (11)$$

are used to find δ and H for all isotopes and temperatures.

9. Volumes are computed for all temperatures using the expression⁽³⁾

$$V_n = \left\{ 5.69 \times 10^2 (BKT)^{1/3} \exp[0.17(BKT)^{-0.373} t_n] \right\}^3 \frac{4\pi}{3}$$

10. Input and computed quantities are printed. Input is actually printed as it is read and calculated quantities as they are calculated. (See Appendix D for sample printout.)

4.2. MAIN ROUTINE (NORMAN)

The main routine has three basic functions:

1. Setup and initial calculation of arrays needed (such as yields and decay coefficients) for the main loop.
2. Execution of the main loop which finds surface concentrations, average concentrations, and profiles.
3. Writing out of results.

4.2.1. Setup and Initial Calculations

The main routine starts by calling subroutine INITAL, which supplies it with necessary input data. Next it computes the array of decay coefficients, d_{inm} , as defined in Section 4.1, item 6; the array of

yields Y_{in} , where Y_{in} is the yield of isotope i at time n ; and the arrays UN and WN. The yields are found by using Eq. (8), Section 4.1, item 7, modified as

$$Y_{in} = Y_{i,n-1} d_{i,n-1,n-1} + Y_{i-1,n-1} (1 - d_{i-1,n-1,n-1})$$

The UN^* and WN arrays are defined by

$$UN_{ins} = E(\delta_{in} \Delta t_n, r_s)$$

$$WN_{in} = \sum_{s=1}^p UN_{ins} w_s$$

where δ_{in} = diffusion coefficient of isotope i at time t_n

Δt_n = n^{th} time interval

r_s = radius of s^{th} particles

w_s = weight of soil in the s^{th} particle size

$E(\delta_{in} \Delta t_n, r_s)$ = solution of diffusion equation for sphere of radius r_s and $\delta_{in} \Delta t_n$ term

Finally, the surface concentrations are calculated for each isotope at time t_1 by the relation

$$C_{i1} \left(\frac{WMOL_i H_{i1} V_1}{RT_1} + WN_{i1} \right) = Y_{i1}$$

4.2.2. Main Loop[†]

The following steps are taken in the main loop for each isotope and each time:

1. Find the terms due to decay of this isotope from previous times.
2. For each precursor of this isotope at each preceeding time, find all possible paths for decay, and for each such path find a diffusion term (see Section 4.8) and a decay term (see Section 4.7).

* $UN_{ins} = D_{inn}^{(s)}$
[†] See Fig. 2

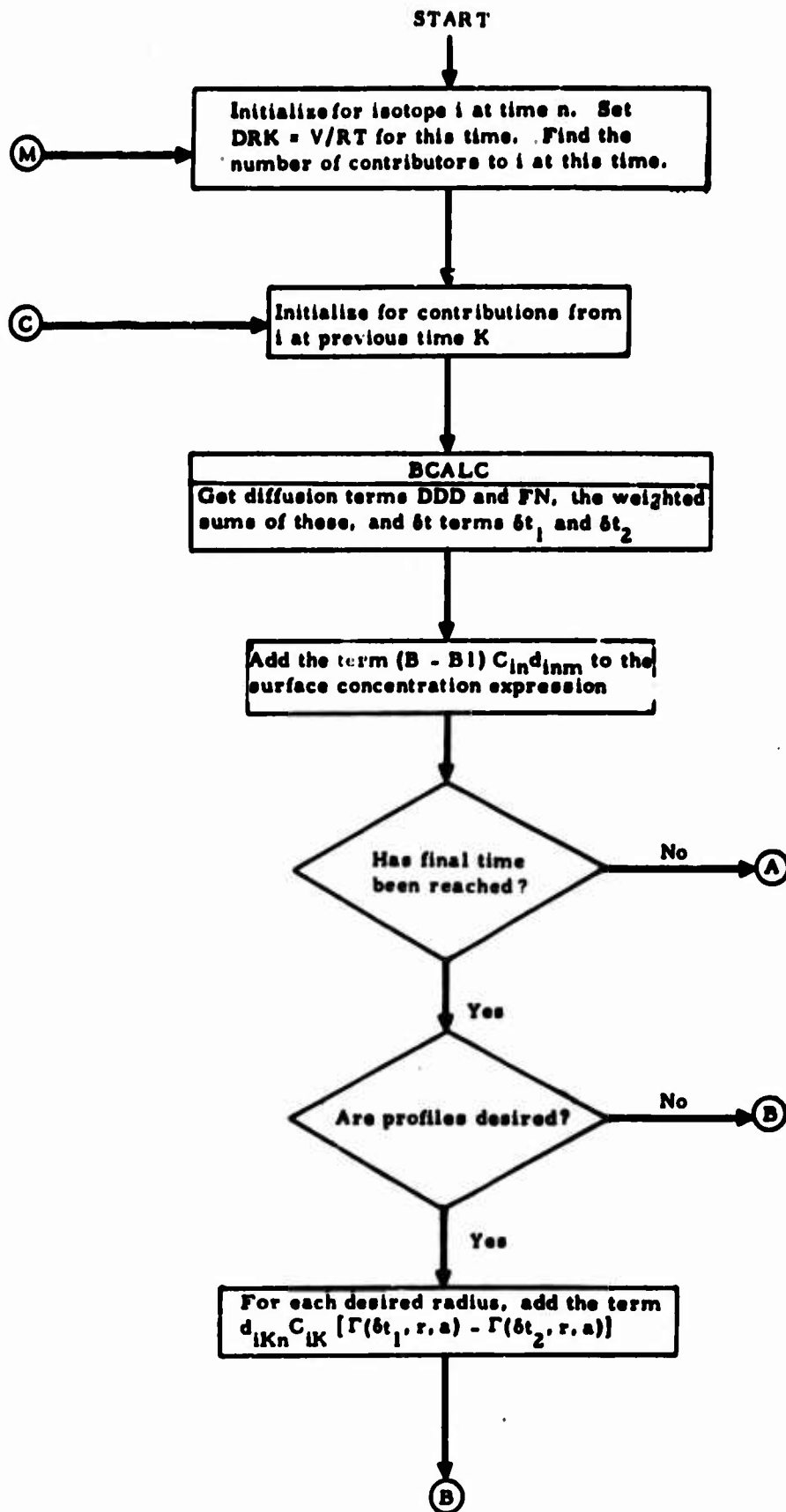


Fig. 2--Flow chart, main loop NORMAN (Sheet 1 of 5)

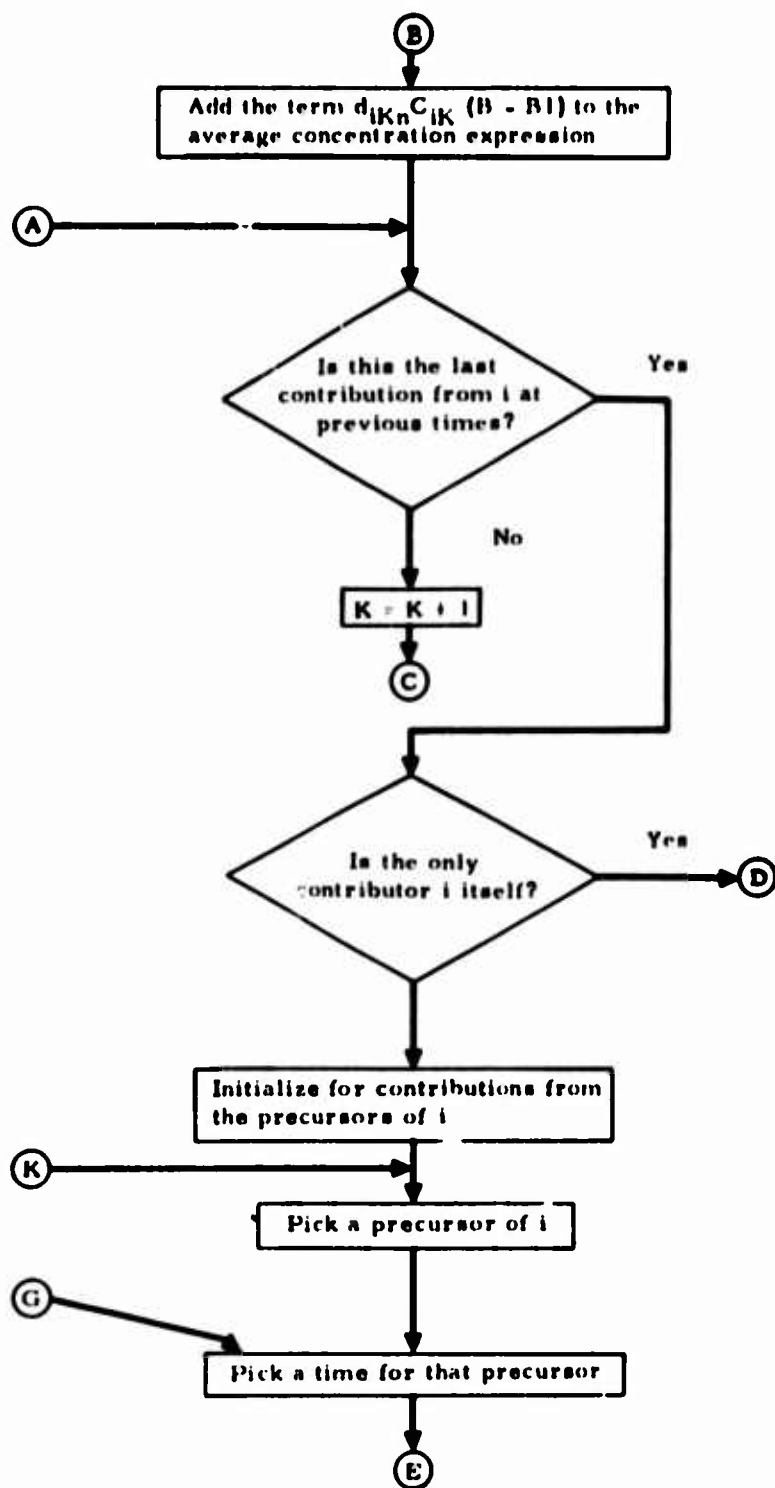


Fig. 2-- Flow chart, main loop NORMAN (Sheet 2 of 5)

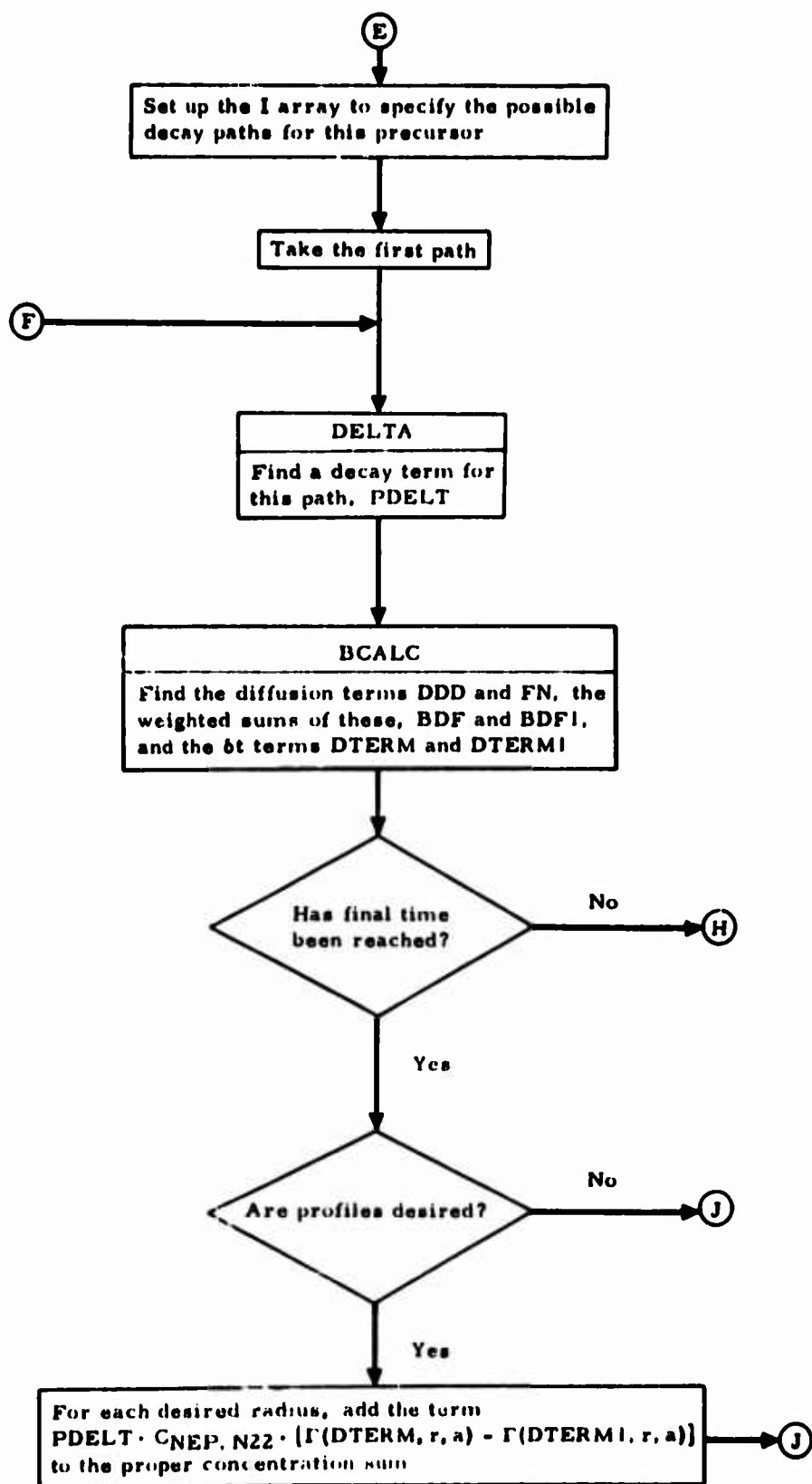


Fig. 2--Flow chart, main loop NORMAN (Sheet 3 of 5)

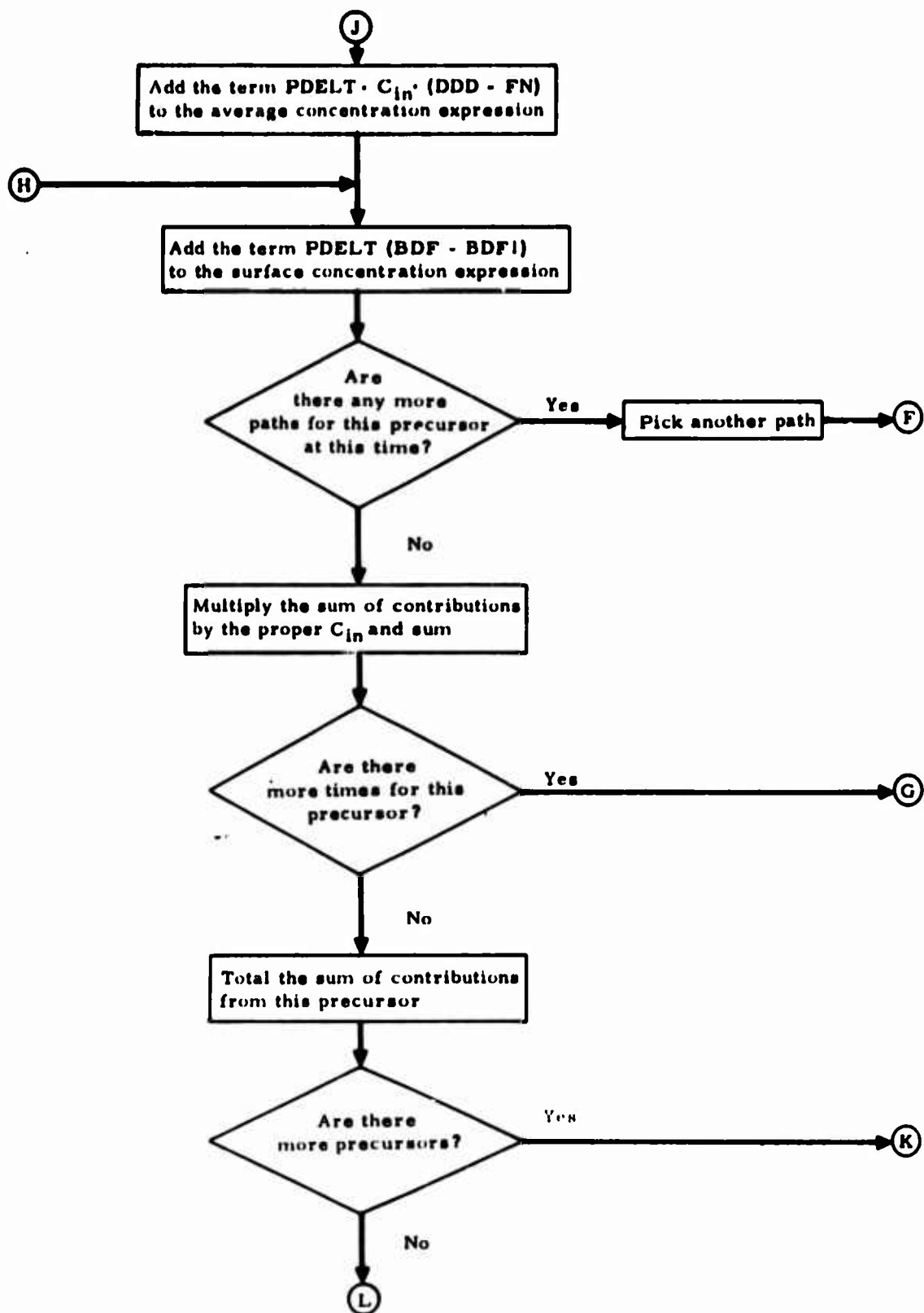


Fig. 2--Flow chart, main loop NORMAN (Sheet 4 of 5)

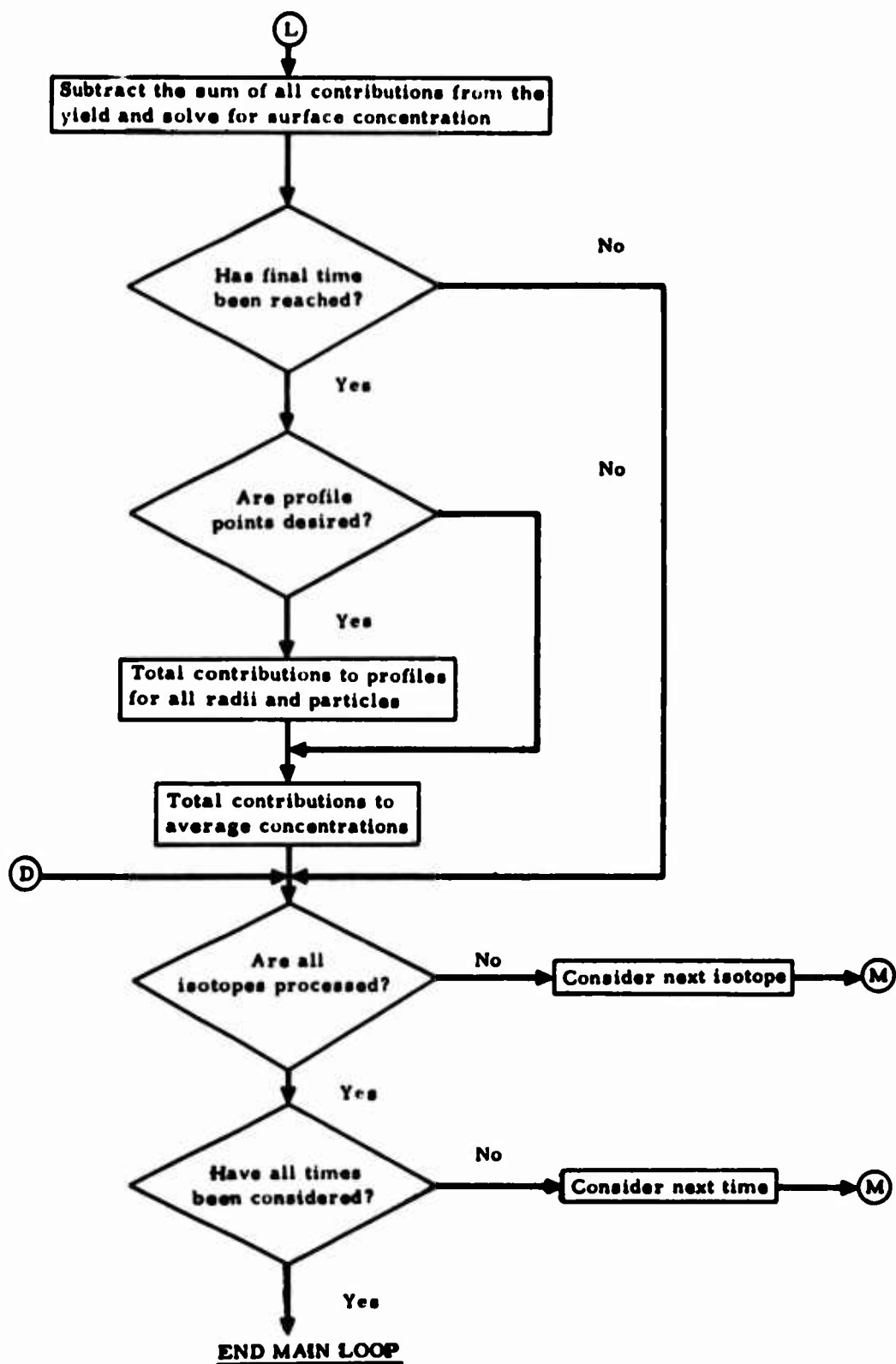


Fig. 2--Flow chart, main loop NORMAN (Sheet 5 of 5)

forming the product as in Eq. (5) and adding to the previous summed contributions. In the event that the final time step has been reached, add the appropriate terms to the average concentration and profile point sums.

