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DIGRTS - A Computer Code for Studying the Diffusion of an Inert Gas in Composite Solids with Reversible Trapping

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Pacific Northwest Laboratories

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THE DIFFUSION OF AN INERT GAS IN
COMPOSITE SOLIDS WITH REVERSIBLE
TRAPPING

by
C. A. Oster

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INTRODUCTION

DIGRTS is a computer program for calculating the concentration distribution of an inert gas diffusing through a composite solid which permits reversible trapping of the gas atoms. The program is coded entirely in FORTRAN IV. The composite solid can consist of up to ten regions. These regions are further subdivided in a manner so that the total number of nodes (subdivision points) is less than or equal to 200. The code can readily be modified should these limits be undesirable. The code permits only constant parameters for describing the diffusion process but the extension to allow time dependent parameters is clearly marked in the program.

In addition to calculations of the concentration distributions, the time dependent release fraction is also computed.

The program is listed in Appendix A and the input data cards for two cases are listed in Appendix B. Appendix C contains some of the results of processing the two cases of Appendix B.

FINITE DIFFERENCE EQUATION USED

The partial differential equations describing the diffusion process are replaced with finite difference equations, which are then solved numerically. The finite difference equations are developed below.

Divide the range of X into J regions. Let X_{rj} denote the right hand end point of region j , and take $X_{r0} = 0$. Thus we have

$$0 = X_{r0} < X_{r1} < \dots < X_{rj}$$

In the development below j takes on integer values from 0 to J inclusive.

The differential equations are

$$\frac{\partial C}{\partial t} = D_j \frac{\partial^2 C}{\partial X^2} - \frac{\partial m}{\partial t} - \frac{\partial M}{\partial t} \quad (1)$$

$$\frac{\partial m}{\partial t} = k_j C - k'_j m \quad (2)$$

$$\frac{\partial M}{\partial t} = K_j C \quad (3)$$

with boundary conditions given by

$$C(X,0) = C^0(X) \quad (4)$$

$$m(X,0) = m^0(X) \quad (5)$$

$$M(X,0) = M^0(X). \quad (6)$$

$C^0(X)$, $m^0(X)$ and $M^0(X)$ are specified functions of X only, and

$$C(0,t) = 0 \quad (7)$$

$$C(X_{rj}, t) = 0 \quad (8)$$

for $t > 0$. In addition the following continuity conditions hold for $t > 0$ at each region boundary:

$$\lim_{X \rightarrow X_{rj-}} C(X,t) = \lim_{X \rightarrow X_{rj+}} C(X,t) \quad (9)$$

$$\lim_{X \rightarrow X_{rj-}} D_j \left(\frac{\partial C}{\partial X} \right) = \lim_{X \rightarrow X_{rj+}} D_{j+1} \left(\frac{\partial C}{\partial X} \right) \quad (10)$$

where $X \rightarrow X_{rj-}$ indicates X approaches X_{rj} from the left and $X \rightarrow X_{rj+}$ indicates the approach is from the right.

Each region j is further divided into subintervals which will be noted by the subscript i . Define the space increment ΔX_i to be the length of the i^{th} subinterval.

$$\Delta X_i = X_i - X_{i-1}$$

where

$$0 \leq X_{i-1} < X_i \leq X_{rj}.$$

We assume that $X_{r_j} = X_i$ for some i and for all j . That is the boundaries X_{r_j} are also points in the mesh used in the numerical process. We approximate the second derivatives by a second order central difference quotient

$$\frac{\partial^2 C}{\partial X^2} \approx \left(\frac{2}{\Delta X_i + \Delta X_{i+1}} \right) \left[\frac{1}{\Delta X_i} C_{i-1} - \left(\frac{1}{\Delta X_i} + \frac{1}{\Delta X_{i+1}} \right) C_i + \frac{1}{\Delta X_{i+1}} C_{i+1} \right].$$

The first derivatives in time are replaced with a first order difference quotient. Let the superscript k denote the time step and write the Crank-Nicolson approximation [1] to Equation (1) as

$$\begin{aligned} \frac{C_i^{(k+1)} - C_i^{(k)}}{\Delta t} = & \frac{D_j}{2} \left(\frac{2}{\Delta X_i + \Delta X_{i+1}} \right) \left\{ \left[\frac{1}{\Delta X_i} C_{i-1}^{(k+1)} - \left(\frac{1}{\Delta X_i} + \frac{1}{\Delta X_{i+1}} \right) C_i^{(k+1)} \right. \right. \\ & \left. \left. + \frac{1}{\Delta X_{i+1}} C_{i+1}^{(k+1)} \right] + \left[\frac{1}{\Delta X_i} C_{i-1}^{(k)} - \left(\frac{1}{\Delta X_i} + \frac{1}{\Delta X_{i+1}} \right) C_i^{(k)} + \frac{1}{\Delta X_{i+1}} C_{i+1}^{(k)} \right] \right\} \\ & - \frac{k_j}{2} [C_i^{(k)} + C_i^{(k+1)}] + \frac{k'_j}{2} [m_i^{(k)} + m_i^{(k+1)}] - \frac{K_j}{2} [C_i^{(k)} + C_i^{(k+1)}]. \end{aligned} \quad (11)$$

where i is such that $X_{r_{j-1}} < X_i < X_{r_j}$ for $j = 1, 2, \dots, J$.

Similarly Equation (2) becomes

$$\frac{m_i^{(k+1)} - m_i^{(k)}}{\Delta t} = \frac{k_j}{2} (C_i^{(k+1)} + C_i^{(k)}) - \frac{k'_j}{2} (m_i^{(k+1)} + m_i^{(k)}).$$

Solving for $m_i^{(k+1)}$ from this equation we obtain

$$m_i^{(k+1)} = \left[\frac{1 - k'_j \left(\frac{\Delta t}{2} \right)}{1 + k'_j \left(\frac{\Delta t}{2} \right)} \right] m_i^{(k)} + \left[\frac{k_j \left(\frac{\Delta t}{2} \right)}{1 + k'_j \left(\frac{\Delta t}{2} \right)} \right] [C_i^{(k+1)} + C_i^{(k)}]. \quad (12)$$

Substituting Equation (12) into Equation (11) yields, after collecting terms and rearranging

$$\begin{aligned}
& \frac{D_j \Delta t}{(\Delta X_i + \Delta X_{i+1}) \Delta X_i} c_{i-1}^{(k+1)} - \left[1 + \frac{D_j \Delta t}{\Delta X_i \Delta X_{i+1}} + \frac{k_j \left(\frac{\Delta t}{2}\right)}{1 + k'_j \left(\frac{\Delta t}{2}\right)} + K_j \left(\frac{\Delta t}{2}\right) \right] c_i^{(k+1)} \\
& + \frac{D_j \Delta t}{(\Delta X_i + \Delta X_{i+1}) \Delta X_{i+1}} c_{i+1}^{(k+1)} \\
& = - \frac{D_j \Delta t}{(\Delta X_i + \Delta X_{i+1}) \Delta X_i} c_{i-1}^{(k)} - \left[1 - \frac{D_j \Delta t}{\Delta X_i \Delta X_{i+1}} - \frac{k_j \left(\frac{\Delta t}{2}\right)}{1 + k'_j \left(\frac{\Delta t}{2}\right)} - K_j \left(\frac{\Delta t}{2}\right) \right] c_j^{(k)} \\
& - \frac{D_j \Delta t}{(\Delta X_i + \Delta X_{i+1}) \Delta X_{i+1}} c_{i+1}^{(k)} - \frac{k'_j \Delta t}{1 + k'_j \left(\frac{\Delta t}{2}\right)} m_i^{(k)} \quad (13)
\end{aligned}$$

Notice that if $c_{i-1}^{(k)}$, $c_i^{(k)}$, $c_{i+1}^{(k)}$ are known then the right hand side of Equation (13) is known.