3. Let α represent the total of the sum of all contributions to the average concentration expression except that term due to absorption diffusion of this isotope from surface concentration C_{in} . Then the surface concentration is found from

$$C_{in} \left(\frac{WMOL_i H_{in} V_n}{RT_n} + WN_{in} \right) = Y_{in} - \alpha$$

4. 2. 3. Output

Certain other calculations, as follows, are made while printing out results.

1. Calculation of the amount of material remaining in the gas phase for each isotope at each time:

$$GAS_{in} = \frac{C_{in} H_{in} V_n WMOL_i}{RT_n}$$

2. Computation of the amount of material in the solid phase (diffused), per isotope, at the final time:

$$SOLID_i = \sum_{s=1}^P A_{is} w_s$$

where A_{is} is the average concentration of isotope i in particle size s .

3. Computation of the weighted mean average concentration for each isotope i :

$$\bar{A}_i = \frac{SOLID_i}{(\text{total weight})}$$

The following quantities are printed:*

- a. T_n , t_n , and C_{in} for each i, n
- b. T_n , t_n , and GAS_{in} for each i, n
- c. T_N , r_s , and A_{is} , N being the final time and for each i, s
- d. $\bar{A}_i$ for each i
- e.† $C_{is}(r)$ for each r, i, s , where $C_{is}(r)$ is the concentration of isotope i in particle s at radius r
- f. A summary of the amounts of material in gas and solid phases at the final temperature

4. 3. FUNCTION DIFFUS (DT, R)

This function computes a solution to the diffusion equation for a spherical body of radius r . The true solution is:⁽⁵⁾

$$D = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp(-n^2 \pi^2 \delta t / r^2) \quad (12)$$

or

$$D = 6 \left(\frac{\delta t}{r^2} \right)^{1/2} \left(\pi^{-1/2} + 2 \sum_{n=1}^{\infty} \text{ierfc} \frac{nr}{\sqrt{\delta t}} \right) - 3 \left(\frac{\delta t}{r^2} \right), \quad (13)$$

where⁽⁶⁾

$$\text{ierfc}(x) = \int_x^{\infty} \text{erfc}(u) du$$

and

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-u^2} du.$$

* See Appendix D for sample output.

† This printout and the calculation are optional (see Section 2).
(See Appendix A for details.)

Function DIFFUS uses the following approximations to these solutions:

$$\text{Let } x = r/\sqrt{\delta t}$$

1. If $x > 3.14$,

$$D = \frac{3}{x} \left(\frac{2}{\sqrt{\pi}} - \frac{1}{x} \right) ,$$

which is a truncation of Eq. (13) with the infinite series neglected.

2. If $2.0 < x \leq 3.14$,

$$D = 1 - \frac{6}{\pi} \left[\exp(-\pi^2/x^2) + \frac{1}{4} \exp(-4\pi^2/x^2) \right]$$

3. If $0.745 < x \leq 2.0$,

$$D = 1 - \frac{6}{\pi} \left[\exp(-\pi^2/x^2) \right]$$

4. If $x \leq 0.745$,

$$D = 1 ,$$

where 2, 3, and 4 are truncations of Eq. (12).

The errors incurred by these approximations are bounded as follows:

$$\begin{aligned} |E_4| &\leq 2.5 \times 10^{-8} \\ |E_3| &\leq 1 \times 10^{-5} \\ |E_2| &\leq 1 \times 10^{-5} \\ |E_1| &\leq 5 \times 10^{-6} \end{aligned}$$

where E_i is the error using approximation i.

4. 4. SUBROUTINE FINAL (AVCON, GAS, R, WT, NAME)

Subroutine FINAL computes the concentration of the last isotope in the various particles assuming that

1. All other isotopes have completely decayed into the last one
2. None of the last isotope has decayed away

3. All of the material in the gas phase when the main process was terminated has condensed onto the particles according to surface area

Let a_{is} = average concentration of isotope i in particle of size s .

$Z_s = r_1 / r_s$, where r_1 is the radius of the largest particles, and

g_i = amount of isotope i in the gas phase when main process was terminated.

Then,

$$f_s = \sum_{i=1}^{LC} a_{is}$$

$$G = \sum_{i=1}^{LC} g_i$$

$$V_s = Z_s w_s \text{ (proportional to the surface area)}$$

$$v = \sum_{s=1}^P V_s$$

where w_s = weight of particles of size s .

Also,

$$F_s = \frac{Z_s G}{v} + f_s$$

and

$$W_s = F_s w_s ,$$

where F_s = total average concentration (includes gas condensation) in particle of size s

W_s = total weight of isotope in particle of size s

f_s = average concentration in particle of size s due to the decay of solids.

The average concentration of the last isotope of the chain, f_s , is considered to be equal to the sum of the average concentrations of all the members of the chain when the main process was terminated. Subroutine FINAL also lists out f , F , and W for each particle size.

4. 5. FUNCTION PROFIL (DT, r, Q)

Function PROFIL computes the concentration at a distance $a = rQ$ from the center of a spherical particle of radius r . The value of the concentration is found from the expression:⁽⁵⁾

$$\frac{C}{C_0} = 1 + \frac{2r}{\pi a} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin \frac{n\pi a}{r} e^{-n^2 \pi^2 \delta t / r^2} \quad (14)$$

or

$$\frac{C}{C_0} = \frac{r}{a} \sum_{n=0}^{\infty} \left\{ \operatorname{erfc} \left[\frac{(2n+1)r - a}{2\sqrt{\delta t}} \right] - \operatorname{erfc} \left[\frac{(2n+1)r + a}{2\sqrt{\delta t}} \right] \right\}, \quad (15)$$

where r = radius of particle

a = distance from center of particle, $a \geq 0.1r$

C_0 = surface concentration (assumed constant)

Function PROFIL computes the value of the ratio C/C_0 using a truncation of Eq. (14) or Eq. (15). In all cases, the series is terminated when either

$$\frac{|S_n - S_{n-1}|}{|S_n|} < \epsilon^*$$

or when $n > 100$, where S_k is Eq. (14) or Eq. (15) truncated to k terms.

The series used is chosen using the following criteria:

If $\delta \Delta t < b_j$, Eq. (15) is used where j is determined as the smallest integer such that

$$r \geq 10^{-j},$$

where $b_j = 10^{1-j - [(j-1)/2]}$

and where $[x]$ = greatest integer I such that $I \geq x$.

Otherwise Eq. (14) is used.

* $\epsilon = 0.01$ at present.

This scheme was determined by examining the values of Eqs. (14) and (15) for various numbers of terms and picking the equation that required the least number of terms.

4.6. FUNCTION ERF(X)

Function ERF computes an approximate value of the error function using a rational approximation. The error function is defined as:

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt .$$

ERF uses the approximation⁽⁵⁾

$$\text{erf}(x) = 1 - (a_1 t + a_2 t^2 + a_3 t^3) e^{-x^2}$$

where

$$t = \frac{1}{1 + px}$$

and

$$p = 0.47047$$

$$a_1 = 0.3480242$$

$$a_2 = -0.0958798$$

$$a_3 = 0.7478556$$

The error E in this approximation is bounded by

$$|E| \leq 2.5 \times 10^{-5} .$$

4.7. SUBROUTINE DELTA (N, NT, I, PR)

Subroutine DELTA computes the decay coefficient, PR, associated with decay of isotope i to the presently considered isotope at time NT. The array I specifies the path being taken, with I(1) specifying the time at which i is considered.

A product of terms of the form*

$$d_{inm} (1 - d_{i, m+1, m+1})$$

is found. The d array is initially calculated in the main routine in such a way that

$$d_{inm} = 1 \quad \text{if } n > m .$$

The general product then has the form

$$PR = d_{inm} (1 - d_{i, m+1, m+1}) d_{k, m+2, \ell} (1 - d_{k, \ell+1, \ell+1}) \cdots d_{n, r, NT-1} ,$$

where i is the subscript of the isotope presently under consideration. The values of n, ℓ , and r depend on the path.

4. 8. SUBROUTINE BCALC (N, NT, I, KLAG, B, DD, DT)

This routine computes the correct δt term associated with the path specified by I and calls DIFFUS to solve for a diffusion term.

The δt term described by Eq. (A-10) is computed from the relation

$$\delta t = \sum_{p=n}^m \delta_{ip} \Delta t_p + \sum_{p=k}^{\ell} \delta_{(i+1)p} \Delta t_p + \cdots + \sum_{p=v}^q \delta_{(i+r)p} \Delta t_p ,$$

where n, m, k, ℓ , $\dots$, v, and q are specified by the I array. The corresponding diffusion terms,

$$D_{i, n, m; i+1, k, \ell; \dots; i+r, v, q}^{(s)}$$

are then found by calling DIFFUS for each s. Depending upon KLAG, either the first D or the second D in Eq. (A-9) is found and stored in the DD array. δt is stored in DT and the expression

$$\sum_{s=1}^P (D_{i, n, m; i+1, k, \ell; \dots; i+r, v, q}^{(s)})^w s$$

is stored in B.

* See Section 4.1, item 6 for definition of d_{inm} .

APPENDIX A
DERIVATION OF EQUATIONS USED

A. 1. THE GENERAL TERM IN THE SURFACE CONCENTRATION EQUATION

An analysis of the case of a single stable isotope with no precursors, which eliminates the decay question, makes it easier to understand the general case. If Eqs. (1) and (2) in Section 3 are rewritten leaving out the isotope identification and letting $w_1 = 1$ and $p = 1$, the following equations are obtained:

$$C_1 G_1 + C_1 D_{11} = Y \quad (A-1)$$

and

$$C_2 G_2 + C_1 D_{12} + (C_2 - C_1) D_{22} = Y, \quad (A-2)$$

where

$$G_N = \frac{V_N M H_N}{RT_N}.$$

Equation (A-2) can be rewritten as follows:

$$C_2 G_2 + C_2 D_{22} + C_1 (D_{12} - D_{22}) = Y.$$

The expression at t_3 is

$$C_3 G_3 + C_1 D_{13} + (C_2 - C_1) D_{23} + [C_3 - (C_2 - C_1) - C_1] D_{33} = Y$$

or

$$C_3 G_3 + C_1 D_{13} + (C_2 - C_1) D_{23} + (C_3 - C_2) D_{33} = Y.$$

The expression at t_4 is

$$C_4 G_4 + C_1 D_{14} + (C_2 - C_1) D_{24} + (C_3 - C_2) D_{34} + (C_4 - C_3) D_{44} = Y.$$

The expression at step N is then

$$C_N G_N + C_1 D_{1N} + \sum_{k=2}^N (C_k - C_{k-1}) D_{kN} = Y . \quad (A-3)$$

Equation (A-3) can be rewritten as follows:

$$C_N G_N + C_1 D_{1N} + \sum_{k=2}^N C_k D_{kN} - \sum_{k=1}^{N-1} C_k D_{k+1, N} = Y$$

or

$$C_N G_N + \sum_{k=1}^N C_k D_{kN} - \sum_{k=1}^{N-1} C_k D_{k+1, N} = Y$$

or, finally, as

$$C_N (G_N + D_{NN}) + \sum_{k=1}^{N-1} C_k (D_{kN} - D_{k+1, N}) = Y . \quad (A-4)$$

Next, consider the general expression with decay from precursors. Figure A.1 represents n isotopes at N time steps; the connecting lines represent the ways in which decay can occur. The numbers occurring with each state represent the number of ways in which that isotope at that time can decay to isotope 1 at t_N . It is apparent that if $N \leq n$, the diagram is triangular and is a Pascal's triangle, the numbers representing binomial coefficients. Thus for $N \leq n$, the total number of terms in the surface concentration expression is

$$2^0 + 2^1 + 2^2 + \dots + 2^{N-1} = 2^N - 1 .$$

For $N > n$, the diagram is a truncated Pascal's triangle. In this case, there are $2^n - 1$ terms from the purely triangular portion, plus

$$\sum_{k=0}^{n-1} \left[\sum_{j=n}^{N-1} \binom{j}{k} \right]$$

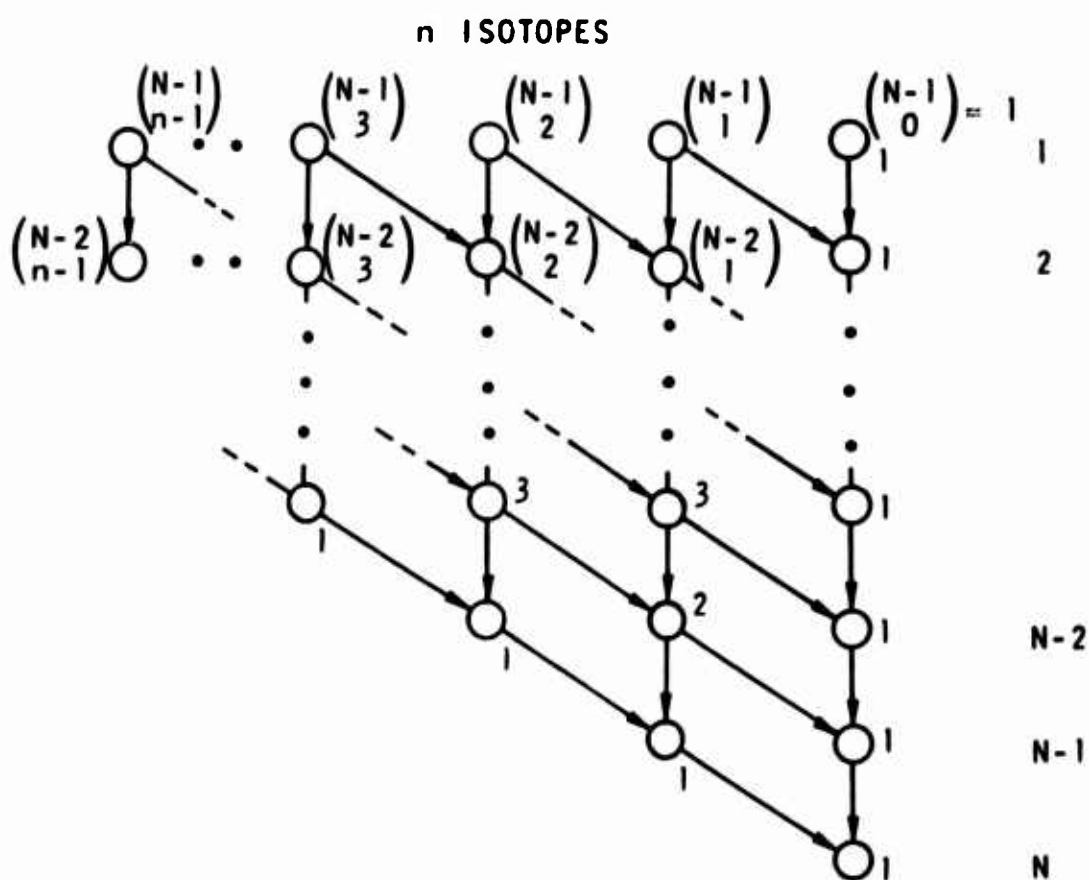


Fig. A. 1--Decay paths for n isotopes through N time steps

from the rectangular portion, giving a total of

$$M = \sum_{k=0}^{n-1} \left[\sum_{j=n}^{N-1} \binom{j}{k} \right] + 2^n - 1 \quad (\text{A-5})$$

In Eq. (A-4), each term in the sum consists of a surface concentration times a diffusion term. In each case the diffusion term is the difference of two diffusion terms, one representing diffusion from t_k to t_N and the other from $t_{(k+1)}$ to t_N . Each of the M terms in the general expression is of a similar form, modified by a decay term.

As an example, consider the terms associated with the position $n = 2$ in Fig. A.1 at t_4 . There are three possible paths for decay to isotope 1. The decay coefficients associated with these paths are

$$\left. \begin{aligned} (1 - d_{211})d_{123} \\ d_{211}(1 - d_{222})d_{133} \\ d_{212}(1 - d_{233}) \end{aligned} \right\} \quad (\text{A-6})$$

where d_{inm}^* represents the decay coefficient of isotope i from time step Δt_n through Δt_m . The corresponding isotope indexed diffusion terms are:

$$\left. \begin{aligned} D_{2,1,1;1,2,4} - D_{1,2,4} \\ D_{2,1,2;1,3,4} - D_{2,2,2;1,3,4} \\ D_{2,1,3;1,4,4} - D_{2,2,3;1,4,4} \end{aligned} \right\} \quad (\text{A-7})$$

where $D_{i,n,m;i+1,k,\ell;\dots;i+r,v,q}$ represents diffusion as isotope i from t_n to t_m , as isotope $i+1$ from t_k to t_ℓ , etc., and as isotope $i+r$ from time t_v to $t_q^\dagger$ (see Eq. (A-10)).

* See Section 4.1, item 6.

† Note that decay is carried only through Step 3, while diffusion is carried through Step 4 (see Section 3).

The total contribution to isotope 1 at t_4 from isotope 2 at t_1 can be written as

$$\begin{aligned}
 C_{21} [(1 - d_{211})d_{123}(D_{2,1,1;1,2,4} - D_{1,2,4}) \\
 + d_{211}(1 - d_{222})d_{133}(D_{2,1,2;1,3,4} - D_{2,2,2;1,3,4}) \\
 + d_{212}(1 - d_{233})(D_{2,1,3;1,4,4} - D_{2,2,3;1,4,4})] \quad (A-8)
 \end{aligned}$$

where again a single particle of unit weight is assumed.

From the above discussion it can be seen that the general term is of the form

$$\begin{aligned}
 C_{in} d_{inm} (1 - d_{i,m+1,m+1}) d_{i+1,m+2,k} (1 - d_{i+1,k+1,k+1}) \cdots \\
 \cdots d_{i+r,\ell,N-1} \left[\sum_{s=1}^P (D_{i,n,m+1;i+1,m+2,k+1;\cdots;i+r,\ell,N}^{(s)} \right. \\
 \left. - D_{i,n+1,m+1;i+1,m+2,k+1;\cdots;i+r,\ell,N}^{(s)} w_s \right] \quad (A-9)
 \end{aligned}$$

where

1. We are considering the contribution to isotope $i + r$ at time N via some path, from isotope i at time n .
2. $m \geq n + 1$
 $k \geq m + 1$
 $\vdots$
 $\ell \geq i + r$
3. There are p particle sizes with weights $w_1, w_2, \dots, w_p$.
4. If $n > m$, $d_{inm} = 1$ as a mathematical convenience.

The quantity $D_{i,n,m;i+1,k,\ell;\cdots;i+r,v,q}^{(s)}$ represents a solution of the diffusion equation for a particle of radius r_s and δt term given by

$$\delta t = \sum_{n=q}^n \delta_{in} \Delta t_n + \sum_{n=k}^{\ell} \delta_{i+1,n} \Delta t_n + \cdots + \sum_{n=v}^q \delta_{i+r,n} \Delta t_n \quad (A-10)$$

where δ_{in} is defined by Eq. (11), Section 4.1, item 8, and Δt_n is defined by Eq. 7, Section 4.1, item 4.

A. 2. AVERAGE CONCENTRATIONS AND PROFILES

As in the case of surface concentrations, the case considered is that of a single stable isotope with no precursors. The basic relationship is

$$\frac{\bar{C}}{C} = D, \quad (A-11)$$

where $\bar{C}$ is an average concentration increment, C is a surface concentration increment, and D is a diffusion term as in Section A. 1. At the first time step, it is clear that

$$\bar{C}_1 = C_1 D_{11}.$$

At the second time step,

$$\bar{C}_2 = C_1 D_{12} + (C_2 - C_1) D_{22},$$

where the first term on the right represents the concentration at time step 1 further diffused and the second term represents material condensed and diffused during time step 2. Similarly, at time step 3,

$$\bar{C}_3 = C_1 D_{13} + (C_2 - C_1) D_{23} + (C_3 - C_2) D_{33},$$

where the three terms represent, respectively, condensation during time steps 1, 2, and 3, and diffusion from those times to time 3. At time step N , it follows that

$$\bar{C}_N = C_1 D_{1N} + \sum_{k=2}^N (C_k - C_{k-1}) D_{k,N}, \quad (A-12)$$

where each term in the sum represents a concentration diffused over the specified time interval.

To obtain an expression similar to Eq. (A-4), Eq. (A-12) is rewritten

as

$$\bar{C}_N = C_1 D_{1N} + (C_N - C_{N-1}) D_{N,N} + \sum_{k=2}^{N-1} C_k D_{k,N} - \sum_{k=2}^{N-1} C_{k-1} D_{k,N} ,$$

or

$$\bar{C}_N = C_N D_{N,N} + \sum_{k=1}^{N-1} C_k D_{k,N} - \sum_{k=1}^{N-1} C_k D_{k+1,N} ,$$

or, finally, as

$$\bar{C}_N = C_N D_{N,N} + \sum_{k=1}^{N-1} C_k (D_{k,N} - D_{k+1,N}) . \quad (A-13)$$

It can be seen that the general expression including decay from precursors consists of terms similar to Eq. (A-9). The number of such terms is the same as that described in Section A.1, since there is a contribution from each isotope at each preceding time step for each possible decay path. Here the expression for average concentration in the s^{th} particle size consists of terms of the form:

$$\begin{aligned} & C_{in} d_{inm} (1 - d_{i,m+1,m+1}) d_{i+1,m+2,k} (1 - d_{i+1,k+1,k+1}) \cdots \\ & \cdots d_{i+r,\ell,N-1} D_{i,n,m+1;i+1,n+2,k+1;\cdots;i+r,\ell,N}^{(s)} \\ & - D_{i,n+1,m+1;i+1,m+2,k+1;\cdots;i+r,\ell,N}^{(s)} \end{aligned} \quad (A-14)$$

summed over all contributions.