Equation (13) is defined at all mesh points X_i except when X_i is a boundary point i.e., $X_i \neq 0, X_{r1}, X_{r2}, \dots, X_{rj}$. At all internal mesh points we utilize Equations (9) and (10). The derivatives in Equation (10) are replaced with difference quotients and Equation (9) used to obtain

$$\frac{D_j}{\Delta X_i} c_{i-1}^{(k+1)} - \left(\frac{n_j}{\Delta X_i} + \frac{n_{j+1}}{\Delta X_{i+1}} \right) c_i^{(k+1)} + \frac{D_{j+1}}{\Delta X_{i+1}} c_{i+1}^{(k+1)} = 0 \quad (14)$$

where i and j are such that $X_i = X_{rj}$.

Equations (12) and (13) can be simplified somewhat by making the following substitutions:

$$\alpha_i = \frac{D_j \Delta t}{(\Delta x_i + \Delta x_{i+1}) \Delta x_i}$$

$$\beta_i = \frac{D_j \Delta t}{(\Delta x_i + \Delta x_{i+1}) \Delta x_{i+1}}$$

$$\gamma_j = \frac{k_j \left(\frac{\Delta t}{2}\right)}{1 + k'_j \left(\frac{\Delta t}{2}\right)}$$

$$\delta_i = 1 + (\alpha_i + \beta_i) + \gamma_j + K_j \left(\frac{\Delta t}{2}\right)$$

$$\epsilon_i = 1 - (\alpha_i + \beta_i) - \gamma_j - K_j \left(\frac{\Delta t}{2}\right)$$

$$\zeta_j = \frac{1 - k'_j \left(\frac{\Delta t}{2}\right)}{1 + k'_j \left(\frac{\Delta t}{2}\right)}$$

$$\eta_j = k'_j \left(\frac{\Delta t}{2}\right) (\zeta_j - 1)$$

Then Equation (13) becomes

$$\begin{aligned} \alpha_i C_{i-1}^{(k+1)} - \delta_i C_i^{(k+1)} + \beta_i C_{i+1}^{(k+1)} \\ = -\alpha_i C_{i-1}^{(k)} - \epsilon_i C_i^{(k)} - \beta_i C_{i+1}^{(k)} - \eta_j m_i^{(k)} \end{aligned} \quad (15)$$

and Equation (12) becomes

$$m_i^{(k+1)} = \zeta_j m_i^{(k)} + \gamma_j [C_i^{(k+1)} + C_i^{(k)}]. \quad (16)$$

The procedure used to solve Equation (1) and (2) are as follows:

$$C_0 = 0 \text{ from Equation (7)}$$

$$C_i \text{ from Equation (15) if } X_i \text{ is not a boundary point}$$

$$C_i \text{ from Equation (14) if } X_i \text{ is a boundary point}$$

$$C_i = 0 \text{ if } X_i = X_{r_j} \text{ by Equation (8).}$$

Equations (14) and (15) couple C_i to its neighbors C_{i-1} and C_{i+1} . Hence we can write down in sequence a set of simultaneous linear equations for $C_i^{(k+1)}$ having a tridiagonal coefficient matrix. Once $C_i^{(k+1)}$ has been obtained $m_i^{(k+1)}$ is obtained from Equation (16). Finally Equation (3) is solved by applying the trapezoidal rule to the right hand side which becomes

$$M_i^{(k+1)} = M_i^{(k)} + K_j \left(\frac{\Delta t}{2} \right) \left[C_i^{(k+1)} + C_i^{(k)} \right]. \quad (17)$$

The release fraction $f(t)$ is obtained by first calculating

$$F(t) = \int_0^{X_{r_j}} [C(X,t) + m(X,t) + M(X,t)] dX \quad (18)$$

then

$$f(t) = 1 - \frac{F(t)}{F(0)}. \quad (19)$$

The integral (18) is approximated by a method described in [2]. Since both $m(X,t)$ and $M(X,t)$ are discontinuous at each interval boundary X_{r_j} the integral is broken into J integrals. The integration algorithm produces an error estimate for each of the J intervals giving some indication of the quality of $f(t)$.

INPUT

Input for DIGRTS is from cards only or from cards and data files. The input is described as individual data packets for various groups of data. These groups are:

- I. Case Identification
- II. Region Description--for each region j
 - A. Time Constants
 - B. Spatial Description
 1. Nongeometric spacing
 2. Geometric spacing
- III. Time Description and Program Control
- IV. Initial Concentrations

All data fields have the FORTRAN format description E10.0. The data deck for a given problem is set up in the order shown in the above data group descriptions. Multiple problems can be processed during a single computer run by simply stacking the individual problem data sets one after the other. The individual data packet may now be described.

The first card of each case is the identification card. This card may contain any alphanumeric character string. There are two restrictions imposed on this card. If columns 1-72 are blank the run is terminated. If the initial concentrations are from an external data file then columns 1-15 must agree with the first 15 characters of the identification of the initial concentrations. (This identification is the case identification of the run which prepared the data file.)

The first card of the j^{th} region contains the time constant data for that region. See Equations (1), (2) and (3). The card has the following format.

Card Columns	Contents
1-10	D_j
11-20	k_j
21-30	k_j'
31-40	K_j

The remainder of the Region Description data packet for region j consists of the spatial subintervals specification. Two options exist here. One permits arbitrary spacing of the subintervals. This spacing is referred to as the nongeometric spacing. The second option permits the description of contiguous subintervals whose lengths vary as a geometric progression. This spacing is referred to as geometric spacing. Both options may be used for any given region.

The nongeometric spacing is achieved by simply listing in increasing order the right hand end points of the intervals. Each end point occupies ten columns on a card permitting up to seven values per card. The sequence of contiguous subintervals is terminated when a blank field is encountered or an endpoint value is less than or equal to its predecessor. (All endpoint values must be positive. Zero is the left endpoint of the first subinterval of region 1.)

The geometric spacing option is introduced by a card containing a -1 in columns 1-10. The ratio of the lengths of two successive subintervals $\Delta X_{i+1}/\Delta X_i$ (in general this value should be greater than or equal to unity) in columns 11-20. Finally columns 21-30 contain the right hand endpoint of the final subinterval described by this card. Some caution must be exercised in using this option as the total number of subintervals must be less than 202. An estimate of the number of subintervals produced by an individual geometric spacing card is given in the next section.

The Region Description part of the data deck is terminated by the Time Description and Program Control card. This card is blank or contains 0 in columns 1-10. This card describes the maximum simulation time (real time), printout frequency, time step options, keys to the initial concentrations and disposition of the final concentrations. This card is described on the following page.

Card Columns	Contents	Description
1-10	Blank on 0	Delimits the Region Description Packets.
11-20	Δt	Maximum time increment used in the computations.
21-30	$t_{\max}$	Maximum value for time t
31-40	Δt_p	Time between print outs
41-50	t_E	Extrapolation time limit. Extrapolation is used to obtain the solution so long as $t \leq t_E$ or until 10 successive time steps are made using a maximum increment of $\Delta t/2$. By taking $t_E = 0$ extrapolation can be suppressed.
51-60	RESTR	If RESTR > 0 the initial concentrations are stored on an unformatted auxiliary file (LUSTRT). Otherwise the initial concentrations are described on cards.
61-70	SAVE	If SAVE > 0 the final set of concentrations are written to an unformatted auxiliary file (LUSAVE) which can be saved and used as initial values on subsequent runs.

The initial concentration distributions $C^0(x)$, $m^0(x)$ and $M^0(x)$ are specified by interpolation on a set of N ($N \leq 202$) values X_n , C_n , m_n , M_n , $n = 1, 2, \dots, N$ where $C_n = C^0(X_n)$, $m_n = m^0(X_n)$, and $M_n = M^0(X_n)$. Now $N-1$ intervals are spanned by these points. The degree d_{Cn} , d_{mn} and d_{Mn} of the polynomial interpolation formula to be used for the n th interval can be specified along with the C_n , m_n , and M_n . Thus the interpolation polynomial of degree d_{Cn} is used to determine $C(x)$ for $X_n \leq x < X_{n+1}$.

In the discussion below let d_n denote d_{Cn} , d_{mn} or d_{Mn} . The definition of an interpolation polynomial of degree d_n requires $d_n + 1$ points (hence $d_n < N$). These points are selected near the n th interval according to the following policy. Suppose the interval of interest is not near the ends, i.e., there are several points either side of X_n . Then the set of interpolating points are given by

d_n	<u>Interpolation Points</u>
0	X_n
1	X_n, X_{n+1}
2	X_{n-1}, X_n, X_{n+1}
3	$X_{n-1}, X_n, X_{n+1}, X_{n+2}$
4	$X_{n-2}, X_{n-1}, X_n, X_{n+1}, X_{n+2}$
5	$X_{n-2}, X_{n-1}, X_n, X_{n+1}, X_{n+2}, X_{n+3}$
$\vdots$	$\vdots$

Let $\left\lfloor \frac{d_n}{2} \right\rfloor$ = largest integer less than or equal to $\frac{d_n}{2}$. If n and d_n are such that $n - \left\lfloor \frac{d_n}{2} \right\rfloor \leq 1$ or $n + \left\lfloor \frac{d_n + 1}{2} \right\rfloor \geq N$ then the set of interpolation points consists of the first or last $d_n + 1$ points respectively.

Generally d_n should be small. This may require a large number of points in those regions where a distribution is changing rapidly. In addition if d_n is odd there are the same number of interpolation points on each side of the n^{th} interval.

Since polynomials are continuous functions the resulting initial distribution is a continuous function of $d_n > 0$.

The current version of the program assumes $C(x)$ is defined as above except when $t = 0$ where $C(x)$ may be discontinuous at $X = X_{r1}$. In this case the limit of $C(x)$ as x approaches x_{r1} from below is $C(x_{r1})$ as defined above but as x approaches x_{r1} from above the value is taken as 0.

The initial concentration distribution cards are described by:

<u>Card Columns</u>	<u>Contents</u>	<u>Description</u>
1-10	x_n	Left end of the n^{th} interpolation interval
11-20	C_n	$C^0(X_n)$
21-30	d_{Cn}	Degree of the C- interpolation polynomial over the n^{th} interpolation interval

(contd)

<u>Card Columns</u>	<u>Contents</u>	<u>Description</u>
31-40	m_n	$m^o(X_n)$
41-50	d_{mn}	Degree of the m- interpolation polynomial over the nth interpolation interval
51-60	M_n	$M^o(X_n)$
61-70	d_{Mn}	Degree of the M- interpolation polynomial over the nth interpolation interval.

This data packet is terminated when columns 1-10 contain a negative number. The total number of cards in this packet including the terminal card, must be less than or equal to 203.

The entire data deck is terminated by a card that is blank in columns 1-72.

SELECTION OF ΔX AND Δt

The Crank-Nicolson algorithm remains stable for all values of ΔX and Δt . Unfortunately the results may not be very accurate. It is desirable to choose these parameters so as to obtain reasonable accuracy at reasonable cost. If Δt and/or ΔX are too small excessive computer time will be required. The following method for selecting ΔX and Δt has been found to give satisfactory results.

First select a reasonable ΔX for the smallest region, say region j
Now choose the smallest ΔX , say $\overline{\Delta X}$ for adjacent regions so that

$$\frac{D_j}{\Delta X_j} \sim \frac{D_{j+1}}{\overline{\Delta X}_{j+1}}$$

while keeping the ΔX 's approximately uniform at regional boundaries. Intermediate ΔX 's need not be uniform but neither should the size of adjacent ΔX 's change greatly.

The choice of Δt is based on the largest value $D/\Delta X^2$ in the spacial grid. Suppose this ΔX is located in region j and denote it by ΔX_j , then choose Δt so that

$$\frac{D_j \left(\frac{\Delta t}{2} \right)}{(\Delta X_j)^2} \sim 1.$$

The total number of points in a problem must not exceed 200. Thus the user of the geometric spacing input option must be able to estimate the number of points generated. The following equation provides such an estimate.

$$n \sim \frac{\log \left[1 + \rho \left(\frac{x_{rj} - x_{rj-1}}{\Delta X_0} \right) \right]}{\log[1 + \rho]}$$

where

x_{rj} is the right hand end and

x_{rj-1} is the left hand end of the interval to be partitioned into n subintervals.

ΔX_0 is the first subinterval and

$(1 + \rho)$ is the ratio of two adjacent subintervals i.e.,

$$1 + \rho = \frac{\Delta X_i}{\Delta X_{i-1}}.$$

Since n must be an integer the value of ρ is recalculated so that n subintervals do exactly span the j^{th} interval. Given n the new value of ρ is obtained by iteration on the function

$$\rho = [1 + \rho A]^{\frac{1}{n}} - 1$$

where

$$A = \frac{x_{rj} - x_{rj-1}}{\Delta X_0}.$$

Convergence is assured so long as

$$\frac{1}{n}(1 + \rho A)^{-\frac{n-1}{n}} A < 1$$

or

$$n > A(1 + \rho A)^{-\frac{n-1}{n}}$$

RESTRICTIONS

The program has fixed dimensioned arrays. These dimensions are large enough to accomodate most problems. Should the case arise where this is not so, the dimensions can be readily altered. The current version of DIGRTS is restricted by the values given in Table 1.