To find profiles, it is desired to find the concentration at specific points within the particle. The basic relation here is (see Ref. 6)

$$\frac{C(a)}{C} = \Gamma(a, r, \delta t) , \quad (A-15)$$

$$\text{where } \Gamma(a, r, \delta t) = 1 + \frac{2r}{\pi a} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin \frac{n\pi a}{r} \exp(-n^2 \pi^2 \delta t / r^2) .$$

As with average concentrations, Eq. (A-15) gives a concentration increment due to diffusion during the given time and with zero initial concentration. For a stable isotope with no precursors we can, in an analogous manner, obtain the expression

$$C_{iN}(a) = C_{iN} \Gamma(a, r, \delta_{iN} \Delta t_N) + \sum_{k=1}^{N-1} C_{ik} \left[\Gamma\left(a, r, \sum_{n=k}^N \delta_{in} \Delta t_n\right) - \Gamma\left(a, r, \sum_{n=k+1}^N \delta_{in} \Delta t_n\right) \right] \quad (A-16)$$

and in the general case obtain a sum of terms similar to Eq. (A.14) with each D replaced by the appropriate Γ .

APPENDIX B

MODEL CALCULATIONS

Some of the initial results of calculations obtained using this program are considered in this appendix. In these calculations examples of a refractory and a volatile chain, 95 and 137, respectively, were selected for study. The results should demonstrate the difference in behavior for extreme cases of refractory and volatile nuclide chains with varying conditions and thus provide limits of fission product behavior during fallout formation. Data sources for these calculations have been listed earlier. In addition to these sources, the standard particle distribution shown in Table B. 1 was developed from one used by Miller, * experimental and estimated diffusion coefficients were employed as measured or estimated in reported studies, and total fissions were scaled as a function of weapon fission yield according to Miller. ⁽¹⁾

Several program variables had to be investigated in order to demonstrate the degree of dependence of the calculational system on these variables. For instance, the variation of results with the size of the temperature increment must be vanishingly small for the selected temperature increment as smaller increments are considered. Also, the variation of results with choice of initial and final calculational temperatures should be defined. Finally, the fact that the particle size distribution employed is idealized—that is, some selected radii represent all of the mass of the particles—should be considered. These points have been investigated and seem to be satisfactorily understood as will be demonstrated as the calculations are presented.

The calculations for the 95 and 137 chains (neglecting $I^{137} \rightarrow Xe^{136}$ and $I^{138} \rightarrow Xe^{137}$) were performed using 2700°K as an initial temperature, 200°K increments, terminating at 900°K, and employing the particle distribution described in Table B. 1. The size of the detonation was taken as 100 KT pure fission. The amount of soil associated with the cloud was 8.5×10^9 g.

* Miller, C. F., private communication, November 1965.

Table B. 1
STANDARD PARTICLE SIZE DISTRIBUTION

Designation	Particle Radius (cm)	Weight Percent of Particle Fraction
T	0. 00030	0. 38
S	0. 0030	28. 92
M	0. 0154	60. 2
L	0. 13	10. 5

The calculated descriptions of behavior of the ^{137} and 95 chains are presented in Figs. B. 1 and B. 2, respectively. In these figures, the average concentration of a particular nuclide in the chain is presented as a function of the last temperature for which the adsorption-diffusion process was calculated. Also included are the gas phase contents of the nuclides at the same temperatures (designated by open circles). In the phenomena described in Fig. B. 1, the curve for the tellurium gas phase content is decreasing as the result of two processes:

1. Te^{137} decay.
2. Absorption of Te^{137} in the fallout particles.

Corresponding processes are involved to different degrees in the description of the gas phase content of any nuclide. In the case of Te^{137} at the lowest temperature, so little of the Te^{137} has been absorbed that the gas phase content curve closely represents the tellurium decay. The gas phase content curves for iodine and xenon also essentially represent radioactive decay phenomena alone, since both of these elements are very volatile. On the other hand, the gas phase content of cesium is dropping sharply with temperature, not because Cs^{137} is decaying but, in this case, because 94% of the cesium in the system has been absorbed by the fallout particles by the 1900°K point and more is absorbed at lower temperatures. Thus, the cesium curve describes mainly the absorption process.

The average concentrations of Te^{137} as they vary with temperature and particle size were also investigated. The large particles, L, as defined in Table B. 1, show a slow but continuous increase in average tellurium concentration as the temperature decreases (see Fig. B. 1).

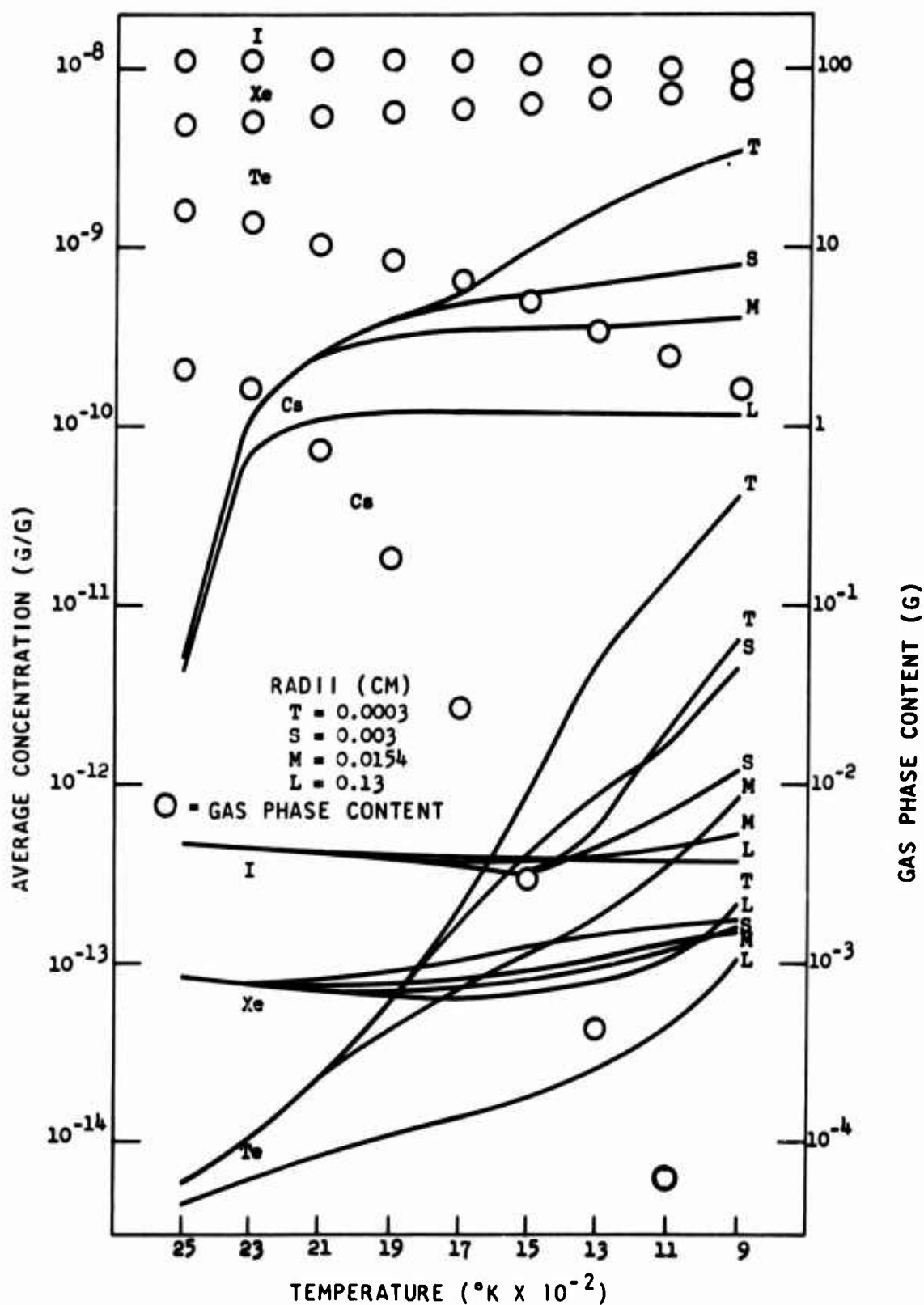


Fig. B. 1--Calculated absorption in fallout of members of 137 chain in g fission product per g fallout as a function of temperature and particle size

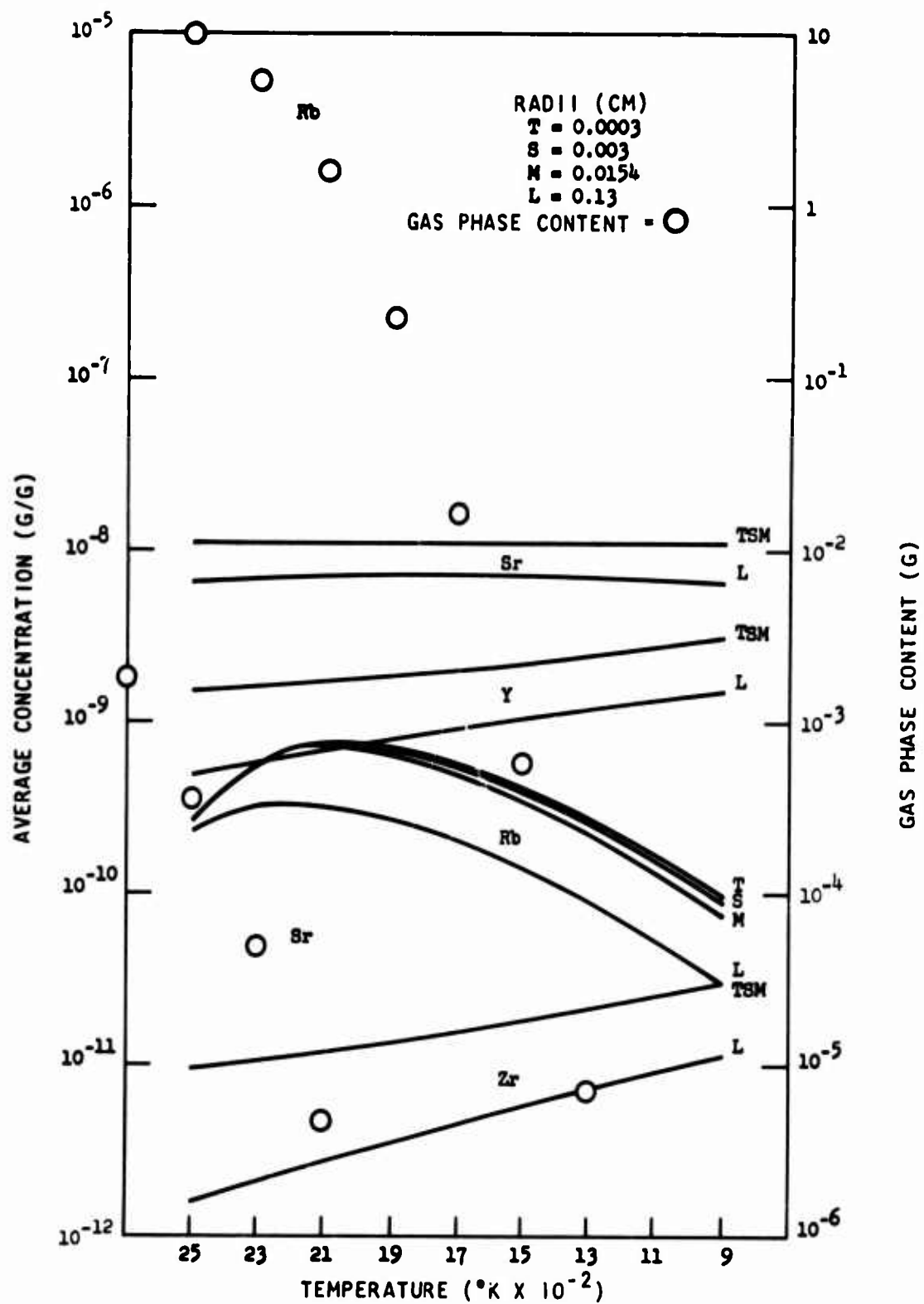


Fig. B.2--Calculated absorption in fallout of members of 95 chain in g fission product per g fallout as a function of temperature and particle size

Also, at the initial temperature the L particles exhibit a slightly lower concentration than the medium-sized particles, M. This point is important because it suggests that at the highest temperature of the calculation, the L particles did not equilibrate with the gas phase; that is, diffusion was not complete. In contrast, the tiny particles, T, the small particles, S, and the M particles exhibit essentially the same average concentration at the initial temperature. Further consideration of Fig. B.1 reveals that the L particles experience a somewhat smaller increase in tellurium concentration than the M particles as the temperature decreases. Also, the S and M curves exhibit a departure from the more sharply rising T curve at two different lower temperatures. Departure points from the T curve occur as the central portions of the L, S, and M particles effectively lose contact with the surface and diffusive transport begins to control the rate of absorption. In addition, at 1300°K absorption into the T particles is diffusion-controlled (at this temperature the surface concentration is calculated to be twice the average concentration).

The behavior of other elements in the 137 chain can also be observed in Fig. B.1. Neither iodine nor xenon is strongly absorbed at even the lowest temperature of this study. The higher temperature portions of the iodine and xenon curves in Fig. B.1 reflect the low absorption and a low temperature coefficient of absorption for these isotopes. At lower temperatures, however, the iodine curves reflect the behavior of the parent tellurium curves. That is, at these temperatures the main iodine concentration in the particles comes from absorbed tellurium decay to iodine, whose loss from the particle is diffusion-controlled. The low temperature increase in xenon concentration in the particles is due to iodine decay, and xenon loss is also diffusion-controlled. This latter process has just become apparent as a result of the lowest temperature calculations shown in Fig. B.1. Similar phenomena can be observed in the cesium absorption curves. Fission cesium is mainly absorbed at 2100°K , where the absorption curves in Fig. B.1 stop their steep ascent. This is the same

temperature region where gas phase cesium starts its sharp decrease. Note that the concentration of cesium in the L particles does not appreciably change at lower temperatures. The remaining gaseous cesium, and that formed in the gas phase decay of xenon, is picked up mainly by the smaller particles because of their large surface to volume ratio. The cesium concentration of the M particles does not change much after 1900°K , while that of the S particles begins to level off at 1700°K . The cesium concentration of the T particles increases sharply, reflecting the continued absorption of cesium produced from xenon (g).

The behavior of the 137 nuclide chain can thus best be explained in terms of diffusion-controlled sorption of tellurium and cesium and decay of the nuclides. Note that the sorption processes depicted in Fig. B.1 account for only a minor portion of the total mass of fission products of this nuclide chain. The rest of the material, at times subsequent to those of this calculation, will go through the process of decaying to cesium and depositing on the outer portions of the fallout particles or on any condensed phase with which it comes in contact. In this study, however, it is assumed that the material remaining in the gas phase at 900°K is surface-deposited on the fallout particles themselves, according to their surface area. In reality, xenon, with a relatively long half life (234 sec), may well separate from portions of the fallout particles before decaying and depositing.

Figure B.2 shows similar data for the 95 chain. The behavior depicted in this figure, except for that of rubidium, represents essentially complete absorption at the highest temperature of the study, 2700°K , and rubidium absorption is essentially complete by 1900°K . The absorption differences between the smaller particles and the L particles result from the nuclides in this chain being incompletely diffused in the larger particles at 2700°K . The splitting of the M, S, and T curves of rubidium results from diffusion control becoming important at lower temperatures for smaller particles, as was discussed previously for tellurium in the 137 chain.

A further description of the effect of initial temperature is appropriate here. Table B.2 contains the 900°K average concentration ratios of L and M for zirconium, yttrium, and strontium and the L/M, M/S, and S/T average concentration ratios for rubidium. For a highly absorbed species, the ratio L/M differs from unity but obviously will approach unity as starting temperatures are increased. However, for rubidium, which is not so highly absorbed, the concentration ratios in various sized particles are independent of the starting temperature; and the smaller the particles, the more nearly this value approaches unity. The calculational values for less highly absorbed species thus appear to be independent of starting temperature.

Table B. 2
CONCENTRATION RATIOS AT 900°K OF PARTICLES OF DIFFERENT
SIZE FOR VARIOUS STARTING TEMPERATURES

Starting Temperature (°K)	Average Concentration Ratio					
	Zr (L/M)	Y (L/M)	Sr (L/M)	Rb (L/M)	Rb (M/S)	Rb (S/T)
2700	0.378	0.497	0.611	0.398	0.844	0.950
3100	0.600	0.754	0.859	0.398	0.844	0.950
3900	0.862	0.924	0.883	0.398	0.844	0.950

The phenomenon of lack of equilibration of nonfractionated nuclides in the larger particles at high temperatures which is seen when the present model is used would seem to indicate some fractionation with size. An investigation of fallout should reveal whether this is indeed the case.

The orientation calculation described above has demonstrated many of the features of the diffusion-controlled model. These features seem to find some support in studies of fallout and certainly should be studied more thoroughly. However, before further questions concerning calculations of fallout phenomena are investigated, some of the strictly mathematical variations within the model calculations should be considered.

An investigation of different-sized temperature stepping intervals was made. In general, in the calculations reported here, 200°K temperature intervals were used. However, these test calculations, which were initiated at 2700°K and were carried through 900°K, were made for the two nuclide chains in both 200° and 100°K increments. Comparing results was more complicated than it first appeared because the final diffusion time corresponded to 800°K in the 200° interval calculations and to 850°K in the 100° interval calculations. In order to avoid this difficulty, both systems were allowed to decay and to absorb the resulting gaseous fission products (mainly Cs¹³⁷) according to surface area, thereby nearly eliminating the final calculational temperature differences. The comparison of results is presented in Table B.3. The only difference that seems significant occurred in the L particle zirconium concentrations, and it can apparently be explained by the difference in initial starting temperatures. The particles had essentially twice the time to diffuse at 2700°K in the case of the 200° increments as in the case of the 100° increments. While a better example might be constructed, it would appear from this study that the size of the temperature increment used in the model may not be very important if chosen as 200°K or less.

Table B. 3
EFFECT OF SIZE OF TEMPERATURE INCREMENT ON
FISSION PRODUCT ABSORPTION

Nuclide	Particle Size	Absorption (g)	
		100°C Temp. Interval	200°C (Std) Temp. Interval
Zr	T	0.456	0.456
	S	34.67	34.63
	M	71.52	71.17
	L	6.86	7.26
Cs	T	14.62	14.63
	S	112.40	112.44
	M	46.92	46.88
	L	1.045	1.042

In the investigation of the effect of the particle size distribution, three different distributions were studied under the same conditions. The distributions employed and the weights of soil associated with each distribution in this case are presented in Table B.4. The amounts of cesium and zirconium fission products (in grams) after decay of precursor fission products are also presented for each fallout particle size as in the previous case. Finally, a ratio of the cesium and zirconium average concentrations associated with each particle size is presented. This ratio is proportional to a fractionation factor ratio comparing these elements. The proportionality constant is 0.649, a nuclide chain yield ratio. Further consideration of Table B.4 reveals that fractionation factors for the very smallest particles far exceed unity, while for the larger particles these factors are less than unity. Fractionation factors in this model are thus quantities that depend on particle size (and also probably on the degree of detachment of the fallout particles from the nuclear cloud before conversion of volatile fission products to condensable ones). Therefore, if this model is correct, observed fractionation factors should be dependent on particle size and thus not accurately definable without ample description of this parameter. Indeed, these factors should be sensitive not only to the particle size in question but also to the particle size distribution. Specifically, one observes using distributions (2) and (3) that fractionation factors for the same size particles can differ considerably. Particle distribution (3) contains a large amount of very small particles. Distributions (1) and (2) are similar, since they both are based on Miller's description. * Note that the distributions (1) and (2) produce similar fractionation factors for similarly sized particles. It seems apparent that in testing this model for reproduction of fractionation factors, one must specify the particle size distribution, a factor often not well documented.

A study was made of the effect of the size of the detonation and the amount of soil in the cloud (that is, the proximity of the detonation to the

* Miller, C. F., private communication, November 1965.