TABLE 1. Problem Limitations due to Program Dimensions

	<u>Maximum Number Permitted</u>
Number of regions, J	10
Number of points including endpoints X_{r0} and X_{rJ}	202
Number of points in Initial Concentration Tables, N	202
Number of values of $f(\cdot)$ plotted	500

EXTRAPOLATION TO THE LIMIT

Economics generally prevents the use of a single value for Δt throughout the entire solution. By choosing a value of Δt for use when t is large, i.e., after the diffusion processes have slowed down, and using extrapolation to the limit techniques it is possible to obtain good solutions which are based on small time steps when the concentrations are changing rapidly and large time steps when the concentrations are changing slowly. These techniques are described by Acton [3, p. 135] and others. The general algorithm used in DIGRTS may now be described.

In this discussion let y denote the solution of any of the differential equations (1), (2) or (3). A solution is obtained for t between t_0 and t_1 using the step Δt first using a one-step procedure to get $y_{1,1}$ (an estimate of y at t_1 using 1 step). Then halving the time step a second estimate $y_{1,2}$ is obtained using $\Delta t/2$ and making 2 steps. Similarly a third estimate $y_{1,3}$ is produced using $\Delta t/4$ and making 4 steps. Using $y_{1,1}$ and $y_{1,2}$ an improved value $y_{2,2} = 2y_{1,2} - y_{1,1}$ is calculated. Similarly, $y_{2,3} = 2y_{1,3} - y_{1,2}$. Now with $y_{2,2}$ and $y_{2,3}$ an improvement of the improved values is obtained from $y_{3,3} = (4y_{2,3} - y_{2,2})/3$.

The value of y can be tested for acceptance at each level, i.e., if $y_{1,2}$ and $y_{1,1}$ compare favorably $y_{1,2}$ is accepted and the above procedure repeated for the time interval t_1 to t_2 . If $y_{1,2}$ and $y_{1,1}$ do not favorably compare then $y_{2,2}$ is calculated and compared with $y_{1,2}$. Again favorable comparison results in $y_{2,2}$ being accepted as the solution at $t = t_1$, and the next time step is made. If $y_{1,2}$ and $y_{2,2}$ do not favorably compare then $y_{1,3}$, $y_{2,3}$ and $y_{3,3}$ are computed. Favorable comparison of $y_{2,3}$ and $y_{3,3}$ results in $y_{3,3}$ being adopted and the next time step is made. Otherwise the procedure computes for $n = 3$, $y_{1,n+1}$ using 2^n steps of size $2^{-n}\Delta t$. Then $y_{2,n+1} = 2y_{1,n+1} - y_{1,n}$, $y_{3,n+1} = (4y_{2,n+1} - y_{1,n+1})/3$. The values of $y_{3,n+1}$ are compared with $y_{3,n}$ and either accepted and t advanced for the next time step or rejected. If rejection is the case then n is incremented and the procedure repeated.

It is possible to produce a time step which is so small that it is economically not feasible to continue. To prevent this from occurring DIGRTS stops extrapolating when $n = 10$, accepts the last value obtained, writes a message to this effect and continues to the next time increment.

The measure of acceptability used in DIGRTS is to compare values of the release fraction $f(t)$ of Equation (19). Let f_n and f_{n+1} denote $f(t)$ based on two successive sets of values obtained by extrapolation. Acceptance is granted if $\left| \frac{f_n - f_{n+1}}{f_{n+1}} \right| < \frac{1}{2} \times 10^{-4}$, otherwise the time step is halved and the procedure repeated.