Table B. 4
EFFECT OF PARTICLE SIZE DISTRIBUTION ON FISSION PRODUCT ABSORPTION

Particle Radius (cm)	Fallout (g)			Fission Product (g)						Ratio		
	Weight (1) (Std)	Weight (2)	Weight (3)	Cs (1)	Cs (2)	Cs (3)	Zr (1)	Zr (2)	Zr (3)	Cs/Zr (1) ²	Cs/Zr (2) ²	Cs/Zr (3) ²
10 ⁻⁶			8.5×10 ⁴			104.6			1.20			87.0
10 ⁻⁵		8.5	4.25×10 ⁵		0.078	52.7		1.17×10 ⁻⁴	6.01		667.0	8.8
10 ⁻⁴		5.95×10 ³	8.5×10 ⁵		5.50	11.0		0.0816	12.02		67.0	0.92
3×10 ⁻⁴	3.23×10 ⁴			14.6			0.444			33.0		
10 ⁻³		1.19×10 ⁶	2.975×10 ⁶		110.7	5.13		16.32	42.06		6.8	0.12
3×10 ⁻³	2.458×10 ⁶			112.4			33.73			3.3		
10 ⁻²		5.95×10 ⁶	2.89×10 ⁶		57.3	1.40		80.9	40.61		0.71	0.034
1.54×10 ⁻²	5.117×10 ⁶			46.9			69.28			0.68		
0.1		1.353×10 ⁶	8.5×10 ⁵		1.45	0.132		16.2	10.54		0.090	0.0125
0.13	8.725×10 ⁵			1.04			10.06			0.10		
1.0		8.415×10 ²	4.25×10 ⁵		9.6×10 ⁻⁵	9.8×10 ⁻³		2.05×10 ⁻³	1.07		0.046	0.0092

²Can be converted to fractionation factors by multiplying by 0.649.

land surface). The calculated final amounts of cesium and zirconium for the various particle sizes as a function of these two quantities are shown in Table B. 5. Note that the calculated fission product distributions in the particles were only slightly different for the various conditions. Specific activities per gram of fallout vary directly with yield and indirectly with the amount of soil, but the relative fission product distribution among the different-sized particles is not greatly affected by these parameters. This reemphasizes the importance of particle size distributions and chemistry in determining the fate of fission products during fallout formation.

Table B. 5

VARIATION OF FISSION PRODUCT ABSORPTION WITH SIZE
AND HEIGHT OF DETONATION EFFECTS FOR A
100-KT FISSION YIELD DETONATION

Particle Radius (cm)	Cesium Absorbed (g)			Zirconium Absorbed (g)		
	Standard	1/100 Soil	10 MT, Total Yield	Standard	1/100 Soil	10 MT, Total Yield
0.0003	14.63	14.76	13.84	0.444	0.539	0.432
0.003	112.44	113.20	110.21	33.73	35.54	32.86
0.0154	46.88	46.06	49.55	69.28	67.76	68.41
0.130	1.042	0.954	1.387	10.06	9.67	11.81

The computer program can also provide fission product profiles. Calculated profiles for both the 137 and 95 chains have been investigated for a 100-KT fission detonation, using 200° temperature increments and the particle size distribution given in Table B. 1. The calculations were initiated at 2700°K for the 137 chain and at 3100°K for the 95 chain. The 900°K profiles for the 95 chain are presented as a function of particle size in Fig. B. 3, and those for the 137 chain are presented in Figs. B. 4, B. 5, and B.6. An unusual abscissa scale is used in these figures solely for the purpose of demonstrating the calculated values more efficiently.

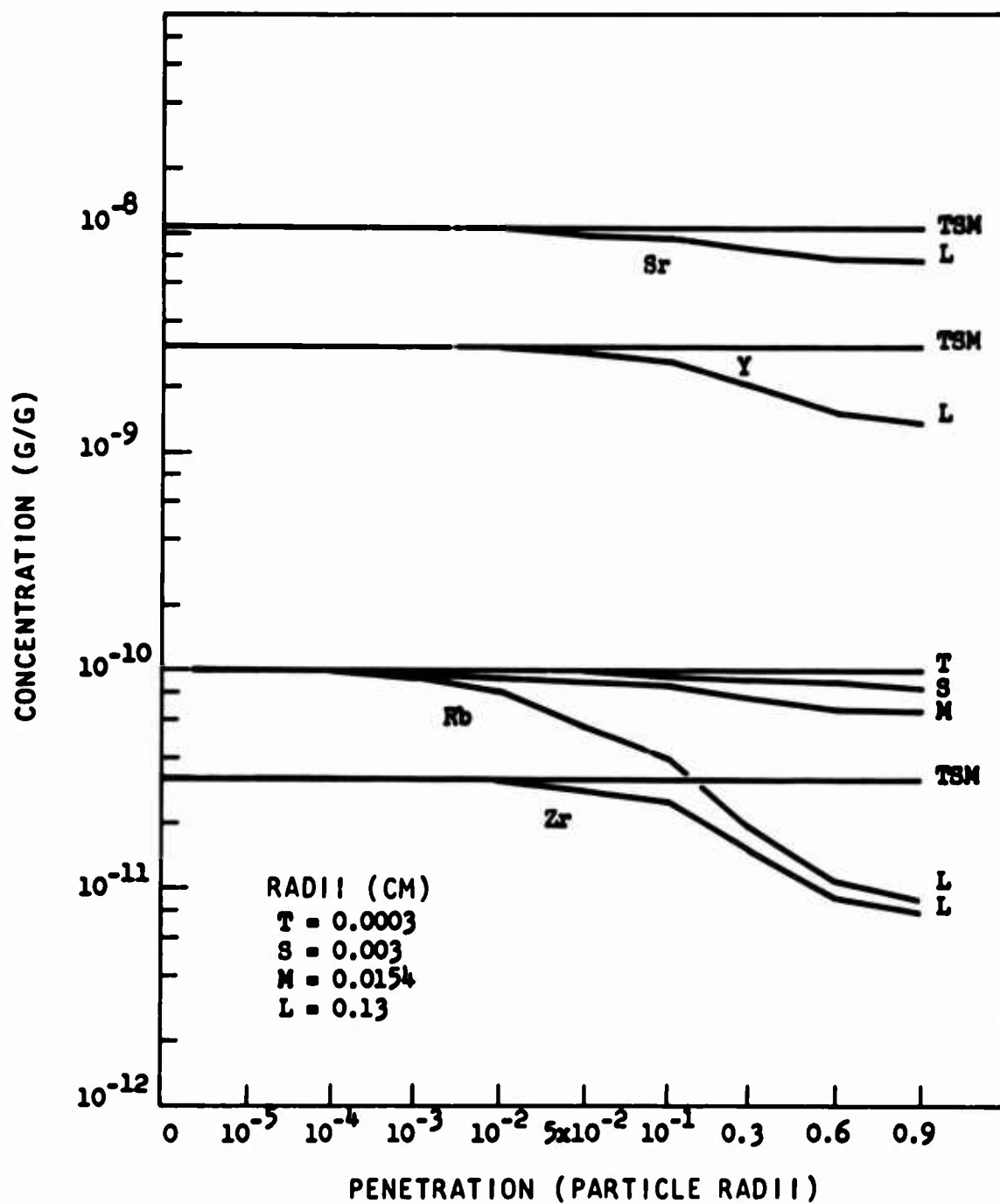


Fig. B. 3--Concentration profiles at 900°K of 95 nuclide chain members as a function of particle size for standard detonation

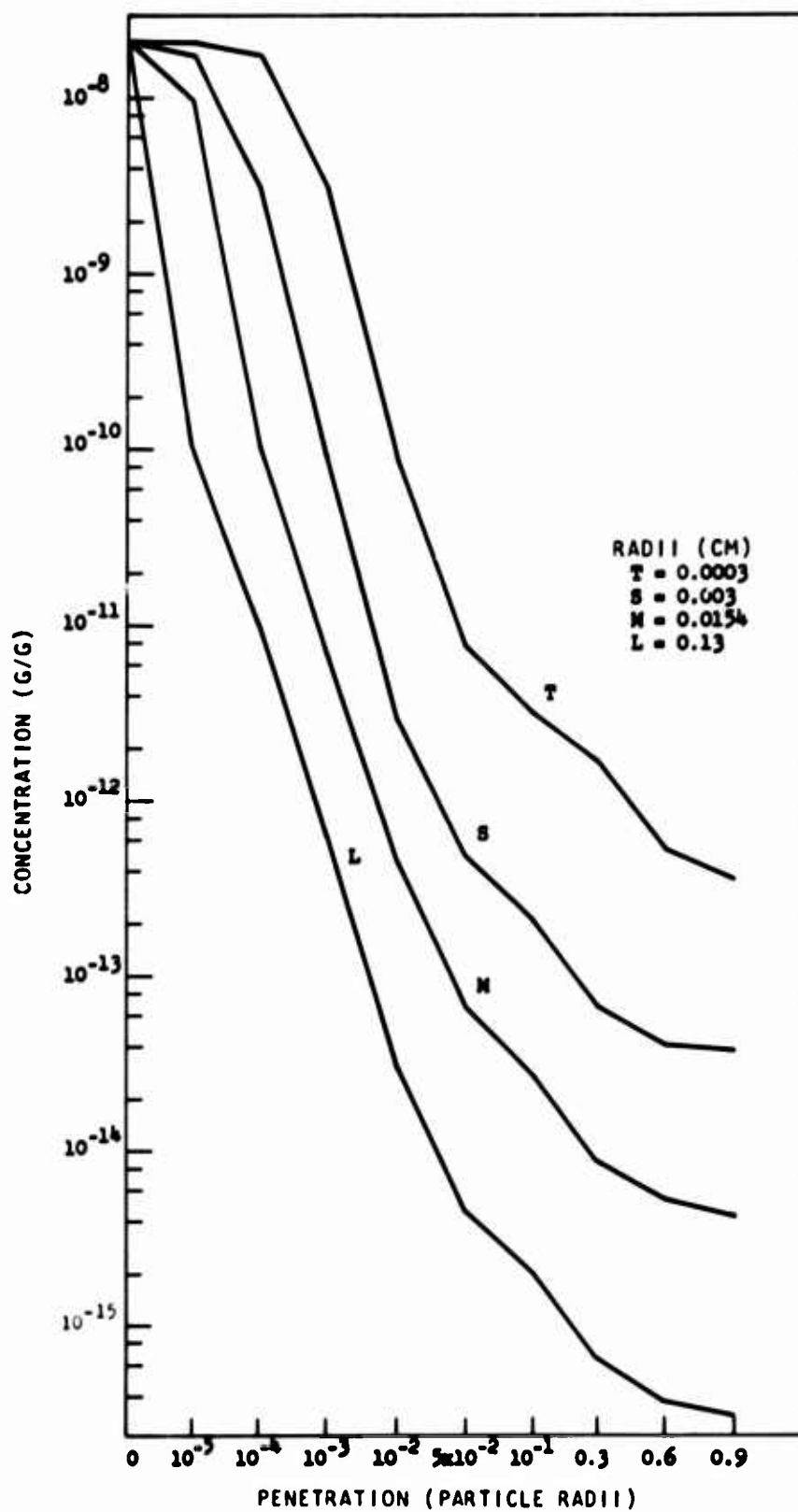


Fig. B.4--Tellurium-137 concentration profiles at 900°K for standard particle size distribution and standard detonation

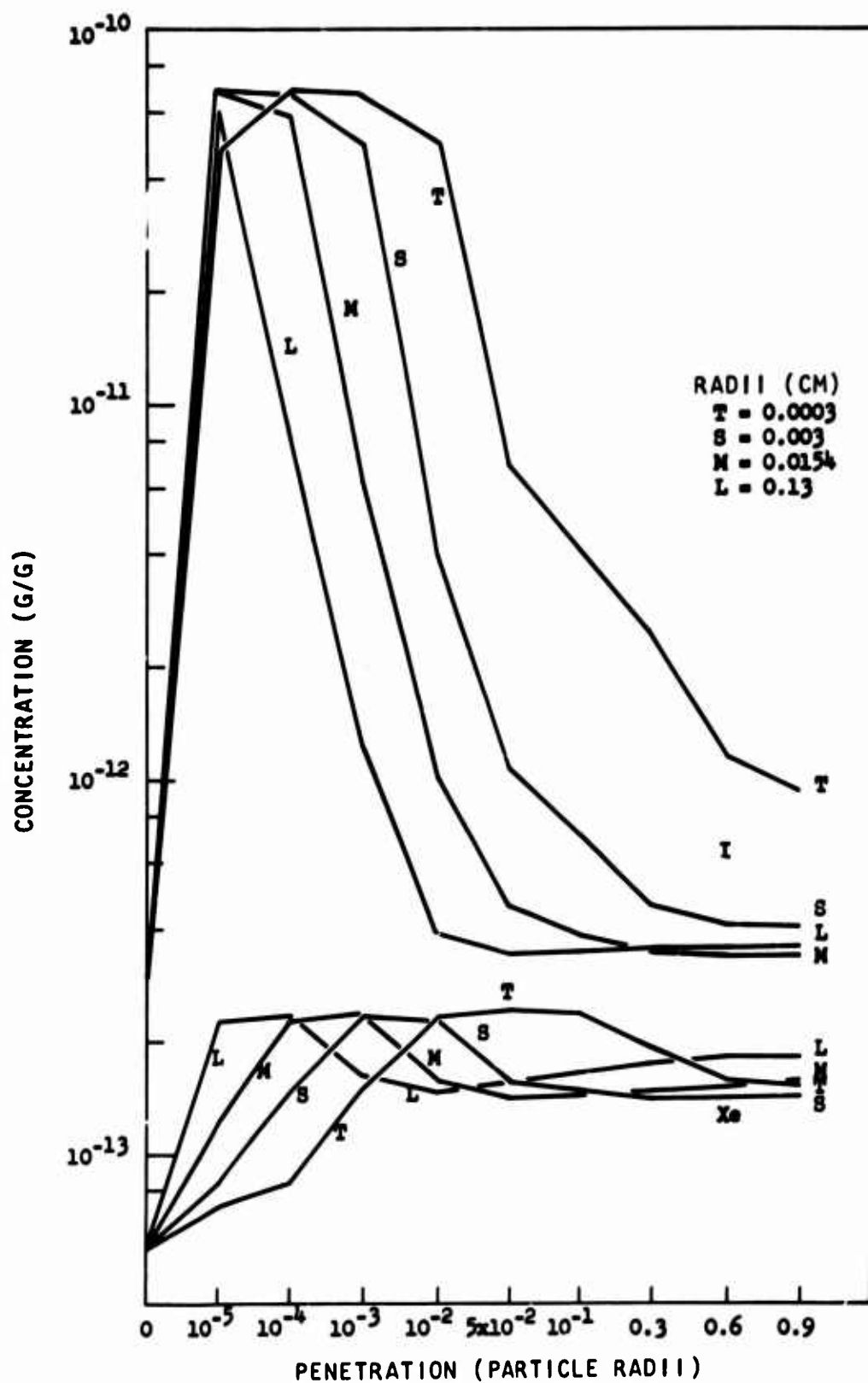


Fig. B. 5--Iodine and xenon-137 concentration profiles at 900°K for standard particle size distribution and standard detonation

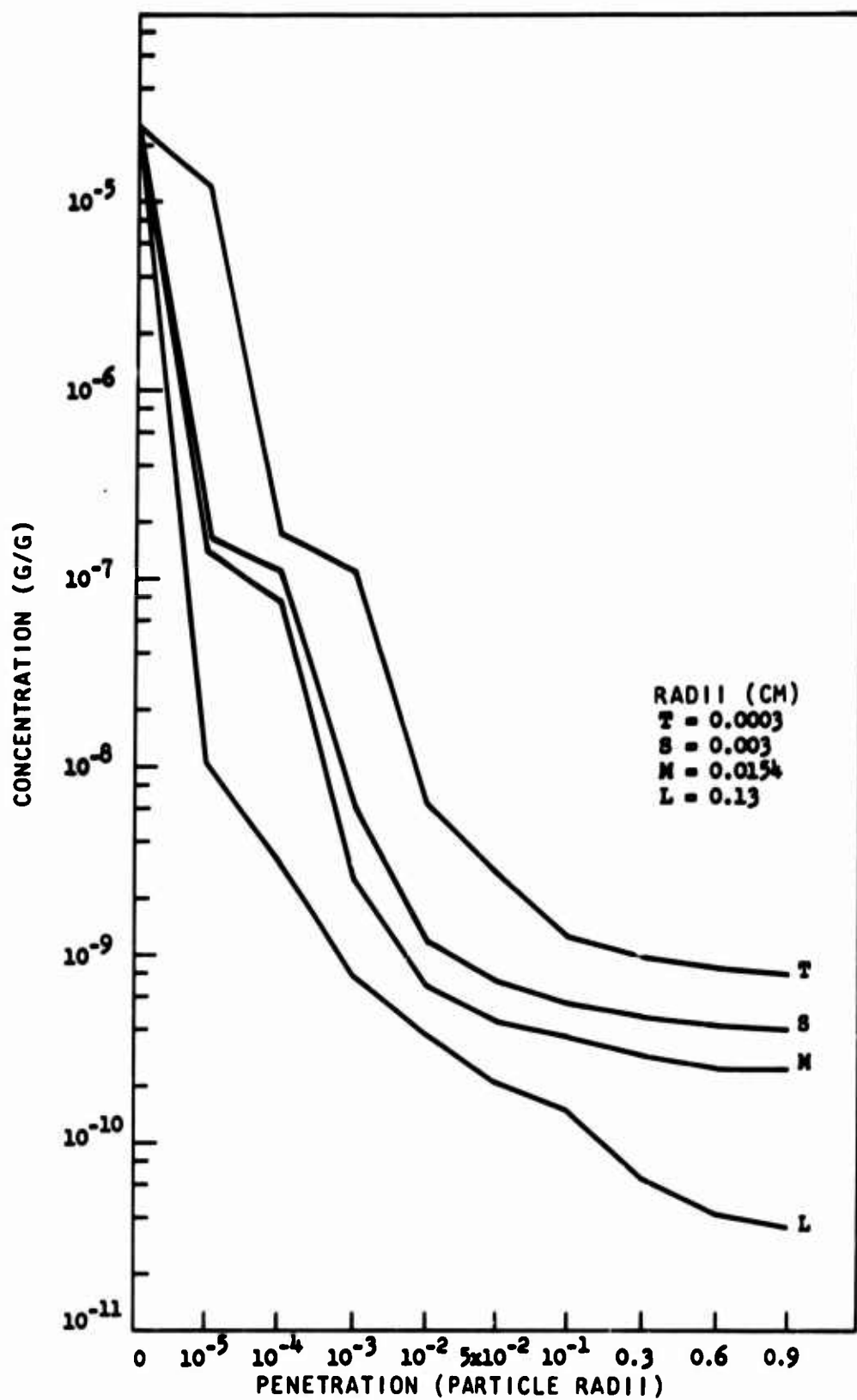


Fig. B.6--Cesium-137 concentration profiles at 900°K for standard particle size and standard detonation

The 900°K profiles for the 95 chain are very simple. They show only small deviations from a flat profile for rubidium in the S, M, and L particles and for the other fission products just in the L particles. The 900°K profiles for the 137 chain are structurally more interesting. The distribution of tellurium within the standard particles at this temperature is shown in Fig. B.4. Calculated tellurium concentrations span eight orders of magnitude in the L particles and five orders of magnitude in the T particles. The concentrations have been drawn as a continuous curve in these diagrams as an aid to the reader and are not to be used in interpolating. The tellurium profiles, then, are characteristic of a moderately volatile fission product (1% condensed at 900°K in this calculation) with a moderately high Henry's law temperature coefficient.

The iodine and xenon profiles (shown in Fig. B. 5) are even more interesting, since they exhibit maxima and minima as a function of radius and particle size. The sharp maxima in the iodine curves can be attributed to absorbed tellurium decay and subsequent diffusion and vaporization of the resulting iodine. The maxima in the xenon curves can be attributed to absorbed iodine decay and diffusion and vaporization of resultant xenon.

The cesium profiles are shown in Fig. B. 6. This set of curves would appear to be exhibiting fine structure that is somewhat dependent on the calculational model. The near-surface behavior of calculated profiles would seem to have an extraneous structure that is a function of the size of the time-temperature steps. The use of shorter time steps should smooth out this profile considerably. However, the general structure of these profiles seems reasonable.

It is interesting to consider the penetration depths used in these mathematical profile calculations. The particle radius $0.0003 \text{ cm} \times 10^{-5}$ fractional penetration gives $0.3 \text{ \AA}$, a value too low on the atomic-size scale to be a credible penetration depth. This can also be said for the 0.0003-cm radius particles at 10^{-4} radius penetration, and the 0.003-cm radius particles at 10^{-5} radius penetration. A value between 15 and $30 \text{ \AA}$, a

borderline penetration, is the next smallest penetration depth plotted. The subsequent minimum value is $130 \text{ \AA}$, a value such that diffusion is reasonable to consider.

A plot of the iodine profiles for the 0.0003-cm radius particles, T , as a function of temperature is shown in Fig. B. 7. These curves demonstrate a general decrease in total iodine loading as the cloud cools. This can be attributed to the expansion of the cloud, high iodine diffusion coefficients, and a low iodine Henry's law temperature coefficient. At the lower temperatures, where iodine is not very mobile, the iodine profile reflects the parent tellurium profile. The difference between the 1100°K and the 900°K profiles is caused by additional tellurium decay to iodine.

This orientation investigation demonstrates the effects of condensed state diffusion in a fallout calculational model embodying this phenomenon. It is interesting to compare this system with the Miller model, where diffusion is deemed infinitely fast above 1673°K and negligibly slow below this temperature. For the case of the highly absorbed nuclide chain, the only noticeable difference is that the calculations for the larger particles in the diffusion-controlled model suggest that equilibrium conditions may not be attained by these particles during fallout formation. Equilibrium conditions are assumed by Miller. In the case of a volatile chain, the diffusion model predicts an absorption behavior which varies with particle size. Miller's model assumes no absorption difference with particle size. In the diffusion model, cooling rate will slightly affect absorption, while in Miller's model it will affect absorption only to the extent that this quantity interacts with fission product decay. Radial concentration gradients are predicted within a fallout particle with the diffusion model, while with Miller's model there are no concentration gradients within a particle, only at the surface of the particle. It seems reasonable to state that the diffusion model provides a more revealing and perhaps a more accurate calculational tool for considering fallout. It is, however, a limited model, and the assumptions underlying the development of the model should not be ignored.

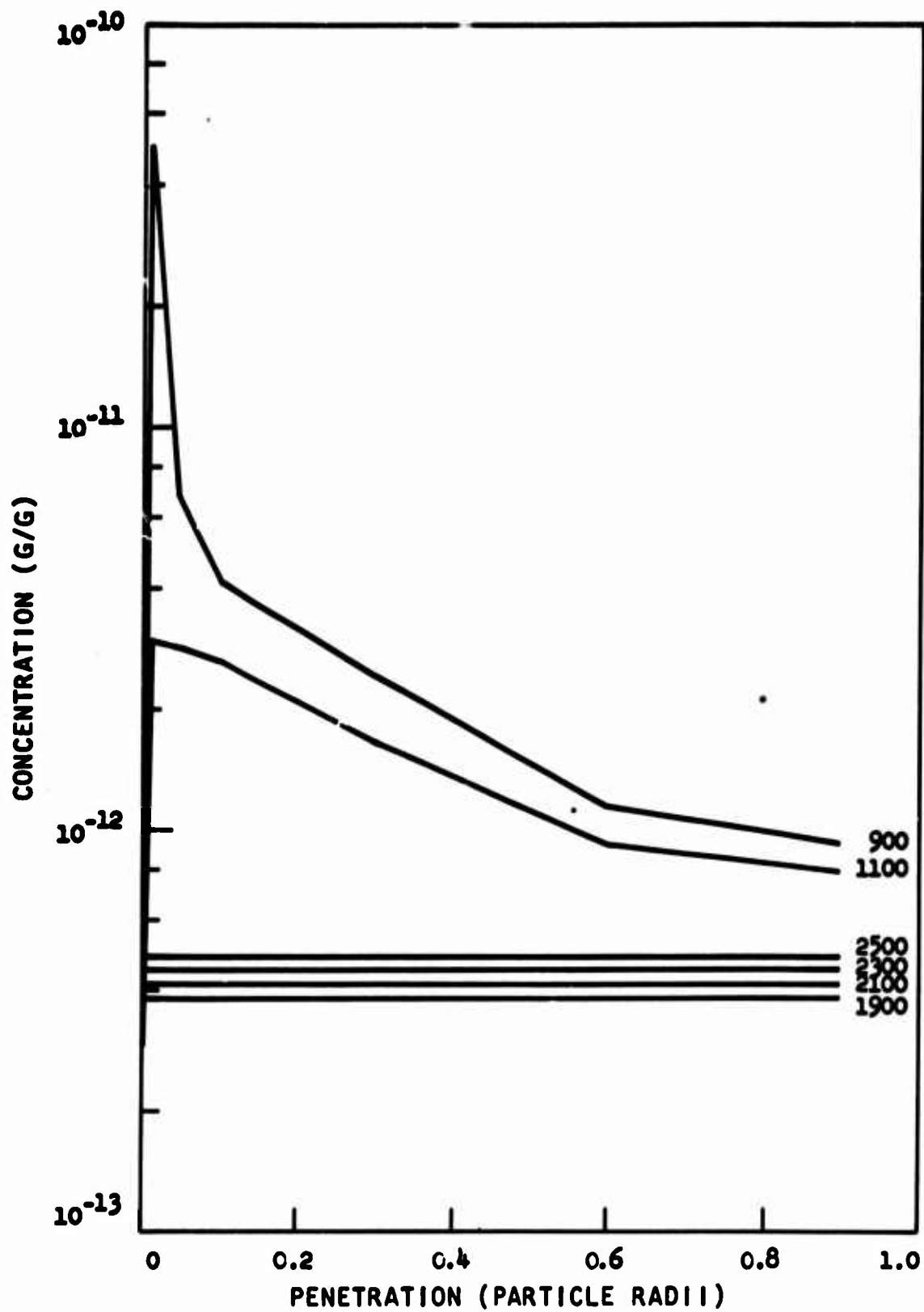


Fig. B. 7--Iodine-137 concentration profiles as a function of final temperature for the 0.0003 cm size particles and the standard detonation

APPENDIX C
CONTROL CARD FORMATS

For identification only

Word	1-12	13	14			
Column	1-22	23-75	77-99			
Format	12A6	13	A4			
Card 1	Case title: may be any set of characters desired	Numerical case designation (564 has been used)	Sub-case designation (for identification)			
Symbol	NTITLE	NCS1	NCS2			

LC ≤ 6
IR ≤ 30
IDPTH ≤ 11

Word	1	2	3	4	5	6
Column	1-5	6-10	11-15	16-20	21-30	31-40
Format	15	15	15	15	F10.0	F10.0
Card 2	Length of chain (number of isotopes)	Number of particle sizes	If equal to 0, do not calculate long term results; if equal to 1, do calculate results	Number of depths to calculate concentrations for (for profiles)	Yield of device (in KT) used in calculating time-temperature distribution	Yield of device (in KT) used in calculating time-temperature distribution
Symbol	LC	IR	ILC	IDPTH	YKT	BKT

If IDPTH = 0, this card is not present
 $0 < Q(1) \leq 1.0$

Word	1	2	3			
Column	1-10	11-20	21-30			
Format	F10.0	F10.0	F10.0			
Card 2a	First distance from center (in radius units) for concentration calculation	Second distance	Third distance	Etc.	Note: Q(0) = 1 gives surface, Q(0) = 1/2 gives half way into particle, etc.	
Symbol	Q(1)	Q(2)	Q(3)			

Word	1	2	3	4	5	6
Column	1-6	7-16	17-26	27-36	37-46	47-56
Format	A6	F10.0	F10.0	F10.0	F10.0	F10.0
Card	Name of isotope	Molecular weight of isotope (in g/mole)	Initial yield of isotope (in g/10 ⁶ fissions)	Constants used to calculate Henry's law constants for this isotope: $\text{Log } H = \text{HC1} + \text{HC2/T}$	Constant used in diffusion coefficient calculation	
Symbol	NAME(L)	WMOL(L)	YIEL	HC1(L)	HC2(L)	DC1(L)

There are LC of card type 3, the last isotopes being first

Word	7	8
Column	57-66	67-76
Format	F10.0	F10.0
Card	Constant used in diffusion coefficient calculation	The half-life of this isotope (in seconds)
Symbol	DC2(L)	HL(L)

Word	1	2	3
Column	1-10	11-20	21-30
Format	F10.0	F10.0	F10.0
Card	The starting (highest) temperature for beginning calculations	The final (lowest) temperature for calculations	The incremental temperature
Symbol	HTMP	ETMP	TEMPV

All temperatures are in °K

Note:

$$\frac{\text{HTMP} - \text{ETMP}}{\text{TEMPV}} \leq 40$$

There are 28 of card
type 5
 $0.0 < PW(K) \leq 1.0$

Word	1	2			
Column	1-10	11-20			
Format	F10.0	F10.0			
Card 5	The radius (in cm) of a particle size	The fraction of soil contained in this particle size			
Symbol:	R(K)	PW(K)			

Word	1				
Column	1-16				
Format	E16.8				
Card 6	Total soil weight contained (in g/Kt)				
Symbol	TWGT				

Word					
Column					
Format					
Card					
Symbol					

APPENDIX D

SAMPLE OUTPUT AND SUBPROGRAM LISTINGS

INPUT DATA

SAMPLE CASE, NORMAN CODE.

LENGTH OF CHAIN = 4
 DEVICE YIELD = .10000000+03 KY
 YIELD = .10000000+03(FOR TIME-TEMP DISTRIBUTION)

ISOTOPE PARAMETERS

NAME	MOLECULAR WEIGHT (G/MOLE)	INITIAL YIELD (ATOMS/10,000 FISSIONS)	MC1	MC2	DC1	DC2	HALF LIFE (SECONDS)
CS	137.	6.0	6.600	17300.0	5.570	20500.0	.40
XE	137.	114.0	4.100	700.0	9.100	20500.0	234.00
I	137.	252.0	3.400	1000.0	7.290	22500.0	24.40
TE	137.	172.4	9.200	11400.0	3.300	15600.0	3.00

STARTING TEMPERATURE = 2900. DEG. KELVIN
 FINAL TEMPERATURE = 900. DEG. KELVIN
 TEMPERATURE INCREMENT = 200. DEG. KELVIN
 TOTAL PARTICLE WEIGHT = 8.50000000+07 G/KY

PARTICLE PARAMETERS & PARTICLE SIZES

RADIUS (CM)	WEIGHT (G)
.000300	3.23000000+07
.003000	2.45819900+09
.015400	5.11599900+09
.130000	8.92500000+03

TIME-TEMPERATURE DISTRIBUTION: 10 STEPS.

TIME INCH	TEMP
5.10650	.75626
5.89304	.81683
6.74542	.88794
7.67571	.97263
8.69962	1.07519
9.83019	1.20136
11.12051	1.36267
12.58839	1.57309
14.30521	1.86057
16.37407	2.27715
	900.0

START TIME FOR CALCULATION OF SURFACE CONCENTRATIONS IS 4.7204 SEC

YIELDS, IN GRAMS, ADJUSTED TO START TIME.

ISOTOPE	YIELD
CS	2.51545820+08
XE	4.69730700+01
I	1.04952669+02
TE	1.65439360+01

DIFFUSION COEFFICIENTS (LINE ONE) AND HEIRY'S LAW CONSTANTS (LINE TWO)

TEMP	CS	XE	I	TE
2700.0	9.49308720-03 1.55809006+00	1.92834660-01 0.93011950+03	9.05037790-02 2.64924034+03	3.32829430-03 6.75506030+04
2500.0	2.34822680-03 4.76630100-01	3.16227760-02 6.60693380+03	1.94938440-02 2.51184630+03	1.14415353-03 3.01995170+04
2300.0	4.53496220-04 1.19745950-01	3.76669890-03 6.24672120+03	3.21655760-03 2.31855480+03	3.29143040-04 1.17372180+04
2100.0	6.42828680-05 2.30093700-02	3.02659150-04 5.84341350+03	3.76456110-04 2.10770350+03	7.43752740-05 3.51024060+03
1900.0	6.03290260-06 3.12618540-03	1.42112250-05 5.38987790+03	2.40475440-05 1.47795070+03	1.22477434-05 9.76353650+02
1700.0	3.24471440-07 2.65173050-04	3.24911180-07 4.87792640+03	1.13424237-06 1.62641340+03	1.32901372-06 1.31877793+02
1500.0	8.00446510-09 1.16591420-05	2.71247340-09 4.29866190+03	1.94908440-06 1.35935630+03	7.94324230-08 2.15443490+01
1300.0	6.32075380-11 1.96023260-07	5.19259860-12 3.64366500+03	9.50006800-11 1.87341880+03	1.94526240-09 1.32762050+00
1100.0	8.58294790-14 7.45980130-10	1.02115328-15 2.90328060+03	6.44624100-14 7.77673650+02	1.31274937-11 2.96930850-02
900.0	6.19753360-18 2.36659030-13	4.52934420-21 2.10001420+03	1.44964470-16 4.65527320+02	9.25113613-15 1.22712520-04

SURFACE CONCENTRATIONS IN G/G

TEMP	TIME	CS	XE	I	TE
2700.0	5.106+00	1.97850050-11	9.27948080-14	5.12442020-13	3.60449230-15
2500.0	5.693+00	5.17861580-11	8.75030070-14	4.76090160-13	5.43337400-15
2300.0	6.745+00	1.33402590-10	4.22951770-14	4.39956150-13	1.65762369-14
2100.0	7.676+00	2.09640170-10	7.72236250-14	4.44667760-13	2.22311140-14
1900.0	8.700+00	4.14980540-10	7.23277880-14	3.71628470-13	5.71540330-14
1700.0	9.833+00	5.75703290-10	6.76943160-14	3.41194250-13	1.93292430-13
1500.0	1.112+01	1.13076421-09	6.34630980-14	3.14446110-13	9.67553720-13
1300.0	1.259+01	7.31660820-09	5.96815490-14	2.94612240-13	8.67935350-12
1100.0	1.431+01	1.93220210-07	5.74340050-14	2.44393330-13	1.94753210-10
900.0	1.637+01	2.49293130-05	5.72266180-14	2.93608840-13	2.05933540-03

AMOUNT OF MATERIAL IN THE GAS PHASE
(IN GRAMS)

ISOTOPE

TEMP	TIME	CS	XE	I	YE
2700.0	5.100+00	2.34744740+00	4.89722820+01	1.44944313+02	1.45+30050+01
2500.0	5.893+00	2.19064010+00	5.10934650+01	1.45890554+02	1.55700241+01
2300.0	6.745+00	1.05912151+00	5.33933620+01	1.05944048+02	1.23924532+01
2100.0	7.676+00	7.88477610+01	5.58932070+01	1.05697472+02	1.05013717+01
1900.0	8.700+00	1.94927950+01	5.86129640+01	1.04930746+02	0.38758710+03
1700.0	9.833+00	2.34709870+02	6.15831460+01	1.03619377+02	0.54203330+03
1500.0	1.112+01	3.15577690+03	6.40426430+01	1.01727363+02	4.95466360+03
1300.0	1.259+01	4.69906200+04	5.84431020+01	9.32629550+01	3.61436760+03
1100.0	1.431+01	6.25290240+05	7.24614900+01	9.54624550+01	2.50307570+03
900.0	1.637+01	3.01224350+06	7.70039060+01	9.19044860+01	1.61952273+03

AVERAGE CONCENTRATIONS PER PARTICLE SIZE
AT FINAL TEMPERATURE 900. DEG CELSIUS

ISOTOPE

PARTICLE RADII
(IN CM)

	CS	XE	I	YE
.00030	3.59673050+09	2.06275100+13	6.70915050+12	4.25040330+11
.00300	8.30925760+10	1.52171700+13	1.20506492+12	4.40337110+12
.01540	4.20978970+10	1.49355310+13	5.17927000+13	6.60214940+13
.13000	1.34016040+10	1.70123950+13	3.62420370+13	1.04160273+13
AVERAGE	5.21472400+10	1.52566390+13	7.24713320+13	1.96332370+12

P P O F I L E P O I N T S

CONCENTRATIONS AT VARIOUS DEPTHS
AT FINAL TEMPERATURE 900. DEG KELVIN

*** CS ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	6.32445-09	1.33118-09	1.05533-09	1.01280-09	9.24212-10	
.003000	1.25965-09	5.73416-10	5.15717-10	4.86937-10	3.44444-10	
.015400	7.21825-10	3.92768-10	3.40076-10	3.04320-10	2.71060-10	
.130000	3.47207-10	1.51910-10	9.32232-11	6.93712-11	4.72192-11	

*** KZ ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	2.31018-13	2.34434-13	2.14135-13	1.92633-13	1.65670-13	
.003000	2.28507-13	1.44232-13	1.53962-13	1.41480-13	1.43079-13	
.015400	1.56731-13	1.44820-13	1.46932-13	1.49524-13	1.52106-13	
.130000	1.45673-13	1.44834-13	1.71597-13	1.76356-13	1.80975-13	

*** I ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	4.93079-11	4.19106-12	3.27276-12	2.44562-12	1.34946-12	
.003000	3.67355-12	7.10290-13	5.46660-13	4.54748-13	4.04552-13	
.015400	1.00400-12	3.78573-13	3.49723-13	3.34723-13	3.33912-13	
.130000	3.83461-13	3.35447-13	3.39240-13	3.42618-13	3.46459-13	

*** TE ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	8.66849-11	3.15110-12	2.35084-12	1.64763-12	7.47300-13	
.003000	2.88242-12	2.05907-13	1.14677-13	6.60401-14	4.13749-14	
.015400	4.42426-13	2.71600-14	1.33915-14	8.45334-15	5.83541-15	
.130000	2.93181-14	2.00482-15	9.73195-16	6.54726-16	4.22769-16	

SUMMARY OF RESULTS AT FINAL TEMP 900. DEG KELVIN

ISOTOPE

	CS	XE	I	TE
AMT IN GAS PHASE	3.4122350-06	7.70039060+01	9.19948660+01	1.61962273+00
AMT IN SOLID PHASE	4.43251550+00	1.29651855-03	6.16006330-03	1.67307940-02
TOTAL	4.43251920+00	7.70032020+01	9.19110950+01	1.63635352+03
YIELD AT FINAL TIME	4.43252020+00	7.70052020+01	9.19110950+01	1.63635323+00
DIFFERENCE	-9.53674320-07	0.00000000	-2.46102290-06	-1.39011610-03

LONG-TERM RESULTS FOR CS ISOTOPE

PARTICLE RADIUS (CM)	AVERAGE CONCENTRATION DUE TO SOLID'S DECAY (G/G)	TOTAL AVERAGE CONCENTRATION (INCLUDES GAS PHASE) (G/G)	TOTAL AMOUNT OF CS IN PARTICLE (G)
.00030	5.64615-93-08	.5256560-07	1.46170734+01
.00300	8.36646370-10	4.57289560-09	1.12310917+02
.01540	4.22515473-10	9.16776270-09	4.60116240+01
.13000	1.34633550-10	1.17062609-09	1.04474537+00

01 FOR NORMAN

COMPILATION BY UNIVAC 1103 FORTRAN-IV DATED 11 NOV 1966 F4008

THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:05:57

MAIN PROGRAM ENTRY POINT 000000

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 002101
0000 *DATA 023461
0002 *BLANK 001676
0003 SING 000023
0004 91 023160
0005 INLOOP 000001

EXTERNAL REFERENCES (BLOCK, NAME)

0006 MARGIN
0007 INITIAL
0010 EXP
0011 DIFFUS
0012 ALO610
0013 BCALC
0014 PROFIL
0015 DELTA
0016 FINAL
0017 DUMP
0020 HEAR25
0021 NADDS
0022 NIO15
0023 NIO25
0024 NSTOPS

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	001161 10L	0001	002020 1000L	0001	002085 1001L	0001	000713 101L	0001	023377 1050E
0000	023067 1075F	0000	023114 1076F	0001	001153 111	0001	000723 111L	0001	021145 12L
0000	023122 1200F	0000	023152 1201F	0000	023213 1202F	0000	023220 1203F	0000	023245 1215F
0000	023254 1208F	0000	023265 1207F	0000	023273 1208F	0000	023304 1209F	0001	000733 121L
0000	023312 1210F	0000	023320 1211F	0000	023352 1212F	0000	023374 1213F	0001	000013 124E
0001	000021 1276	0001	001137 13L	0001	000743 131L	0001	000335 1325	0001	001131 14L
0001	000051 1416	0001	000130 1556	0001	000141 1606	0001	000154 1653	0001	000157 1753
0001	001076 18L	0001	001107 19L	0001	000213 2026	0001	000300 21L	0001	000231 2115
0001	000245 2146	0001	000056 22L	0001	000266 2216	0001	000333 2363	0001	000155 24L
0001	001700 232L	0001	000401 2543	0001	000424 2606	0001	000457 2703	0001	000395 28L
0001	000535 3046	0001	000555 3116	0001	000634 3266	0001	000700 3343	0001	001324 3716
0001	001044 3766	0001	000753 40L	0001	000310 401L	0001	001254 4000	0001	001304 3853
0001	001332 47L	0001	001175 5L	0001	000362 501L	0001	000365 502L	0001	001322 5035
0001	001234 503L	0001	001237 504L	0001	001431 5106	0001	001441 5163	0001	001361 5275

NORMAN --- MAIN PROGRAM

0001	001470	5346	0001	001472	5376	0001	001514	5476	0001	001535	5615	0001	001545	5655
0001	001553	5736	0001	001550	600L	0001	001507	6016	0001	000020	601L	0001	000007	5612
0001	001206	602L	0001	001572	6056	0001	001615	6176	0001	000043	6335	0001	001652	6475
0001	001660	6455	0001	001666	6526	0001	001725	6656	0001	001734	6745	0001	001745	7425
0001	001756	7106	0001	001770	7166	0001	002001	7245	0001	002266	A	0002	001334	AC
0002	R 000000	ALU610	0002	R 001626	AT4	0000	Q 017036	ADAV	0001	Q 000374	AVCJ4	0001	Q 002276	0
0000	R 023002	BDF	0000	R 023003	QDF1	0000	Q 023004	BDS	0001	Q 022755	LA	0000	R 022763	0
0000	R 017394	COAC	0004	R 003000	OCY	0000	R 000716	DOH	0002	Q 000374	DFC	0003	Q 017130	0
0001	R 000300	UIFFUS	0000	R 022752	DRK	0000	Q 022751	DT	0003	Q 022751	DTCL4	0000	Q 022764	0
0000	R 022753	DVD	0010	R 000000	EXP	0000	Q 000660	F4	0000	Q 000366	GAS	0002	Q 000754	0
0000	I 000360	I	0003	I 000007	IDPTH	0000	Q 022741	IEPR	0003	I 000006	IL5	0003	I 000001	0
0000	I 022767	ISUB	0000	I 022772	II	0000	I 022744	J	0003	I 022746	K	0003	I 022765	0
0000	I 022762	KRIK	0005	I 000000	L	0003	I 000000	LC	0003	I 022750	LCC	0003	I 022743	0
0000	I 022756	KWK	0000	I 022742	0	0002	I 000360	NAE	0003	I 000303	NC51	0003	I 000006	0
0000	I 022767	NEL	0000	I 022771	NEP	0000	I 022770	NET	0001	I 022757	IT	0003	I 022754	0
0003	I 000002	NTOT	0000	I 022774	02	0000	I 022775	022	0003	I 022775	02	0003	I 022776	0
0000	I 022777	NS	0000	I 023000	06	0000	Q 023001	PDFLT	0014	R 000000	PROFIL	0003	Q 000010	0
0002	R 001342	R	0000	R 022750	BCST	0000	Q 017014	SOLIJ	0000	Q 022745	SUM	0003	Q 000006	0
0002	R 001506	I	0002	R 001556	TEMP	0000	Q 017022	TOTAL	0003	Q 000305	TAT	0003	Q 023005	0
0000	R 000754	U4	0002	R 001436	VOL	0002	R 000356	W4OL	0004	Q 023000	W4	0002	R 001400	0
0002	R 000000	YLD	0000	R 023005	YTY									

*** MAIN PROGRAM FOR NORMAN PROBLEM ***

PROGRAM COMPUTES SURFACE CONCENTRATIONS OF CHAINS OF ISOTOPES.