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APPENDIX A

PROGRAM LISTING

```

PROGRAM DIGRTS(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
1 LUSTRT,LUSAVE,TAPE1=LUSTRT,TAPE2=LUSAVE)
C
C---- DIGRTS - D(IFFUSION OF) I(NERT) G(AS WITH) R(EVERSIBLE)
C          T(RAPPING IN COMPOSITE) S(SOLIDS)
C
LOGICAL ERINPT,ERR,NOEXTR,ERINIT
C
COMMON          ABCD(202,4),XX(202),C(202),SMALLM(202),BIGM(202),
1 DX(201),ALPHA(200),BETA(200)
COMMON /ARRAYS/ JMAX,NR(10),XR(10),D(10),B4LIF(10),TRPLIF(10),
1 CAPK(10),GAMMA(10),ETA(10),ZETA(10),SMXR(10),BMXR(10)
COMMON /EXTRAP/ NOPTS,
1 OLDC(202),OLDSM(202),OLDBM(202),OLDSMR(10),OLDBMR(10),
2 C00 (202),SM00 (202),BM00 (202),SMXR00(10),BMXR00(10),
3 C10 (202),SM10 (202),BM10 (202),SMXR10(10),BMXR10(10),
4 C20 (202),SM20 (202),BM20 (202),SMXR20(10),BMXR20(10),
5 C11 (202),SM11 (202),BM11 (202),SMXR11(10),BMXR11(10),
6 C21 (202),SM21 (202),BM21 (202),SMXR21(10),BMXR21(10)
COMMON /TITLE / TITLE(80)
COMMON / CZERO/ R
COMMON /OTHER / NDXSMF,SMALLF(501)
COMMON /COM / T
COMMON /LUIO / LUIN,LUOUT
C
INTEGER TITLE, TYTLE(80),BLANK
DIMENSION TTT(501)
EQUIVALENCE (TTT(1),ABCD(1,1)),(TYTLE(1),ABCD(1,4))
C
DATA MAXREG,MAXPTS,MAXPLT/10,202,501/
DATA BLANK/1H /
C
99 FORMAT(7E10.0)
98 FORMAT(7HOREGION I5,1P5E15.7,12H WAS DROPPED)
97 FORMAT(44HOTOO MANY POINTS, TOTAL EXCEEDS CAPACITY OF 15)
96 FORMAT(49H0INITIAL CONDITIONS PRODUCE NON-POSITIVE INTEGRAL)
95 FORMAT(33H0TIME HISTORY OF RELEASE FRACTION/)
94 FORMAT(80H0 J NR XR D K
1-PRIME CAP K /)
93 FORMAT(1X2I5,1P5E13.4)
92 FORMAT(1H0//29H COMPUTATIONAL TIME STEP...1PE13.4/
1 29H MAXIMUM TIME..... E13.4/
2 29H PRINT OUT TIME INTERVAL... E13.4/
3 29H EXTRAPOLATION TIME LIMIT.. E13.4/
4 29H RESTRT..... E13.4/
5 29H SAVE..... E13.4)
91 FORMAT(39H0NO INTERMEDIATE POINTS, CASE BYPASSED.)
90 FORMAT(60H0RECOMPUTED DELTA-X NOT FOUND WHEN GEOMETRIC SPACING IS
1USED)
89 FORMAT(33H EXTRAPOLATION INTERRUPTED AT T =1PE15.7,
111H, WHEN DT =E15.7)
88 FORMAT(53H0TOO MANY POINTS IN INITIAL DISTRIBUTION, CAPACITY ISI5)
87 FORMAT(87H0NO. OF POINTS IN INITIAL DISTRIBUTION ON RESTART FILE CO
1ONFLICTS WITH THOSE FROM CARDS./I5,27H POINTS ON RESTART FILE AND
2 I5,19H POINTS FROM CARDS,I5,28H REGIONS ON RESTART FILE AND
3 I5,20H REGIONS FROM CARDS.)
86 FORMAT(80A1)
85 FORMAT(1H180A1)
84 FORMAT(29H1CASE TITLE IS.....80A1,3H.../
1 29H AND RESTART DATA TITLE IS...80A1,3H.../
83 FORMAT(25H0RESTART DATA TITLE IS...80A1,3H...)

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      82 FORMAT(70H0THE ABOVE CONCENTRATION DISTRIBUTIONS HAVE BEEN SAVED F
      10R RESTARTING.)
C
C
C---- LOGICAL IN/OUTPUT UNITS
C
C   STARTING VALUES MAY BE READ FROM TAPE LUSTRT.
C   FINAL VALUES MAY BE WRITTEN TO TAPE LUSAVE.
C   CARD READER IS LUIN
C   PRINTER IS LUOUT
C
C   LUSTRT=1
C   LUSAVE=2
C   LUIN =5
C   LUOUT=6
C
C   MAXIJ=MAXPTS-2
C   EPSLN=1.E-7
100 NOPTS=1
C   ERINPT=.FALSE.
C   ERR   =.FALSE.
C   XRJM1=0.
C   OLDX=0.
C   DXJ=1.E-6
C   J=0
C   IJ=0
C
C*****
C*
C* * * INPUT * * *      INPUT INSTRUCTIONS FOR DIGRTS      * * * INPUT * *
C*
C*
C*--- INPUT - - - INDIVIDUAL PROBLEMS CAN BE STACKED BACK TO BACK
C*                EACH PROBLEM IS TREATED SEPARATELY AS A DATA PACKET
C*                ALL DATA CARDS HAVE THE FORTRAN FORMAT(7E10.0)
C*
C*TITLE CARD - ANY ALPHANUMERIC CHARACTER STRING FOR CASE DESCRIPTION.
C*                IF COLUMNS 1-72 ARE BLANK THE RUN IS TERMINATED.
C*                IF INITIAL CONCENTRATIONS ARE ON LUSTRT (RESTRT .GT. 0)
C*                THEN COLUMNS 1-15 MUST AGREE WITH THE TITLE OF THE DATA
C*                ON LUSTRT.
C*
C*REGION DESCRIPTIONS
C*   THERE CAN BE UP TO MAXREG (=10) REGIONS IN EACH PACKET (PROBLEM)
C*
C*--TIME CONSTANTS
C*--- CARD J.1 CONTAINS THE FOLLOWING DESCRIPTORS FOR REGION J
C*   COLUMNS 1-10  DJ      = DIFFUSION COEFFICIENT
C*   COLUMNS 11-20 B4LIFJ = 1/(MEAN LIFE OF ATOMS
C*                        BEFORE BEING TRAPPED)
C*   COLUMNS 21-30 TRPLIJ = 1/(MEAN LIFE OF TRAPPED
C*                        ATOMS)
C*   COLUMNS 31-40 CAPKJ  = TIME CONSTANT IN BIGM EQUATION
C*
C*--SUBREGION SPATIAL DESCRIPTION
C*
C*--- NON-GEOMETRIC SPACING INPUT OPTION