SUMMARY OF MAJOR VARIABLE NAMES

00100	1.	C	DECAY(I,J,K)	DECAY COEFFICIENT OF ISOTOPE I FROM TIME J TO TIME K.
00100	2.	C	GAST(I)	AMOUNT OF ISOTOPE I IN THE GAS PHASE.
00100	3.	C	AVCON(I,J)	AVERAGE CONCENTRATION OF ISOTOPE I IN PARTICLE SIZE J.
00100	4.	C	PH(I),DND(I)	DIFFUSION TERMS ASSOCIATED WITH PARTICLE SIZE J.
00100	5.	C	SURCON(I,J)	SURFACE CONCENTRATION OF ISOTOPE I AT TIME J.
00100	6.	C	I(K)	ARRAY OF SUBSCRIPTS DESCRIBING A DECAY PATH.
00100	7.	C	SOLUT(I)	AMOUNT OF ISOTOPE I IN THE SOLID PHASE.
00100	8.	C	CONC(I,J,K)	CONCENTRATION OF ISOTOPE I IN PARTICLE SIZE J AT A RELATIVE RADII (K).
00100	9.	C	Q(K)	ARRAY OF RELATIVE RADII FOR CALCULATING CONC

(SEE SUBROUTINE INITIAL FOR ADDITIONAL VARIABLE DEFINITIONS.)

00101	25.	C	COMMON YLD(6,40),NAE(40),VOL(6),DFC(6,40),HEN(6,40),AK(6),K(30),J
00101	26.	C	/T(30),VOL(40),T(40),TEVP(40),DATA(40)
00103	27.	C	COMMON/SING/LC,IR,NTOT,NC51,NC52,YST,IL6,IDPTH,0
00104	28.	C	COMMON/BI/DCY(6,40,40),BN(6,40)
00105	29.	C	COMMON/TICL00P7L

NORMAN --- MAIN PROGRAM.

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00106 30. DIMENSION SURCON(6,40),I(6)
00107 31. DIMENSION GAS(6)
00110 32. DIMENSION AVCON(6,30)
00111 33. DIMENSION FNT(30),DOOT(30)
00112 34. DIMENSION UN(6,40,30)
00113 35. DIMENSION SOLID(6),TOTAL(6),DIF(6)
00114 36. DIMENSION AVAV(6)
00115 37. DIMENSION CONC(6,30,11),O(11)
00116 38. DATA KCST/.0820597/
00116 39. C
00116 40. C SUBROUTINE INITIAL READS ALL PARAMETERS FOR THIS CASE
00116 41. C AND PRINTS OUT ALL INPUT.
00116 42. C INITIAL ALSO PREPARES INPUT TO BE COMPATIBLE WITH MAIN PROGRAM
00116 43. C
00120 44. CALL MARGIN(4,62)
00121 45. IERREQ
00122 46. 3 CALL INITIAL
00122 47. C
00122 48. C LOOP 20 FINDS ALL DECAY COEFFICIENTS.
00122 49. C
00123 50. DO 20 N=1,LC
00126 51. DO 20 N=1,NTOT
00131 52. DO 20 J=1,NTOT
00134 53. SUM=0.
00135 54. IF(J=N)21,22,23
00140 55. 23 DO 24 K=N,J
00143 56. 24 SUM=SUM+T(K)
00145 57. 60 TO 21
00146 58. 22 SUM=T(J)
00147 59. 21 DCYTH=N,J*EXP(-K*(T-SUM))
00150 60. 20 CONTINUE
00150 61. C
00150 62. C INITIALIZATION OF PROFILE POINTS AND AVERAGE CONCENTRATIONS.
00150 63. C
00154 64. DO 25 K=1,IR
00157 65. DO 25 L=1,LC
00162 66. IF(IDPTH.EQ.0)50 TO 25
00164 67. DO 26 ISUB=1,ISPTH
00167 68. 26 CONC(L,K,ISUB)=0.
00171 69. 25 AVCON(L,K)=0.
00171 70. C
00171 71. C SUBSECTION TO CALCULATE YIELDS FOR ALL TIMES AND ELEMENTS.
00171 72. C YLD(L,J)=YIELD AT TIME J FOR ELEMENT L.
00171 73. C
00174 74. DO 300 J=2,NTOT
00177 75. YLD(L,J)=YLD(L,J-1)+DCYTH(L,J-1)*J-1)
00200 76. LCC=LC-1.
00201 77. DO 301 L=1,LC
00204 78. 301 YLD(L,J)=YLD(L,J-1)+DCYTH(L,J-1)+YLD(L+1,J-1)*(1.-DCYTH(L+1,J-1)*J-1)
00204 79. .17)
00206 80. 300 CONTINUE
00206 81. C
00206 82. C SUBSECTION TO CALCULATE THE MN ARRAY. MN(L,J)=SUM OVER ALL
00206 83. C PARTICLES OF THE HEIGHT OF THE PARTICLES TIMES THE SURFACE

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NORMAN --- MAIN PROGRAM.

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00206 84. C CONCENTRATION RATIO. THE SURFACE CONCENTRATION RATIO IS THE
00206 85. C SOLUTION TO THE DIFFUSION EQUATION, USING AS A DT TERM THE
00206 86. C DIFFUSION COEFFICIENT OF ELEMENT L DURING THE JTH TIME INTERVAL.
00206 87. C
00210 88. DO 400 JEL,NTOT
00213 89. DO 400 L=L,LC
00216 90. DT=DFC(L,J)*DT(J)
00217 91. SUM=0.
00220 92. DO 401 K=L,IR
00223 93. UH(L,J,K)=1.
00224 *DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTegers MAY NOT BE MEANINGFUL.
00224 94. IF(DT*.GE.(1.8*R(K)*.2))GO TO 401
00226 95. UH(L,J,K)=DIFFUS(DT,R(K))
00227 96. 401 SUM=SUM+UH(L,J,K)*DT(K)
00231 97. 400 UH(L,J)=SUM
00231 98. C
00231 99. C SUBSECTION TO CALCULATE THE SURFACE CONCENTRATION (SURCON) FOR
00231 100. C EACH ISOTOPE AT TIME STEP ONE.
00231 101. C
00234 102. DRK=VOL(1)/(RCST*E-P(1))
00235 103. DO 500 L=L,LC
00240 104. IF(ALGLOG(EN(L,1))+ALOG10(DRK).GT.35.) GO TO 501
00242 105. DVO=AMOL(L)*EN(L,1)*DRK*UH(L,1)
00243 106. GO TO 502
00244 107. 501 DVO=1.E37*UH(L,1)
00245 108. 502 CONTINUE
00246 109. IF(DVO)500,1000,500
00251 110. 500 SURCON(L,1)=VLD(L,1)/DVO
00251 111. C
00251 112. C *** MAIN LOOP ***
00251 113. C
00251 114. C CALCULATION OF SURFACE CONCENTRATIONS FOR EACH ISOTOPE AT EACH
00251 115. C TIME.
00251 116. C
00253 117. DO 600 NTIME=2,NTOT
00256 118. DRK=VGLNTIME/(RCST*TEMP(NTIME))
00257 119. DO 600 L=L,LC
00262 120. KRA=LC-[L]
00262 121. C
00262 122. C KRA-1 IS THE NUMBER OF PREDECESSORS CONTRIBUTING TO ISOTOPE L AT
00262 123. C TIME NTIME.
00262 124. C
00263 125. MAK=MINO(KRA,NTIME)
00264 126. NTE=NTIME-1
00265 127. SUM=0.
00266 128. 111750
00266 129. C
00266 130. C LOOP 601 FINDS CONTRIBUTIONS TO ISOTOPE L FROM L AT PRECEDING
00266 131. C TIME STEPS.
00266 132. C
00267 133. DO 601 K=L,NT
00272 134. 112750-K
00272 135. C
00272 136. C SCALE FINDS A DIFFUSION TERM.

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00272	137.	C	
00273	138.		CALL @CALC(I,K,I,1,0,000,DIERR)
00274	139.		KRIK=I
00275	140.		I(2)=I(2)-1
00276	141.		CALL @CALC(I,KRIK,I,1,0,0,FI,DIERR)
00277	142.		BRES=I
00300	143.		SUMSU=I+ BRESURCON(L,K)*DCY(L,K,IT)
00301	144.		IF(ITIME,NE,NTOTED TO 601
00301	145.	C	
00301	146.	C	IF FINAL TIME, FIND CONTRIBUTIONS TO AVERAGE CONCENTRATIONS
00301	147.	C	A/D PROFILE POINTS.
00301	148.	C	
00303	149.		DO 6012 M=1,IR
00306	150.		IF(DPTH,EG,DTG TO 6012
00310	151.		DO 6013 ISU=1,DPTH
00313	152.		CONCL=4,ISU)=CONCL+1,ISU)+DCY(L,K,IT)*SURCON(L,K)*(PROFIL(I)*
00313	153.		*N(RM)*Q(1506))-PROFIL(DIER(I,R(M),Q(1506)))
00314	154.		6013 CONTINUE
00316	155.		6012 AVCON(L,M)=AVCON(L,M)+DCY(L,K,IT)*SURCON(L,K)*(DQ(4I-FM(K))
00320	156.		601 CONTINUE
00322	157.		A=SUM
00323	158.		IF(WK,EG,DTG TO 602
00323	159.	C	
00323	160.	C	LOOP 603 FINDS CONTRIBUTIONS TO ISOTOPE L FROM ITS PREDECESSORS.
00323	161.	C	
00325	162.	C	DO 605 N=1,2,3,4,5
00325	163.	C	
00325	164.	C	VALUE OF NEL IS THE SUBSCRIPT OF PREDECESSOR OF ISOTOPE L.
00325	165.	C	
00330	166.		SUM=0.
00331	167.		NET=NEL-1
00332	168.		NEP=NEL+L-1
00332	169.	C	
00332	170.	C	LOOP 5 FINDS CONTRIBUTIONS FROM ISOTOPE NED AT TIME 162.
00332	171.	C	
00333	172.		DO 5 IT=1,NT
00336	173.		N2=NTIME-11
00337	174.		I(17211
00340	175.		B=0.
00340	176.	C	
00340	177.	C	THE I ARRAY SPECIFICS THE DECAY PATH FROM IEP AT 162
00340	178.	C	TO L AT NTIME.
00340	179.	C	
00341	180.		N2=11-NEL
00342	181.		I(2)=1
00343	182.	101	IF(NEL,EG,DTG TO 40
00345	183.		N3=N2-I(2)-1
00346	184.		I(3)=1
00347	185.	111	IF(NEL,EG,DTG TO 40
00351	186.		N3=N3-I(3)-1
00352	187.		I(4)=1
00353	188.	121	IF(NEL,EG,DTG TO 40
00355	189.		N3=N3-I(4)-1
00356	190.		I(5)=1

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NORMAN --- MAIN PROGRAM.
00357 191. 131 IF (NEL.EQ.5) GO TO 40
00361 192. N5=N5-I(5)-1
00362 193. I(6)=1
00363 194. C
00362 195. C DELTA FINDS THE DECAY TERM ASSOCIATED WITH THIS PATH.
00362 196. C
00363 197. C 40 CALL DELTA(NEL,NTIME,I,PDDEL)
00363 198. C
00363 199. C BCALC FINDS THE DIFFUSION TERMS ASSOCIATED WITH THIS PATH.
00363 200. C
00364 201. CALL BCALC(NEL,NTIME,I,1,BDF,DOO,DTER4)
00365 202. CALL BCALC(NEL,NTIME,I,0,BDF,1,FN,DTER4)
00366 203. IF (NTIME.NE.NTOT) GO TO 19
00366 204. C
00366 205. C AT THE FINAL TIME, FIND AVERAGE CONCENTRATION AND PROFILE POINT
00366 206. C CONTRIBUTIONS.
00366 207. C
00370 208. DO 18 N21,NR
00373 209. IF (IDPTH.EQ.0) GO TO 18
00375 210. DO 18O ISUB=1,1DPTH
00400 211. CUNC(L,N,ISUB)=CUNC(L,N,ISUB)+PDDEL*SURCON(NEP,N2P)*(H*DFIL(UTER4
00400 212. *R(N)*G1SUB))-PROFIL(DYER4,R(N)*G1SUB))
00401 213. 18O CONTINUE
00403 214. 18 AVCON(L,N)=AVCON(L,N)+PDDEL*SURCON(NEP,N2P)*(DOO(I)*F(N))
00405 215. 19 B36=B36+BDF*3DF1
00405 216. C
00405 217. C B IS THE SUM OF ALL CONTRIBUTIONS FOR THESE STATES.
00405 218. C
00406 219. C B=B+B36*PDDEL
00407 220. GO TO (5,10,11,12,13,18),NEL
00410 221. 14 * (6)=1(6)+1
00411 222. IF (I(6)=46) 40,40,13
00414 223. 13 I(5)=1(5)+1
00415 224. IF (I(5)=45) 13,13,12
00420 225. 12 I(4)=1(4)+1
00421 226. IF (I(4)=44) 12,12,11
00424 227. 11 I(3)=1(3)+1
00425 228. IF (I(3)=43) 11,11,10
00430 229. 10 I(2)=1(2)+1
00431 230. IF (I(2)=42) 10,10,16
00434 231. 16 B=B+SURCON(NEP,N22)
00435 232. 5 SURCON(NEP,N22)
00437 233. 603 A=A+SUM
00441 234. 002 IF (ALOG10(NTIME/NTIME)+ALOG10(DO0)*G1,N5,1) GO TO 503
00443 235. DVO=DNK+XOL(L)*HEN(L,NTIME)+H(L,NTIME)
00444 236. GO TO 504
00445 237. 503 DVO=1.E37+H(L,NTIME)
00446 238. 504 CONTINUE
00447 239. IF (DVO) 666,1001,666
00452 240. 666 YV=YV+DVO*(NTIME)-A
00453 241. T1=DVO-H(L,NTIME)
00454 242. SURCON(L,NTIME)=YV/DVO
00455 243. IF (NTIME.NE.NTOT) GO TO 600
00457 244. DO 47 N21,NR

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NORMAN --- MAIN PROGRAM.	
00462 245.	IF (IDPTH.EQ.0) GO TO 47
00464 246.	DO 470 ISUB=1, IDPTH
00467 247.	CONC(L,M,ISUB)=CONC(L,M,ISUB)+SURCON(L,NTOT)*PROFIL(DFC(L,NTOT))*T(
00467 248.	NTOT)*R(M)/3(ISUB)
00470 249.	470 CONTINUE
00472 250.	47 AVCON(L,M)=AVCON(L,M)+SURCON(L,NTOT)*DPI(L,NTOT,M)
00474 251.	600 CONTINUE
00474 252.	C
00474 253.	C
00474 254.	C
00474 255.	C
00474 256.	C
00474 257.	C
00477 258.	WRITE(6,1075) MCS1,MCS2,NAME(L),L=1,LC
00507 259.	DO 1090 J=1,NTOT
00512 260.	1090 WRITE(6,1076) TEMP(J),ATM(J),SURCON(L,J),L=1,LC
00512 261.	C
00512 262.	C
00512 263.	C
00523 264.	WRITE(6,1200) MCS1,MCS2,NAME(L),L=1,LC
00533 265.	DO 80 J=1,NTOT
00536 266.	DO 81 L=1,LC
00541 267.	81 GAS(L)=SURCON(L,J)*HE(L,J)*VOL(J)*MOL(L)/(MCS1*TEMP(J))
00543 268.	80 WRITE(6,1076) TEMP(J),ATM(J),GAS(L),L=1,LC
00543 269.	C
00543 270.	C
00543 271.	C
00554 272.	WRITE(6,1201) MCS1,MCS2,TEMP(NTOT),NAME(L),L=1,LC
00565 273.	DO 43 J=1,IR
00570 274.	43 WRITE(6,1202) R(J),AVCON(L,J),L=1,LC
00570 275.	C
00570 276.	C
00570 277.	C
00600 278.	LOOP 88 FINDS SUMMARY RESULTS.
00603 279.	DO 88 L=1,LC
00604 280.	SOLID(L)=0.
00607 281.	DO 89 K=1,IR
00611 282.	89 SOLID(L)=SOLID(L)+AVCON(L,K)*WT(K)
00612 283.	AVAV(L)=SOLID(L)/IR
00613 284.	TOTAL(L)=SOLID(L)+GAS(L)
00615 285.	88 DIP(L)=(TOTAL(L)-VOLD(L,NTOT))
00623 286.	WRITE(6,1210) (AVAV(L),L=1,LC)
00625 287.	IF (IDPTH.EQ.0) GO TO 252
00625 288.	WRITE(6,1211) MCS1,MCS2,TEMP(NTOT)
00625 289.	C
00625 290.	C
00632 291.	C
00635 292.	DO 250 L=1,LC
00644 293.	WRITE(6,1212) NAME(L),TOTRT,K=1,IR
00647 294.	DO 251 K=1,IR
00657 295.	251 WRITE(6,1213) RT(K),CONCL(K,IR),IR,IR
00657 296.	250 CONTINUE
00657 297.	C
00657 298.	C
00657 299.	C
00657 300.	PRINT SUMMARY RESULTS.

NORMAN --- MAIN PROGRAM

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00661 299. 252 WRITE(6,1204)TEMP(NTOT),NCS1,NCS2,(NAME(L),L=1,LC)
00672 300. WRITE(6,1205)(GAS(L),L=1,LC)
00700 301. WRITE(6,1206)(SOLID(L),L=1,LC)
00706 302. WRITE(6,1207)(TOTAL(L),L=1,LC)
00714 303. WRITE(6,1208)(VLD(L),L=1,LC)
00722 304. WRITE(6,1209)(DIF(L),L=1,LC)
00730 305. IF(ILE.EQ.0)GO TO 3
00732 306. CALL FINAL(AVCON,GAS,R,NT,NAME(1))
00733 307. GO TO 3
00733 308. C
00733 309. C ERROR STOPS
00733 310. C
00734 311. 1000 WRITE(6,1050)NAME(L),NMOL(L),HEM(L,1),NM(L,1),T(1),TEMP(1),VOL(1)
00745 312. CALL DUMP
00746 313. 1001 WRITE(6,1050)NAME(L),NMOL(L),HEM(L,NTIME),NM(L,NTIME),T(NTIME),TE4
00746 314. XP(NTIME),VOL(NTIME)
00757 315. CALL DUMP
00757 316. C
00757 317. C F O R M A T S
00757 318. C
00760 319. 1050 FORMAT(1H0,5X,35H*** ERROR: PROGRAM CANNOT CONTINUE./10X,20HTHE SUR
00760 320. FACE CONCENTRATION OF GAS,1X,12HIS I-FINITE./15X,19HMOLECULAR WEI
00760 321. GHT = ,E16.8/15X,23HWEIGHTS LAW CONSTANT = ,E16.8/15X,54HIN = ,E10.
00760 322. X8/15X,17HINCREASE = ,E16.8/15X,14HOPERATOR = ,F9.1/15X,15
00760 323. XH VOLUME OF CLOUD = ,E16.8)
00761 324. 1075 FORMAT(1H0,50X,31H SURFACE CONCENTRATIONS IN U/G ,15X,9H CASE NO. ,
00761 325. /13,1H,,A9/28X,7HISOTOPE//13X,4HTEMP,6X,4HTIME,6X,46,5(13X,46,5)
00762 326. 1076 FORMAT(1X,7,1,2X,1P8,3,6(13X,1P16,8))
00763 327. 1200 FORMAT(1H1,48X,35H OUTPUT OF MATERIAL IN THE GAS PHASE,61X,10HIN G
00763 328. ,RANST30X,9H CASE NO. ,13,1H,,A9/28X,7HISOTOPE//13X,4HTEMP,6X,4HTIME
00763 329. ,9X,46,5(13X,46,5))
00764 330. 1201 FORMAT(1H1,62X,40H AVERAGE CONCENTRATIONS PER PARTICLE SIZE,14X,9H C
00764 331. ASE NO. ,13,1H,,A9/49X,21HAT FINAL TEMPERATURE ,F5.0/11H DEG KELVI
00764 332. N/28X,7HISOTOPE//2X,15H PARTICLE RADIUS,7H(1X C9)13X,46,5(13X,
00764 333. 46,5))
00765 334. 1202 FORMAT(1H1,41X,33H SUMMARY OF RESULTS AT FINAL TEMP ,F5.0/11H DEG K
00766 335. 1204 FORMAT(1H1,41X,33H SUMMARY OF RESULTS AT FINAL TEMP ,F5.0/11H DEG K
00766 336. ,ELVT,10X,9H CASE NO. ,13,1H,,A9/28X,7HISOTOPE//26X,46,5(13X,46,5))
00767 337. 1205 FORMAT(1H0,17H AVERAGE IN GAS PHASE,6(13X,1P16,8))
00770 338. 1206 FORMAT(1H0,17H AVERAGE IN SOLID PHASE,1X,1P16,8,5(13X,1P16,8))
00771 339. 1207 FORMAT(1H0,54H TOTAL,12X,6(13X,1P16,8))
00772 340. 1208 FORMAT(1H0,54H YIELD AT FINAL TIME,1X,1P16,8,5(13X,1P16,8))
00773 341. 1209 FORMAT(1H0,10H DIFFERENCE,7X,6(13X,1P16,8))
00774 342. 1210 FORMAT(1H0,5X,7H AVERAGE,5X,6(13X,1P16,8))
00775 343. 1211 FORMAT(1H1,52X,26H R O F I L E P O I N T 5,21X,9H CASE NO. ,13,1H
00775 344. ,A9/28X,7HISOTOPE//2X,15H PARTICLE RADIUS,7H(1X C9)13X,46,5(13X,
00775 345. 46,5))
00776 346. 1212 FORMAT(1H0,5X,7H AVERAGE,5X,6(13X,1P16,8))
00776 347. ,A9/28X,7HISOTOPE//2X,15H PARTICLE RADIUS,7H(1X C9)13X,46,5(13X,
00777 348. 46,5))
00777 349. 1213 FORMAT(1H1,52X,26H R O F I L E P O I N T 5,21X,9H CASE NO. ,13,1H
00777 349. 46,5))
01000 E40

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END OF LISTING. 1 *DIAGNOSTIC* MESSAGE(S).

SUBROUTINE INITIAL

01 FOR INITIAL

COMPILATION BY UNIVAC 1106 FORTRAN-IV DATED 11 NOV 1966 F4000
THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:04

SUBROUTINE INITIAL ENTRY POINT 001103

STORAGE USED (BLOCK, NAME, LENGTH)

0001	SCODE	001114
0000	DATA	000626
0002	BLANK	001676
0003	SING	000023

EXTERNAL REFERENCES (BLOCK, NAME)

0004	ALOG
0005	DIFFUS
0006	EXP
0007	NRJUS
0010	NIC15
0011	NIC25
0012	NRJUS
0013	NEAP65

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000054	10L	0000	000164	100F	0000	000275	101F	0000	000310	102F	0000	000337	102F	
0000	000360	104F	0000	000402	105F	0000	000406	106F	0000	000436	107F	0000	000457	107F	
0000	000464	109F	0000	000502	110F	0000	000506	111F	0000	000534	112F	0000	000541	112F	
0000	000545	114F	0000	000563	115F	0001	000605	116G	0001	000703	12L	0001	000567	16L	
0001	000050	1406	0001	000067	1466	0001	000625	16L	0001	000107	16H9	0001	000635	16L	
0001	000606	19L	0000	000162	200UF	0000	000271	2001F	0000	000306	2002F	0000	000343	2003F	
0000	000345	2004F	0001	000304	21L	0001	000177	216G	0001	000223	22L	0001	000204	2383	
0001	000334	2606	0001	000350	2706	0001	000471	3276	0001	000507	3376	0001	000532	3536	
0001	000554	3676	0001	000612	4046	0001	000635	416G	0001	000716	4383	0001	000727	4435	
0001	000743	4536	0001	000745	4566	0001	001004	476G	0001	001014	4763	0001	001022	4825	
0001	001032	5106	0001	001036	5206	0001	000451	61L	0001	000440	63L	0001	000403	66L	
0001	000453	65L	0001	000541	77L	0001	000542	78L	0002	001334	AA	0004	000009	1336	
0002	R	001626	ATM	0000	R	000131	PKT	0000	R	000160	CCN1	0000	R	000124	C1
0000	R	000150	C2	0003	R	000142	C3	0000	R	000125	C4	0000	R	000350	CC2
0000	R	000102	CCP	0002	R	000374	DPC	0005	R	000000	DIFFUS	0000	R	000000	EXP
0000	R	000006	MC1	0000	R	000014	MC2	0002	R	000754	ME1	0000	R	000156	12.1
0000	R	000134	HTMP	0000	I	000132	I	0003	I	000007	TDPTH	0003	I	000000	19
0000	I	000127	J	0000	I	000137	K	0000	I	000156	KK12	0000	I	000000	LC
0000	I	000157	LCC	0002	I	000360	NAME	0003	I	000003	NCS1	0003	I	000110	RTITLE
0003	I	000002	MTOT	0000	R	000126	PI	0000	R	000044	PM	0002	R	001342	7
0002	R	001506	I	0002	R	001536	TEMP	0000	R	000152	TEMP1	0000	R	000151	TEMP
0000	R	000141	IIV	0000	R	000155	TT	0000	R	000149	TEMP	0003	R	000005	TEMP
0002	R	001436	VOL	0002	R	000366	WVOL	0002	R	000400	W1	0000	R	000139	WRT

SUBROUTINE INITIAL

0002 R 000000 YLD 0000 R 00015 ZDC 0000 R 000140 ZDT 0000 2 000147 ZSHI 0000 2 000143 ZTI

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00101 1. SUBROUTINE INITIAL
00102 2. COMMON YLD(6,40),HAYE(6),FVOL(6),DFC(6,40),HEN(6,40),AK(6),H(30),A
00103 3. /T(30),VOL(40),T(40),TEMP(40),ATM(40)
00104 4. COMMON/SING/LC,IR,NTOT,NC51,NC52,TY,ILG,IDPH,MO
00105 5. DIMENSION YI(6),MC1(6),MC2(6),DC1(6),DC2(6),HL(6),PU(30),DOP(6)
00106 6. DIMENSION Q(11)
00107 7. DIMENSION NTITLE(12)
00108 8. DATA '174.66E37,C4/2.381G26IE-5/,PI/3.14159265/
00109 9. SUBROUTINE READS ALL DATA AND CALCULATES INITIAL INPUTS NEEDED.
00110 10. C
00111 11. C VARIABLE DEFINITIONS
00112 12. C
00113 13. C LC LENGTH OF CHAIN.
00114 14. C YAT YIELD OF DEVICE USED IN CALCULATING YIELDS (IN KT)
00115 15. C BAT YIELD USED FOR CALCULATING VOLUME, WEIGHT, TEMPERATURES,
00116 16. C AND TIME INCRS. (IN KT)
00117 17. C IR NUMBER OF PARTICLES
00118 18. C NAME ARRAY CONTAINING NAMES OF ISOTOPIES.
00119 19. C FVOL ARRAY CONTAINING MOLECULAR WEIGHTS OF ISOTOPIES (IN GR/MOL)
00120 20. C VI ARRAY CONTAINING INITIAL YIELDS AT YEO. (IN ATOMS
00121 21. C PER 10,000 FISSIONS)
00122 22. C DFC ARRAY OF DIFFUSION COEFFICIENTS.
00123 23. C HEN ARRAY OF HENRY'S LAW CONSTANTS.
00124 24. C AK ARRAY OF K, WHERE
00125 25. C -LOG(1/2)EK*(HALF LIFE)
00126 26. C R ARRAY OF PARTICLE RADII. (IN CM.)
00127 27. C AT ARRAY OF PARTICLE WEIGHTS (IN GR/MS).
00128 28. C VOL ARRAY OF CLOUD VOLUMES (IN LITERS).
00129 29. C T ARRAY OF TIME INCREMENTS. (IN SEC)
00130 30. C TEMP ARRAY OF TEMPERATURES. (IN DEG CELSIUS)
00131 31. C HL ARRAY OF HALF-LIVES. (IN SECONDS)
00132 32. C P2 ARRAY OF PERCENT OF TOTAL WEIGHT PER PARTICLE SIZE.
00133 33. C NTOT TOTAL NUMBER OF TIME TEMPERATURE STEPS.
00134 34. C HTEMP THE STARTING (HIGHEST) TEMPERATURE.
00135 35. C LTEMP THE FINAL (LOWEST) TEMPERATURE.
00136 36. C TCRPV THE INCREMENTAL TEMPERATURE.
00137 37. C Y6GT TOTAL HEIGHT OF PARTICLES.
00138 38. C YIV TOTAL INITIAL VOLUME OF CLOUD.
00139 39. C MC1,MC2 ARRAYS OF CONSTANTS USED IN CALCULATING HENRY'S LAW
00140 40. C CONSTANTS. LOG(HENRY'S LAW) = MC2/TEMP.
00141 41. C DC1,DC2 ARRAYS OF CONSTANTS USED IN CALCULATING DIFFUSION
00142 42. C COEFFICIENTS. LOG(DIFFUSION) = DC2/TEMP.
00143 43. C
00144 44. C READ INPUT DATA AND PRINT ISOTOPE PARAMETERS.
00145 45. C
00146 46. READ(5,115) (NTITLE(I),J=1,12),NC51,NC52
00147 47. READ(5,2000) LC,IR,ILG,IDPTH,YAT,BAT
00148 48. IF (IDPTH.EQ.0) GO TO 10

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SUBROUTINE INITIAL
00136 49. READ(5,2002) (I(I), I=1, IOPM)
00144 50. 10 WRITE(6,100) (N(I), I=1, IOPM)
00157 51. DO 90 L=1, LC
00162 52. READ(5,2001) NAME(L), ZMOL(L), YI(L), HCI(L), HC2(L), DC1(L), DC2(L), HL(L)
00162 53. /)
00174 54. 90 WRITE(6,101) NAME(L), ZMOL(L), YI(L), HCI(L), HC2(L), DC1(L), DC2(L), HL(L)
00174 55. /)
00207 56. READ(5,2002) HTEMP, ETMP, TEMPV
00214 57. READ(5,2003) (R(K), K=1, IR)
00223 58. READ(5,2004) TWGT, TIV
00227 59. C3=-.546*(R(KT))**(-.373)
00227 60. C
00227 61. C TEST STARTING TEMPERATURE--- IF SPECIFIED TEMPERATURE IS SUCH
00227 62. C THAT ALL F VALUES ARE UNITY, REDUCE STARTING TEMP. BY ONE
00227 63. C INCREMENT.
00227 64. C
00230 65. 22 ZTMP=HTEMP-TEMPV/2.
00231 66. ZTEMP=ZTMP-TEMPV/7C3
00232 67. DO 20 L=1, LC
00235 68. ZDC=10.*R(DC1(L))-DC2(L)/ZTMP)
00236 69. ZDT=ZDC*ZTM
00237 70. ZSUX=0.
00240 71. 20 ZSUM=ZSUM+DIFFUS(ZDT,R(I))
00242 72. IF (ZSUM-1) 51, 7, 51 GO TO 21
00244 73. HTEMP=ZTMP-TEMPV
00245 74. GO TO 22
00245 75. C
00245 76. C PRINT WEIGHT, TEMPERATURE AND VOLUME PARAMETERS.
00245 77. C
00246 78. 21 WRITE(6,102) HTEMP, ETMP, TEMPV
00253 79. WRITE(6,103) TAST
00253 80. C
00253 81. C CALCULATE WEIGHTS PER PARTICLE SIZE AND PRINT.
00253 82. C
00256 83. TAT=T*GT*OKT
00257 84. DO 91 K=1, IR
00262 85. 91 W(K)=TWGT*PR(K)
00264 86. WRITE(6,104) IR
00267 87. DO 92 K=1, IR
00272 88. 92 WRITE(6,105) W(K), TAT(K)
00277 89. C2=(OKT)**(-.01)
00277 90. C
00277 91. C COMPUTE INITIAL TIME (TINT), INCREMENTAL TIMES (T(I)), AND
00277 92. C TOTAL TIMES ATN(I)).
00277 93. C
00300 94. TINT=1006/HTEMP/(C1*C2)/7C3
00301 95. J=1
00302 96. TEMPC=HTEMP
00303 97. 64 TTEMP=TEMP-TEMPV
00304 98. TEMPT(J)=TEMPC+TTEMP/72.
00305 99. T(J)=ZALOG(TTEMP/TEMP)/C3
00306 100. IF (TTEMP-ETMP) 61, 60
00311 101. 60 J=J+1
00312 102. IF (J-40) 62, 53

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SUBROUTINE INITIAL

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00315 103.      62 TEXPL=TIMEP
00316 104.      60 TO 64
00317 105.      63 WRITE(6,106)TEMP(40)
00322 106.      NTOT=40
00323 107.      60 TO 65
00324 108.      61 NTOT=J
00325 109.      65 ATN(1)=TINT+T(1)/2.
00326 110.      DO 66 J=2,NTOT
00331 111.      66 ATN(J)=ATA(J-1)+T(J)+T(J-1))/2.
00331 112.      C
00331 113.      C PRINT TIME-TEMPERATURE DISTRIBUTION.
00331 114.      C
00333 115.      WRITE(6,107)NTOT
00336 116.      DO 70 J=1,NTOT
00341 117.      70 WRITE(6,108)ATN(J),T(J),TEMP(J)
00347 118.      WRITE(6,114)TINT
00347 119.      C
00347 120.      C COMPUTE INITIAL YIELDS IN GRAMS.
00347 121.      C
00352 122.      DO 71 L=1,LC
00355 123.      *DIAGNOSTIC* THE LIST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
00355 123.      IF(ML(L).EQ.0.) GO TO 77
00357 124.      AK(L)=-69315/ML(L)
00360 125.      60 TO 78
00361 126.      77 AK(L)=0.
00362 127.      76 YI(L)=CS*WOL(L)*YKT*YI(L)
00363 128.      71 CONTINUE
00363 129.      C
00363 130.      C CALCULATE YIELDS AT START TIME.
00363 131.      C
00365 132.      HLM=1.E38
00366 133.      DO 14 L=1,LC
00371 134.      IF(ML(L).LT.1.E-5) GO TO 14
00373 135.      HLM=AMIN(HLM,ML(L))
00374 136.      14 CONTINUE
00376 137.      HLM=ML/10.
00377 138.      IF(HLM.GT.TINT) HLM=TINT
00401 139.      TTE=HLM
00402 140.      KNUZ=0
00403 141.      19 DO 15 L=1,LC
00406 142.      15 DDP(L)=EXP(-AK(L)*HLM)
00410 143.      LCC=LC-1
00411 144.      16 IF(LC.EQ.1) GO TO 16
00413 145.      DO 73 L=1,LCC
00416 146.      73 YI(L) =YI(L)*DDP(L)+YI(L+1)*(1.-DDP(L+1))
00420 147.      18 YI(LC)=YI(LC)*DDP(LC)
00421 148.      TTE=HLM
00422 149.      IF(TTE.LT.TINT) GO TO 16
00424 150.      IF(KNUZ.EQ.1) GO TO 13
00426 151.      IF(ABS(TTE-TINT).LT.1.E-5) GO TO 13
00430 152.      KNUZ=1
00431 153.      HLM=TINT-TTE+HLM
00432 154.      60 TO 19
00433 155.      13 DO 17 L=1,LC

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SUBROUTINE INITIAL

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00436 150. 17 YLD(L,1)=YI(L)
00436 157. C
00436 158. C PRINT OUT ADJUSTED YIELDS.
00436 159. C
00440 160. 74 WRITE(6,109)
00442 161. DO 75 L=1,LC
00445 162. 75 WRITE(6,110)NAME(L),YLD(L,1)
00445 163. C
00445 164. C CALCULATE DIFFUSION COEFFICIENTS AND HENRY'S LAW CONSTANTS.
00445 165. C
00452 166. DO 80 J=1,NTOT
00455 167. DO 30 L=1,LC
00460 168. MEN(L,J)=10.0*(HCL(L)-HCL2(L)/TEMP(J))
00461 169. DO 80 J=1,NTOT
00461 170. C PRINT DIFFUSION AND HENRY'S LAW COEFFICIENTS.
00461 171. C
00461 172. C
00464 173. WRITE(6,111)NCS1,HCS2,NAME(L),L=1,LC)
00474 174. DO 50 J=1,NTOT
00477 175. WRITE(6,112)TEMP(J),(DFC(L,J),L=1,LC)
00506 176. 50 WRITE(6,113)(HEN(L,J),L=1,LC)
00506 177. C
00506 178. C CALCULATE VOLUME FOR ALL TIMES.
00506 179. C
00515 180. C
00515 181. C
00517 182. C
00522 183. 40 VOL(J)=CON*TEMP(COHL*AT*Q(J))**3
00524 184. 2000 FORMAT(4I5,2F10.3)
00525 185. 100 FORMAT(1H,51X,25H1000 INPUT DATA 007755X,12X,0.1A,04C5E
00525 186. /O,13.1M,04//
00525 187. /I1 = 12/10X,15HDEVICE YIELD = 516.3524 KT/1000GHEM OF CH4
00525 188. /6H(FROM TIME-TEMP DISTRIBUTION))//56X,14HISOTOPE DATA REFERS//42X,4H1A
00525 189. /7C,9X,9HMOLECULAR WEIGHT INITIAL,9X,3HCH4,12X,3H12C,12X,3H13C,12X,3H
00525 190. /DC2,12X,4HMF/22X,4HHEIGHT,9X,5HYIELD,70X,4H1FC/20X,9H1 G/100 ME,
00525 191. /9X,15HISOTOPES/17X,00H063X,9H1SECTORS/35X,9H1STATIONS/1)
00526 192. 2001 FORMAT(46,7F10.0)
00527 193. 101 FORMAT(15X,4G,12X,F8.0,3X,F7.10X,F8.3,7X,F8.1,7X,F8.3,7X,F8.1,7GF
00530 194. /8.2)
00530 195. 2002 FORMAT(10F10.0)
00531 196. 102 FORMAT(11H0.9X,25HSTARTING TEMPERATURE = ,F6.0,12H DEG. KELVIN/10X,
00531 197. /20HFINAL TEMPERATURE = ,F6.0,12H DEG. KELVIN/10X,25HTEMPERATURE TI
00531 198. /CNEMENT = ,F6.0,12H DEG. KELVIN)
00532 199. 2003 FORMAT(2F10.0)
00533 200. 2004 FORMAT(2E16.8)
00534 201. 103 FORMAT(10X,24HTOTAL PARTICLE WEIGHT = ,PE16.8,6H G/KYT)
00535 202. 104 FORMAT(11H0.10X,19-PARTICLE PARAMETERS/10X,12,1X,10HPARTICLE SIZES/
00535 203. .12X,6H0RADIUS,12X,6HHEIGHT/10X,9H1C7/10X,4H1C1)
00536 204. 105 FORMAT(10X,F10.6,5X,1PE16.8)
00537 205. 106 FORMAT(11H0.9X,52HTHE ARE TOO MANY TIME-TEMPERATURE STEPS SPECIFI
00537 206. /ED./10X,40HTHE LOWEST TEMPERATURECONSIDERED ALL FE,1X,F7.1015H DE
00537 207. /6REES KELVIN)
00540 208. 107 FORMAT(11H0.9X,20HTIME-TEMPERATURE DISTRIBUTION,1X,12,7H STEPS./12
00540 209. /X,40HTIME,10X,40HTIME,10X,40HTEMP/26X,9H1C7)

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SUBROUTINE INITIAL

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00541 210. 108 FORMAT(1H,9X,F9.50X,F9.501X,F7.1)
00542 211. 109 FORMAT(1H0,20X,41HYIELD5, 14 GRATS, ADJUSTED TO START TIME./10X,7H
00543 212. /15010PE,10X,5HYIELD)
00544 213. 110 FORMAT(1H,9X,A6,6X,1PE16.8)
00545 214. 111 FORMAT(1H1,24X70HDIFUSION COEFFICIENTS (LINE ONE) AND HENRY'S LAW
00546 215. / CONSTANTS (LINE TWO),3X,9MCASE NO. 13,1H,0A7/9X,4HTEMP,2A,6(13X
00547 216. /,A6)/)
00548 217. 112 FORMAT(1H0,1X,F9.1,7X,6(3X,1PE16.8))
00549 218. 113 FORMAT(17X,6(13X,1PE16.8))
00550 219. 114 FORMAT(1H0,9X,56HSTART TIME FOR CALCULATION OF SURFACE CONCENTRATI
00551 220. / 0.5 IS ,F9.5,4H SEC)
00552 221. 115 FORMAT(12A6,13,1X,A6)
00553 222. RETURN
00554 223. END

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END OF LISTING. 1 *DIAGNOSTIC* MESSAGE(S).