C*   CARDS J.2 ... CONTAIN THE RIGHT HAND ENDPOINTS OF THE
C*   SUBINTERVALS OF REGION J   XJ1,XJ2,...,XJN
C*   THE SEQUENCE OF XJ. IS TERMINATED WHEN XJK-XJK-1 .LE. 0.
C*   OR A BLANK CARD OR INPUT FOR GEOMETRIC SPACING

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DIG0610
DIG0620
DIG0630
DIG0640
DIG0650
DIG0660
DIG0670
DIG0680
DIG0690
DIG0700
DIG0710
DIG0720
DIG0730
DIG0740
DIG0750
DIG0760
DIG0770
DIG0780
DIG0790
DIG0800
DIG0810
DIG0820
DIG0830
DIG0840
DIG0850
DIG0860
DIG0870
DIG0880
DIG0890
DIG0900
DIG0910
DIG0920
DIG0930
DIG0940
DIG0950
DIG0960
DIG0970
DIG0980
DIG0990
DIG1000
DIG1010
DIG1020
DIG1030
DIG1040
DIG1050
DIG1060
DIG1070
DIG1080
DIG1090
DIG1100
DIG1110
DIG1120
DIG1130
DIG1140
DIG1150
DIG1160
DIG1170
DIG1180
DIG1190
DIG1200
DIG1210

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C*
C*--- GEOMETRIC SPACING INPUT OPTION (INCLUDES UNIFORM SPACING CASE)
C* CARDS J.2 ... CONTAIN THE FOLLOWING DATA
C* COLUMNS 1-10 -1.
C* COLUMNS 11-20 GEOMETRIC SPACING RATIO OF DX(.+1)/DX(.)
C* COLUMNS 21-30 RIGHT HAND ENDPOINT OF LAST SUBINTERVAL HERE
C* THE SEQUENCE IS TERMINATED WITH A BLANK CARD OR INPUT FOR THE
C* NON-GEOMETRIC SPACING OPTION.
C*
C* THE REGION DESCRIPTION CARDS ARE TERMINATED BY THE TIME CARD
C* DESCRIBED NEXT.
C*
C*TIME DESCRIPTION AND PROGRAM CONTROL CARD
C*
C* COLUMNS 1-10 BLANK OR 0
C* COLUMNS 11-20 DELTAT = COMPUTATIONAL TIME STEP
C* COLUMNS 21-30 TMAX = MAXIMUM SIMULATION TIME
C* COLUMNS 31-40 DPRINT = PRINTOUT TIME STEP
C* COLUMNS 41-50 EXTRAT = EXTRAPOLATION TIME LIMIT
C* SOLUTION OBTAINED BY EXTRAPOLATION UNTIL
C* TIME EXCEEDS EXTRAT, THEN NO
C* EXTRAPOLATION OCCURS.
C* COLUMNS 51-60 RESTRT IF RESTRT .GT. 0 INITIAL VALUES ARE ON
C* LUSTRT. ELSE THEY ARE ON CARDS.
C* COLUMNS 61-70 SAVE IF SAVE .GT. 0 THE FINAL SET OF
C* CONCENTRATIONS ARE WRITTEN TO LUSAVE
C* FOR PRESERVATION.
C*
C*INITIAL CONCENTRATIONS (IF RESTRT .LE. 0)
C*
C* THERE CAN BE UP TO MAXPTS+1 (=203) CARDS IN THE FOLLOWING PACKET
C* OF INITIAL DISTRIBUTION TABLES.
C*
C* COLUMNS 1-10 XX
C* COLUMNS 11-20 C(XX)
C* COLUMNS 21-30 DEGREE OF POLYNOMIAL INTERPOLATION TO BE USED
C* FOR C(.) WHEN X IS BETWEEN XX AND THE NEXT
C* VALUE OF XX.
C* COLUMNS 31-40 SMALLM(XX)
C* COLUMNS 41-50 DEGREE OF POLYNOMIAL INTERPOLATION TO BE USED
C* FOR SMALLM(.)
C* COLUMNS 51-60 BIGM(XX)
C* COLUMNS 61-70 DEGREE OF POLYNOMIAL INTERPOLATION TO BE USED
C* FOR BIGM(.)
C* THE LAST CARD OF THIS PACKET MUST HAVE A NEGATIVE NUMBER IN
C* COLUMNS 1-10.
C*
C*
C*THE LAST CARD OF THE DATA DECK MUST BE BLANK IN COLUMNS 1-72
C*
C*****
C
C--- READ TITLE CARD
READ (LUIN,86) TITLE
DO 200 I=1,72
IF (TITLE(I).NE.BLANK) GO TO 300
200 CONTINUE
GO TO 4
300 WRITE (LUOUT,85) TITLE

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1	READ (LUIN,99)	DJ,B4LIFJ,TRPLIJ,CAPKJ,EXTRAT,RESTR,SAVE	DIG1830
	IF(DJ.LT.0.) GO TO 4		DIG1840
	IF(J.EQ.0) WRITE (LUOUT,94)		DIG1850
	IF(DJ.EQ.0.) GO TO 3		DIG1860
	NRJ=0		DIG1870
	IF(J.LT.MAXREG) GO TO 2		DIG1880
101	J=J+1		DIG1890
	WRITE (LUOUT,98) J,XRJ,DJ,B4LIFJ,TRPLIJ,CAPKJ		DIG1900
	ERINPT=.TRUE.		DIG1910
	GO TO 1		DIG1920
2	READ (LUIN,99) (XX(JJ),JJ=1,7)		DIG1930
	IF(XX(1).EQ.0.) GO TO 402		DIG1940
	IF(XX(1).LT.0.) GO TO 1002		DIG1950
C----	NON-GEOMETRIC INPUT OPTION		DIG1960
	DO 302 JJ=1,7		DIG1970
	DXK=XX(JJ)-OLDX		DIG1980
	IF(DXK.LE.0.) GO TO 2		DIG1990
	DXJ=DXK		DIG2000
	IF(IJ.LT.MAXIJ) GO TO 102		DIG2010
	IF(ERR) GO TO 202		DIG2020
	FRR=.TRUE.		DIG2030
	WRITE (LUOUT,97) MAXPTS		DIG2040
	GO TO 202		DIG2050
102	IJ=IJ+1		DIG2060
202	NRJ=NRJ+1		DIG2070
	DX(IJ)=DXJ		DIG2080
	XRJ=XX(JJ)		DIG2090
	OLDX=XX(JJ)		DIG2100
302	CONTINUE		DIG2110
	GO TO 2		DIG2120
402	IF(XRJ.LE.XRJM1) GO TO 101		DIG2130
	IF(NRJ.LE.0) GO TO 101		DIG2140
	J=J+1		DIG2150
C	NRJ = NUMBER OF SEGMENTS		DIG2160
C	XRJ = RIGHT HAND END POINT		DIG2170
	NR (J)=NRJ		DIG2180
	XR (J)=XRJ		DIG2190
	D (J)=DJ		DIG2200
	B4LIF (J)=B4LIFJ		DIG2210
	TRPLIF(J)=TRPLIJ		DIG2220
	CAPK (J)=CAPKJ		DIG2230
	NOPTS=NOPTS+NRJ		DIG2240
	XRJM1=XRJ		DIG2250
	WRITE (LUOUT,93) J,NRJ,XRJ,DJ,B4LIFJ,TRPLIJ,CAPKJ		DIG2260
	GO TO 1		DIG2270
C----	GEOMETRIC SPACING INPUT OPTION		DIG2280
1002	JJ=0		DIG2290
	ARE=XX(2)-1.		DIG2300
	IF(ABS(ARE).LT.EPSLN) GO TO 2002		DIG2310
	RATIO=(XX(3)-OLDX)/DXJ		DIG2320
	ALOGT=1.+ARE*RATIO		DIG2330
	IF(ALOGT.LE.0.) GO TO 1802		DIG2340
	IF(XX(2).LE.0.) GO TO 1802		DIG2350
	N=ALOG(ALOGT)/ALOG(XX(2))+.5		DIG2360
	IF(N.LE.0) GO TO 1802		DIG2370
	EXPON=1./FLOAT(N)		DIG2380
	ICOUN=0		DIG2390
1102	RNEW=(1.+ARE*RATIO)**EXPON-1.		DIG2400
	IF(ARE.EQ.0.) GO TO 2002		DIG2410
	IF(ABS((RNEW-ARE)/ARE)-EPSLN) 1302,1302,1202		DIG2420
1202	ARE=RNEW		DIG2430

ICOUN=ICOUN+1	DIG2440
IF(ICOUN.LE.100) GO TO 1102	DIG2450
ERR=.TRUE.	DIG2460
WRITE (LUOUT,90)	DIG2470
1302 ONEPR=1.+RNEW	DIG2480
1402 JJ=JJ+1	DIG2490
IF(IJ.LT.MAXIJ) GO TO 1502	DIG2500
IF(ERR) GO TO 1602	DIG2510
ERR=.TRUE.	DIG2520
WRITE (LUOUT,97) MAXPTS	DIG2530
GO TO 1602	DIG2540
1502 IJ=IJ+1	DIG2550
1602 NRJ=NRJ+1	DIG2560
DX(IJ)=DXJ	DIG2570
XRJ=OLDX+DXJ	DIG2580
DXJ=ONEPR*DXJ	DIG2590
IF(JJ.LT.N) GO TO 1702	DIG2600
XRJ=XX(3)	DIG2610
DX(IJ)=XRJ-OLDX	DIG2620
OLDX=XRJ	DIG2630
GO TO 2	DIG2640
1702 OLDX=XRJ	DIG2650
GO TO 1402	DIG2660
1802 N=1	DIG2670
1902 RNEW=0.	DIG2680
GO TO 1302	DIG2690
C---- UNIFORM SPACING CASE	DIG2700
2002 N=(XX(3)-OLDX)/DXJ+.5	DIG2710
N=MAX0(N,1)	DIG2720
DXJ=(XX(3)-OLDX)/FLOAT(N)	DIG2730
GO TO 1902	DIG2740
C	DIG2750
3 JMAX=J	DIG2760
IF(NOPTS.LE.MAXPTS) GO TO 204	DIG2770
WRITE (LUOUT,97) MAXPTS	DIG2780
4 STOP	DIG2790
104 WRITE (LUOUT,91)	DIG2800
GO TO 100	DIG2810
204 ERINIT=.FALSE.	DIG2820
R=XR(1)	DIG2830
T=0.	DIG2840
IF(RESTRT.GT.0.) GO TO 504	DIG2850
C---- READ TABULAR INITIAL VALUES FROM CARDS	DIG2860
NDXSMF=0	DIG2870
304 READ (LUIN,99) (TTT(I),I=1,7)	DIG2880
IF(TTT(1).LT.0.) GO TO 5	DIG2890
IF(NDXSMF.LT.MAXPTS) GO TO 404	DIG2900
IF(ERINIT) GO TO 304	DIG2910
WRITE (LUOUT,88) MAXPTS	DIG2920
ERINIT=.TRUE.	DIG2930
GO TO 304	DIG2940
404 NDXSMF=NDXSMF+1	DIG2950
C00 (NDXSMF)=TTT(1)	DIG2960
OLDC (NDXSMF)=TTT(2)	DIG2970
C10 (NDXSMF)=TTT(3)	DIG2980
OLDSM(NDXSMF)=TTT(4)	DIG2990
SM10 (NDXSMF)=TTT(5)	DIG3000
OLDBM(NDXSMF)=TTT(6)	DIG3010
BM10 (NDXSMF)=TTT(7)	DIG3020
GO TO 304	DIG3030
C---- INITIAL VALUES ARE ON TAPE LUSTRT	DIG3040

504	READ (LUSTRT) TYTLE,N,M,T,TOTO	DIG3050
	IF(N.EQ.NOPTS) GO TO 704	DIG3060
604	WRITE (LUOUT,84) TITLE,TYTLE	DIG3070
	WRITE (LUOUT,87) N,NOPTS,M,JMAX	DIG3080
	ERINIT=.TRUE.	DIG3090
	GO TO 5	DIG3100
704	IF(M.NE.JMAX) GO TO 604	DIG3110
C----	FIRST 15 CHARACTERS MUST AGREE WITH INPUT TITLE	DIG3120
	DO 804 I=1,15	DIG3130
	IF(TITLE(I).NE.TYTLE(I)) GO TO 604	DIG3140
804	CONTINUE	DIG3150
	WRITE (LUOUT,83) TYTLE	DIG3160
	READ (LUSTRT) (C(I),SMALLM(I),BIGM(I),I=1,N)	DIG3170
	READ (LUSTRT) (SMXR(I),BMXR(I),I=1,M)	DIG3180
5	IF(ERINPT) GO TO 4	DIG3190
	IF(ERR) GO TO 4	DIG3200
	IF(ERINIT) GO TO 4	DIG3210
C		DIG3220
C----	INPUT DATA ALL READ IN	DIG3230
C		DIG3240
	WRITE (LUOUT,92) R4I IF.I,TRPLIJ,CAPKJ,EXTRAT,RESTRT,SAVE	DIG3250
	DELTAT=B4LIFJ	DIG3260
	TMAX=TRPLIJ	DIG3270
	IF(DELTAT.LE.0.) DELTAT=TMAX/10.	DIG3280
	KPRINT=CAPKJ/DELTAT+.5	DIG3290
	KPRINT=MAX0(KPRINT,1)	DIG3300
C		DIG3310
C----	THE INDEXING CONVENTION USED HERE HAS DX(I),ALPHA(I),BETA(I)	DIG3320
C	AND XX(I) ASSOCIATED WITH C(I+1) FOR I=1,2,...,IJMAX, AND	DIG3330
C	DX(IJMAX+1) AND XX(IJMAX+1) ASSOCIATED WITH C(IJMAX+2)	DIG3340
C		DIG3350
	IJMAX=NOPTS-2	DIG3360
	IF(IJMAX.LT.1) GO TO 104	DIG3370
	XRJ=0.	DIG3380
	DO 105 J=1,IJMAX	DIG3390
	RHS=2./(DX(J)+DX(J+1))	DIG3400
	ALPHA(J)=RHS/DX(J)	DIG3410
105	BETA(J)=RHS/DX(J+1)	DIG3420
	IF(RESTRT.LE.0.) CALL STRTNO	DIG3430
	NDXSMF=1	DIG3440
	SMALLF(1)=0.	DIG3450
	TOTO=TRAPZR(T)	DIG3460
	T=0.	DIG3470
	CALL PRINT	DIG3480
	C(1)=0.	DIG3490
	IF(TOTO.GT.0.) GO TO 205	DIG3500
	WRITE (LUOUT,96)	DIG3510
	GO TO 4	DIG3520
205	IJKMAX=TMAX/DELTAT+.05	DIG3530
	IF(IJKMAX.LE.1) IJKMAX=2	DIG3540
	IPLOT=TMAX/(FLOAT(MAXPLT-1)*DELTAT)+.05	DIG3550
	IPLOT=MAX0(IPLOT,1)	DIG3560
	HAFDLT=DELTAT/2.	DIG3570
	ITTER=0	DIG3580
C		DIG3590
C----	START OF TIME LOOP (IJK IS THE TIME INDEX)	DIG3600
C		DIG3610
	IJK=1	DIG3620
	DT=DELTAT	DIG3630
	DT02=DT/2.	DIG3640
	NOEXTR=.FALSE.	DIG3650

IF(T.GE.EXTRAT) NOEXTR=.TRUE.	DIG3660
305 IF(NOEXTR) GO TO 605	DIG3670
C---- SET FOR EXTRAPOLATION TO LIMIT	DIG3680
TNEXT=T+DELTAT	DIG3690
EF1=TOTO	DIG3700
DO 405 J=1,NOPTS	DIG3710
OLDC (J)=C (J)	DIG3720
OLDSM(J)=SMALLM(J)	DIG3730
405 OLDBM(J)=BIGM (J)	DIG3740
DO 505 J=1,JMAX	DIG3750