SUBROUTINE FINAL

01 FOR FINAL

COMPILATION BY UHIVAC 1108 FORTRAN-IV DATED 11 NOV 1966 F4008
THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:09

SUBROUTINE FINAL ENTRY POINT 000123

STORAGE USED (BLOCK, NAME, LENGTH)

0001	*CODE	000152
0000	*DATA	000345
0002	*BLANK	000000
0003	SING	000006

EXTERNAL REFERENCES (BLOCK, NAME)

0004	NAMEUS
0005	NI015
0006	NI025

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000234	100F	0000	000320	101F	0001	000014	107G	0001	000015	113J	0001	000016	118G		
0001	000037	131G	0001	000052	180G	0001	000100	158G	0001	000000	FC	0001	000001	FC5		
0000	R	000074	FW	0000	R	000250	GT	0000	I	000233	I	0003	I	000226		
0000	I	000227	K	0000	I	000251	L	0003	I	000300	LC	0003	I	000226		
0003	000002	MTOT	0003	000015	TWT	0000	R	000170	V	0003	I	000232	AV	0003	I	000132

00101	1.	SUBROUTINE FINAL	AVCON(6,30),GAS(6),Z(30),Z(30)	FI 1A0010
00103	2.	DIMENSION	AVCON(6,30),GAS(6),Z(30),Z(30)	FI 1A0210
00104	3.	DIMENSION	FC(30),FCS(30),FV(30),Z(30),V(30)	FI 1A0210
00105	4.	COMMON	SI(4G/LC,IR,NTOT,NCS1,NCS2,EXT	FI 1A0230
00106	5.	DO	10 J=1,IR	FI 1A0510
00111	6.	FCS(J)=0.		FI 1A0510
00112	7.	DO	11 K=1,LC	FI 1A0520
00115	8.	11 FCS(J)=FCS(J)+AVCON(K,J)		FI 1A0530
00117	9.	10 CONTINUE		FI 1A0540
00121	10.	GT=0.		FI 1A0550
00122	11.	DO	20 L=1,LC	FI 1A0570
00125	12.	20 GT=GT+GAS(L)		FI 1A0570
00127	13.	VFE0.		FI 1A0570
00130	14.	DO	30 K=1,IR	FI 1A0580
00133	15.	Z(K)=Z(117)R(K)		FI 1A0580
00134	16.	V(K)=Z(K)+V(K)		FI 1A0580
00135	17.	30 VFE=VFE+V(K)		FI 1A0580
00137	18.	DO	40 I=1,IR	FI 1A0580
00142	19.	FC(I)=Z(117)G(I)+VFE(I)		FI 1A0580

SUBROUTINE FINAL		
00143	20.	48 F4(I)=FC(I)*NT(I)
00143	21.	C
00143	22.	C PRINT DATA.
00143	23.	C
00145	24.	WRITE(6,100)NAME,ICS1,ICS2,NAVE
00153	25.	DJ 50 K=1,71
00156	26.	50 WRITE(6,101)R(K),FC5(K),FC(K),FY(K)
00165	27.	100 RETURN
00166	28.	NO. 013.14.74/79X.15-PARTICLE RADIUS.5X.21-NAVERAGE CONCENTRATION.0.011010
00166	29.	.5X.27-TOTAL AVERAGE CONCENTRATION.0.5X.15-TOTAL AVERAGE CONCENTRATION.0.011010
00166	30.	.12X.20-DUE TO SOLIDS DECAY.0.5X.20-TOTAL AVERAGE CONCENTRATION.0.011010
00166	31.	.24 IN PARTICLE/36X.7H(6"/54).22X.7H(6"/54).20X.4H(C4)
00167	32.	101 FORMAT(13X,F7.5,12X,1PE14.3,15X,1PE14.3,13X,1PE14.3)
00170	34.	END

END OF LISTING. 0 DIAGNOSTIC MESSAGE(S).

SUBROUTINE BCALC

01 FOR BCALC
 COMPILATION BY UNIVAC 1106 FORTRAN-IV DATED 11 NOV 1966 F4008
 THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:12

SUBROUTINE BCALC ENTRY POINT 000157

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CUL 000225
 0000 *DATA 000030
 0002 *BLANK 001676
 0003 SING 000005
 0004 BI 023160
 0005 INLOOP 000001

EXTERNAL REFERENCES (BLOCK, NAME)

0006 DIFFUS

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000116 11L 0001 000110 12L 0001 000043 1315 0001 000131 1603 0001 000027 20L
 0001 000153 30C 0001 000027 30L 0002 001134 AK 0002 001625 ATN 0003 000000 20V
 0002 R 000374 CFC 0006 R 000000 DIFFUS 0000 R 000000 EMISLH 0002 000754 EPI 0003 I 000001 20
 0001 000002 J 0000 I 000010 K 0005 I 000000 L 0003 000000 LC 0004 I 000005 20
 0002 000360 NAME 0003 000003 MCS1 0003 000004 MCS2 0001 000003 TEL 0004 I 000005 20
 0000 I 000011 HGG 0003 000002 TOT 0000 I 000005 SI 0001 000007 20V
 0000 R 000001 SVSU4 0002 R 001546 T 0002 001556 TEMP 0002 R 001342 X 0004 R 000004 20V
 0004 022600 BI 0002 R 001800 Y 0002 000000 YLN 0002 001436 YCL 0002 000365 20V

00101 1. SUBROUTINE BCALC(N,T,I,KLAG,S,DD,DT)
 00101 2. C SUBROUTINE TO CALCULATE SOLUTIONS TO THE DIFFUSION EQUATION.
 00101 3. C FIRST SECTION COMPUTES THE PROPER DT VALUE.
 00103 4. DIMENSION ITG)
 00104 5. COMMON YLD(5,40),IAE(6),XVL(6),DEC(6,40),MEI(6,40),AK(6),R(30),T
 00104 6. /T(30),VOL(40),T(40),TEMP(40),AT(40)
 00105 7. COMMON/SING/LC,IR,NTOT,MCS1,MCS2
 00106 8. COMMON/BI/DCY(6,40),ZOT/ENT(6,40)
 00107 9. COMMON/INLOOP/L
 00110 10. DIMENSION DD(11)
 00111 11. DATA EPISLN/.0001/
 00113 12. SVSU=0
 00114 13. J=3
 00115 14. NEL=N
 00116 15. SUM=0
 00117 16. NI=NT-T(1)

SUBROUTINE BCALC

Q1 FOR BCALC
 COMPILE BY UNIVAC 1106 FORTRAN-IV DATED 11 NOV 1966 F#005
 THIS COMPILE WAS DONE ON 19 DEC 66 AT 21:06:12

SUBROUTINE BCALC ENTRY POINT 000157

STORAGE USED (BLOCK, NAME, LENGTH)

0001	*CODE	000225
0000	*DATA	000030
0002	*BLANK	001676
0003	SING	000005
0004	BI	023160
0005	INLOOP	000001

EXTERNAL REFERENCES (BLOCK, NAME)

0006 DIFFUS

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000116	11L	0001	000110	12L	0001	000043	131S	0001	000131	100J	0001	000027	20L				
0001	000153	30L	0001	000067	20L	0002	001134	AK	0002	001025	AY	0003	000003	2CV				
0002	R	000374	LFC	0006	R	000000	DIFFUS		0000	R	000000	EPISLN	0003	I	000001	10		
0000	I	000002	J	0000	I	000010	K		0005	I	000000	L	0003	I	000005	10		
0002	000360	NAME	0003	000003	1CS1	0003	000004	NC52	0000	I	000003	DEL	0003	I	000007	200		
0000	I	000011	NC5	0003	000002	1TOT	0000	I	000005	11	0002	R	001342	2	0003	R	000004	510
0000	M	000001	SVSU4	0002	M	001506	1		0002	001556	TEMP	0002	001436	2CL	0003	000365	200L	
0004	022600	BI	0002	R	001800	1T	0002	000000	YLN									

00101 1. SUBROUTINE BCALC(N,IT,I,KL,AG,9,DD,DT)
 00101 2. C SUBROUTINE TO CALCULATE SOLUTIONS TO THE DIFFUSION EQUATION.
 00101 3. C FIRST SECTION COMPUTES THE PROPER DT VALUE.

00103 4. DIMENSION I(6)
 00104 5. COMMON YLD(5,40),IA,E(6),AQL(6),DEC(6,40),HEI(6,40),AK(a),X(30),Y
 00105 6. /T(30),VOL(40),T(40),TEMP(40),ATHT(40)
 00106 7. COMMON/SING/LC,IR,1TOT,NC51,NC52
 00107 8. COMMON/BI/DTY(6,40,20),BI(6,40)
 00107 9. COMMON/INLOOP/L
 00110 10. DIMENSION DUT(1)
 00111 11. DATA EPISLN/.0001/
 00113 12. SVSU=0
 00114 13. J=3
 00115 14. NEL=0
 00116 15. SUM=0
 00117 16. NIE=0-1(1)

```

00120 17. M1=M1*(2)+1
00121 18. IF(KLAG)50,50,20
00124 19. 50 M1=M1+1
00125 20. IF(M1-GT-M1)GO TO 60
00127 21. 20 NEP=NEL+L-1
00130 22. DO 10 K=M1,M1
00133 23. SUM=SUM+DFC(NEP,K)*I(K)
00134 24. IF(ABS(SVSUM-SUM).LT.ABS(EPSLM*SVSUM)) GO TO 11
00136 25. S/SUM=SUM
00137 26. 10 CONTINUE
00141 27. 60 NEL=NEL-1
00142 28. IF(NEL-1)11,12,13
00145 29. 13 M1=M1+1
00146 30. M1=M1*(J)+1
00147 31. J=J+1
00150 32. GO TO 20
00151 33. 12 M1=M1+1
00152 34. M1=M1
00153 35. GO TO 20
00154 36. 11 DT=SUM
00155 37. SUM=0
00156 38. NG=N1-I(1)+1
00157 39. DO 30 K=1,IR
00162 40. DJ(K)=1.0
00163 41. *DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTegers MAY NOT BE MEANINGFUL.
00163 41. IF(DT-GE-(1.0+9(K)*2))GO TO 30
00165 42. DJ(K)=DIFFUS(DT,R(K))
00166 43. 30 SUM=SUM+DJ(K)*DT(K)
00170 44. B=SUM
00171 45. RETURN
00172 46. END

```

END OF LISTING. 1 *DIAGNOSTIC* MESSAGE(S).

SUBROUTINE DELTA

01 FOR DELTA
 COMPILATION BY UNIVAC 1100 FORTRAN-IV DATED 11 NOV 1966 F0009
 THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:15

SUBROUTINE DELTA ENTRY POINT 000172

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 000221
 0000 *DATA 000043
 0002 *BLANK 000000
 0003 B1 023160
 0004 I-LOOP 000001

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000111 IOL 0001 000021 I106 0001 000052 I2L 0001 000084 I203 0001 000127 I206
 0001 000156 I536 0001 000152 I7L 0003 R 000000 DCY 0000 R 000000 DELT 0000 R 000016 PLT
 0000 I 000011 ISUM 0000 I 000007 J 0000 I 000012 K 0004 I 000000 L 0000 I 000010 M
 0000 I 000013 N02 0000 I 000014 N03 0000 I 000015 N04 0000 I 000006 NE 0003 000000 NY

00101 1. SUBROUTINE DELTA(NIT, IOPR)
 00103 2. DIMENSION I(6), DELT(6)
 00104 3. COMMON/317DCY(6*0,0), ZN(6*0)
 00105 4. COMMON/I-LOOP/L
 00106 5. NEER=1
 00107 6. DO 10 J=1, NE
 00112 7. N01=N-J&L
 00113 8. ISUM=I-I(1)
 00114 9. IF(J-I) 11, 12, 11
 00117 10. 11 DO 14 K=2, J
 00122 11. 14 ISUM=ISUM+I(K)
 00124 12. ISUM=ISUM+2*J-2
 00125 13. 12 N02=ISUM
 00126 14. N03=ISUM+I(J+1)
 00127 15. N04=N03*1
 00130 16. DELT=1.
 00131 17. IF((N03*LE.0).OR.(N02*LE.0) 1760 TO 10
 00133 18. DELT=DCY(N01, N02, N03)
 00134 19. 10 DELT(J)=DELTA(1-DCY(N01, N02, N03))
 00136 20. ISUM=I-I(1)
 00137 21. DO 15 K=2, N
 00142 22. 15 ISUM=ISUM+I(K)
 00144 23. ISUM=ISUM+2*NE
 00145 24. DELT(N)=1.
 00146 25. IF((ISUM*LE.0) 1760 TO 17
 00150 26. DELT(N)=DCY(L, ISUM, NIT-1)
 00151 27. 17 PRE1.

SUBROUTINE DELTA

00152 28. 00 10 K10N
00155 29. 10 PREP*DELTA
00157 30. RETURN
00160 31. END

END OF LISTING. 0 *DIAGNOSTIC* MESSAGE(S).

FUNCTION DIFFUS

01 FOR DIFFUS
 COMPILE BY UNIVAC 1108 FORTRAN-IV DATED 11 NOV 1966 F#009
 THIS COMPILE HAS DONE ON 19 DEC 66 AT 21:06:18

FUNCTION DIFFUS ENTRY POINT 000000

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 000066
 0000 *DATA 000021
 0002 *BLANK 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 SORT
 0004 EXP

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000021 10L 0001 000020 12L 0000 R 000001 CONST 0000 R 000002 C1 0000 R 000003 C2
 0000 R 000000 DIFFUS 0000 R 000000 EXP 0000 R 000000 SORT 0000 R 000000 Y

00101 1. FUNCTION DIFFUS(OT,R)
 00103 2. DATA CONST,C1,C2/1.128379,.60792710,-9.4596044/
 00107 3. X=R/SORT(OT)
 00110 4. IF(X-3.1415926)10,20
 00113 5. 20 DIFFUS=3.*(CONST-1./4)/X
 00116 6. 12 RETURN
 00119 7. 10 Y=X**2
 00122 8. DIFFUS=1.-C1*EXP(C2/Y)
 00125 9. IF(X-2.)12,12.15
 00128 10. 15 DIFFUS=DIFFUS-C1*EXP(C2/Y)/Y.
 00131 11. RETURN
 00134 12. END

END OF LISTING. 0 *DIAGNOSTIC MESSAGE(S).

COMPILATION BY UNIVAC 1108 FORTRAN-IV DATED 11 NOV 1966 FAUNA
THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:20

FUNCTION PROFIL **ENTRY POINT 000342**

 STORAGE USED (BLOCK, NAME, LENGTH) |

05C000 JC93 1000

0000	*DATA	000043
0000	0000	0000

0002 JUL 0000

EXTERNAL REFERENCES (BLOCK, NAME)

WISCONSIN

EXP 0004

1475 5000

0006 ERF

0007 NEXPLS

 STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME) |[illegible]

00101 I. FUNCTION PROFILE(L,Y,Z)

[illegible]

FUNCTION PROFIL

00122	16.	N=1	PROF0130
00123	17.	SUM=0.	PROF0130
00124	18.	20 PSUM=SUM	PROF0130
00125	19.	SUM=SUM+((-1)*PI*27A)*EXP((-2)*PI*27A*PI*50/(A**2)))/PI	PROF0130
00126	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00127	20.	IF (ABS(SUM-PSUM).LE.(1.E-2)*ABS(SUM)) GO TO 21	
00128	21.	N=N+1	PROF0130
00129	22.	IF (N-100)20*20*21	PROF0130
00130	23.	21 PROFIL=1.+(2.*PI*27A)*SUM	PROF0130
00131	24.	RETURN	PROF0130
00132	25.	40 N=1	PROF0130
00133	26.	SUM=0.	PROF0130
00134	27.	41 PSUM=SUM	PROF0130
00135	28.	SUM=SUM+((-1)*PI*27A)*EXP((-2)*PI*27A*PI*50/(A**2))	PROF0130
00136	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00137	29.	IF (ABS(SUM-PSUM).LE.(1.E-2)*ABS(SUM)) GO TO 30	
00138	30.	N=N+1	PROF0130
00139	31.	IF (N-100)41*41*42	PROF0130
00140	32.	42 PROFIL=1.+(2.*PI*27A)*SUM	PROF0130
00141	33.	RETURN	PROF0130
00142	34.	C	PROF0130
00143	35.	C	PROF0130
00144	36.	C	PROF0130
00145	37.	30 CIE1/12.*SUM*PI*PI	PROF0130
00146	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00147	38.	IF ((A-RT)*C1.CE.3.5)*50 TO 60	PROF0130
00148	39.	SUM=0.	PROF0130
00149	40.	N=0	PROF0130
00150	41.	31 PSUM=SUM	PROF0130
00151	42.	SUM=SUM+((-1)*PI*27A)*EXP((-2)*PI*27A*PI*50/(A**2))	PROF0130
00152	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00153	43.	IF (ABS(SUM-PSUM).LE.(1.E-2)*ABS(SUM)) GO TO 32	PROF0130
00154	44.	N=N+1	PROF0130
00155	45.	IF (N-100)31*31*32	PROF0130
00156	46.	40 SUM=0.	PROF0130
00157	47.	32 PROFIL=1.+(2.*PI*27A)*SUM	PROF0130
00158	48.	RETURN	PROF0130
00159	49.	E.O	PROF0130

END OF LISTING. 6 *DIAGNOSTIC* MESSAGE(S).

FUNCTION ERF

01 FOR ERF
 COMPILE BY UNIVAC 1105 FORTRAN-IV DATED 11 NOV 1956 F4008
 THIS COMPILATION WAS DONE JUN 19 DEC 66 AT 21:06:23

FUNCTION ERF ENTRY POINT 000050

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 300034
 0000 *DATA 000013
 0002 *BLANK 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 EXP

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000 R 000000 ERF 0003 R 000030 EXP 0000 R 000001 Y

00101 1. FUNCTION ERF(X)

00101	1.	FUNCTION ERF(X)	ERF	0010
00101	2.	C		0020
00101	3.	C	COMPUTES ERROR FUNCTION WITH AN ERROR OF LESS THAN 2.5E-5.	0030
00101	4.	C	SEE HANDBOOK OF MATH. FUNCTIONS WITH FORMULAS, GRAPHS AND TABLES.	0040
00101	5.	C	TABLES, MARCH 1955. NBS APPLIED MATHEMATICS SERIES 55, PAGE 294	0050
00101	6.	C	PARAGRAPH 7.1.25.	0060
00101	7.	C		0070
00103	8.	Y=1.711+.47067EX		0080
00104	9.	ERF=1.-T*(.3480242+T*(.09513798+T*(.7478556)))*EXP(-X**2)		0090
00105	10.	RETURN		0100
00106	11.	END		0110

END OF LISTING. 0 *DIAGNOSTIC MESSAGE(S).

FUNCTION: WANGIM

FIGURE 10

ASSEMBLED BY UNIVAC IIIB ASSEMBLER VERSION 9 LEVEL 01/4

ASSEMBLED BY UNIVAC IIIB ASSEMBLER VERSION 9 LEVEL 01/4

THIS ASSEMBLY WAS DONE ON 19 DEC 66 AT 21:05:26

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DATE	DESCRIPTION	AMOUNT	BALANCE
1900	TO BALANCE	100000	100000
1901	BY SALES	100000	200000
1902	TO PURCHASES	100000	100000
1903	BY SALES	100000	200000
1904	TO PURCHASES	100000	100000
1905	BY SALES	100000	200000
1906	TO PURCHASES	100000	100000
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1976	TO PURCHASES	100000	100000
1977	BY SALES	100000	200000
1978	TO PURCHASES	100000	100000
1979	BY SALES	100000	200000

DATE	DESCRIPTION	AMOUNT	CHECK NO.	BANK	INITIALS
10/1/78	DEPOSIT	100.00		CHASE	
10/2/78	PAYROLL	50.00	101	CHASE	
10/3/78	RENT	25.00	102	CHASE	
10/4/78	UTILITIES	15.00	103	CHASE	
10/5/78	SALES	75.00	104	CHASE	
10/6/78	DEPOSIT	120.00		CHASE	
10/7/78	PAYROLL	55.00	105	CHASE	
10/8/78	RENT	25.00	106	CHASE	
10/9/78	UTILITIES	15.00	107	CHASE	
10/10/78	SALES	80.00	108	CHASE	
10/11/78	DEPOSIT	110.00		CHASE	
10/12/78	PAYROLL	52.00	109	CHASE	
10/13/78	RENT	25.00	110	CHASE	
10/14/78	UTILITIES	15.00	111	CHASE	
10/15/78	SALES	78.00	112	CHASE	
10/16/78	DEPOSIT	115.00		CHASE	
10/17/78	PAYROLL	53.00	113	CHASE	
10/18/78	RENT	25.00	114	CHASE	
10/19/78	UTILITIES	15.00	115	CHASE	
10/20/78	SALES	79.00	116	CHASE	
10/21/78	DEPOSIT	118.00		CHASE	
10/22/78	PAYROLL	54.00	117	CHASE	
10/23/78	RENT	25.00	118	CHASE	
10/24/78	UTILITIES	15.00	119	CHASE	
10/25/78	SALES	81.00	120	CHASE	
10/26/78	DEPOSIT	122.00		CHASE	
10/27/78	PAYROLL	56.00	121	CHASE	
10/28/78	RENT	25.00	122	CHASE	
10/29/78	UTILITIES	15.00	123	CHASE	
10/30/78	SALES	82.00	124	CHASE	
10/31/78	DEPOSIT	125.00		CHASE	

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DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) General Atomic Division General Dynamics Corporation San Diego, California		2a. REPORT SECURITY CLASSIFICATION Unclassified	
		2b. GROUP	
3. REPORT TITLE A CALCULATIONAL MODEL FOR CONDENSED STATE DIFFUSION CONTROLLED FISSION PRODUCT ABSORPTION DURING FALLOUT FORMATION			
4. DESCRIPTIVE NOTES (Type of report and inclusive dates)			
5. AUTHOR(S) (Last name, first name, initial) Korts, Richard F. and Norman, John H.			
6. REPORT DATE January 10, 1967		7a. TOTAL NO. OF PAGES 91	7b. NO. OF REFS 5
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d.		9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	
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11. SUPPLEMENTARY NOTES		12. SPONSORING MILITARY ACTIVITY Office of the Civil Defense, Office of the Secretary of the Army, Washington, D.C. 20310	
13. ABSTRACT A program is presented to compute fallout fission product absorption in an expanding, cooling, uniform field of gas and fallout particles where the rate of fission product absorption is controlled by fission product surface concentrations as given by Henry's law constants and diffusion of these fission products into the fallout particles. The calculations are made a nuclide chain at a time, employing nuclear device and fission product parameters. Program output includes average concentration versus particle size for each absorbed fission product at a pre-selected lower temperature and the amount of that fission product in the gas phase, with an option for the calculation of fission product radial profiles versus particle size.			

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Surface concentration Concentration profiles Fallout formation Fission products Absorption Diffusion						

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