OLDSMR(J)=SMXR(J)	DIG3760
505 OLDBMR(J)=BMXR(J)	DIG3770
OLDT=T	DIG3780
IEXTRA=0	DIG3790
NOSTEP=0	DIG3800
DT=4.*DT	DIG3810
MAXSTP=(TNEXT-T)/DT+0.05	DIG3820
MAXSTP=MAX0(MAXSTP,1)	DIG3830
DT=(TNEXT-T)/FLOAT(MAXSTP)	DIG3840
DT02=DT/2.	DIG3850
605 DO 6 J=1,JMAX	DIG3860
C	DIG3870
C	DIG3880
*****	DIG3890
C*	DIG3900
C* IF D(.),B4LIF(.),TRPLIF(.) AND/OR CAPK(.) BECOME NON-CONSTANT	DIG3910
C* THE CHANGE SHOULD BE MADE HERE	DIG3920
C*	DIG3930
*****	DIG3940
C	DIG3950
C	DIG3960
DT02KP=DT02*TRPLIF(J)	DIG3970
DEN=1.+DT02KP	DIG3980
GAMMA (J)=B4LIF(J)/DEN*DT02	DIG3990
ZETA (J)=(1.-DT02KP)/DEN	DIG4000
ETA (J)=DT02KP*(ZETA(J)+1.)	DIG4010
6 CONTINUE	DIG4020
C	DIG4030
C---- SET UP COEFFICIENT MATRIX	DIG4040
C	DIG4050
IJ=0	DIG4060
DO 9 J=1,JMAX	DIG4070
IMAXM1=NR(J)-1	DIG4080
DIFJ=D(J)*DT02	DIG4090
GJ=GAMMA(J)+CAPK(J)*DT02	DIG4100
ZJ=ETA(J)	DIG4110
IF(IMAXM1.LE.0) GO TO 8	DIG4120
C---- SET UP REGION(J) EQUATIONS	DIG4130
DO 7 I=1,IMAXM1	DIG4140
IJ=IJ+1	DIG4150
AJ=ALPHA(IJ)*DIFJ	DIG4160
BJ=BETA (IJ)*DIFJ	DIG4170
RHS=AJ+BJ+GJ	DIG4180
DJ=1.+RHS	DIG4190
EJ=1.-RHS	DIG4200
RHS=AMAX1(ABS(AJ),ABS(BJ))	DIG4210
RHS=AMAX1(ABS(DJ),RHS)	DIG4220
ABCD(IJ,1)= AJ/RHS	DIG4230
ABCD(IJ,2)=-DJ/RHS	DIG4240
ABCD(IJ,3)= BJ/RHS	DIG4250
C---- SET UP RIGHT HAND SIDE	DIG4260

RHS=(-AJ*C(IJ)-EJ*C(IJ+1)-BJ*C(IJ+2)-ZJ*SMALLM(IJ+1))/RHS	DIG4270
7 ABCD(IJ,4)=RHS	DIG4280
8 IF(J.EQ.JMAX) GO TO 9	DIG4290
C---- SET UP INTERFACE EQUATION	DIG4300
IJ=IJ+1	DIG4310
AJ =D(J)/DX(IJ)	DIG4320
DJ =D(J+1)/DX(IJ+1)	DIG4330
BJ =-AJ-DJ	DIG4340
RHS=AMAX1(ABS(AJ),ABS(BJ))	DIG4350
RHS=AMAX1(ABS(DJ),RHS)	DIG4360
ABCD(IJ,1)=AJ/RHS	DIG4370
ABCD(IJ,2)=BJ/RHS	DIG4380
ABCD(IJ,3)=DJ/RHS	DIG4390
ABCD(IJ,4)=0.	DIG4400
9 CONTINUE	DIG4410
ABCD(1,4)=ABCD(1,4)-ABCD(1,1)*C(1)	DIG4420
ABCD(1,1)=0.	DIG4430
C---- NOW SOLVE FOR NEW C(IJ) WHICH WILL BE IN XX(IJ-1)	DIG4440
CALL DIAG3(ABCD,IJMAX,XX)	DIG4450
XX(IJMAX+1)=C(IJMAX+2)	DIG4460
C---- GET NEW SMALLM(IJ) AND BIGM(IJ)	DIG4470
PART=2.*C(1)	DIG4480
IJ=1	DIG4490
DO 17 J=1,JMAX	DIG4500
IMAX=NR(J)	DIG4510
ZJ=ZETA (J)	DIG4520
GJ=GAMMA(J)	DIG4530
CAPKDT=CAPK(J)*DT02	DIG4540
C---- GET LEFT END VALUE OF SMALLM(.) AND BIGM(.)	DIG4550
IF(IJ.EQ.1) GO TO 13	DIG4560
PART=OLDCIJ+XX(IJ-1)	DIG4570
13 SMALLM(IJ)=ZJ*SMALLM(IJ)+GJ*PART	DIG4580
BIGM(IJ)=BIGM(IJ)+CAPKDT*PART	DIG4590
DO 16 I=1,IMAX	DIG4600
IJ=IJ+1	DIG4610
OLDCIJ=C(IJ)	DIG4620
PART=OLDCIJ+XX(IJ-1)	DIG4630
IF(I.EQ.IMAX) GO TO 16	DIG4640
SMALLM(IJ)=ZJ*SMALLM(IJ)+GJ*PART	DIG4650
BIGM(IJ)=BIGM(IJ)+CAPKDT*PART	DIG4660
16 C(IJ)=XX(IJ-1)	DIG4670
C---- GET RIGHT END VALUE OF SMALLM(.) AND BIGM(.)	DIG4680
SMXR(J)=ZJ*SMXR(J)+GJ*PART	DIG4690
BMXR(J)=BMXR(J)+CAPKDT*PART	DIG4700
17 CONTINUE	DIG4710
SMALLM(IJ)=0.	DIG4720
BIGM (IJ)=0.	DIG4730
T=T+DT	DIG4740
IF(NOEXTR) GO TO 517	DIG4750
NOSTEP=NOSTEP+1	DIG4760
IF(NOSTEP.LT.MAXSTP) GO TO 605	DIG4770
C---- MAKE EXTRAPOLATION	DIG4780
CALL EXTRA(IEXTRA)	DIG4790
EFO=EF1	DIG4800
EF1=TRAPZR(T)	DIG4810
IF(EF1.EQ.0.) GO TO 417	DIG4820
IF(ABS((EFO-EF1)/EF1)-.5E-4) 417,417,117	DIG4830
117 IF((DELTAT/DT).LE.1024.) GO TO 617	DIG4840
WRITE (LUOUT,89) T,DT	DIG4850
GO TO 417	DIG4860
617 IEXTRA=IEXTRA+1	DIG4870

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NOSTEP=0
MAXSTP=2*MAXSTP
DT=DT02
DT02=DT02/2.
DO 217 J=1,NOPTS
C      (J)=OLDC (J)
SMALLM(J)=OLDSM(J)
217 BIGM (J)=OLDBM(J)
DO 317 J=1,JMAX
SMXR(J)=OLDSMR(J)
317 RMXR(J)=OLDRMR(J)
T=OLDT
GO TO 605
417 IF(ABS((DT-HAFDLT)/HAFDLT)-.5E-4) 817,817,717
717 ITTER=0
817 ITTER=ITTER+1
IF(ITTER.GT.10) NOEXTR=.TRUE.
TOTT=EF1
IF(T.GE.EXTRAT) NOEXTR=.TRUE.
IF(.NOT.NOEXTR) GO TO 917
DT=DELTAT
DT02=DT/2.
917 IF(MOD(IJK,IPLOT).NE.0) GO TO 18
517 IF(NOEXTR) TOTT=TRAPZR(T)
IF(NDXSMF.GE.MAXPLT) GO TO 18
NDXSMF=NDXSMF+1
SMALLF(NDXSMF)=1.-TOTT/TOTO
18 IF(IJK.EQ.IJKMAX) GO TO 20
IF(MOD(IJK,KPRINT).EQ.0) CALL PRINT
20 IJK=IJK+1
IF(IJK.LE.IJKMAX) GO TO 305
CALL PRINT
IF(SAVE.GT.0.) WRITE (LUOUT,82)
DELTPL=FLOAT(IPLOT)*DELTAT
DO 21 I=1,NDXSMF
TIMMM=FLOAT(I-1)*DELTPL
TIMMM=ABS(TIMMM)
21 TTT(I)=SQRT(TIMMM)
WRITE (LUOUT,85) TITLE
WRITE (LUOUT,95)
CALL TOLP(TTT,SMALLF,NDXSMF,1,NDXSMF)
IF(SAVE.LE.0.) GO TO 100
WRITE (LUSAVE) TITLE,NOPTS,JMAX,T,TOTO
WRITE (LUSAVE) (C(I),SMALLM(I),BIGM(I),I=1,NOPTS)
WRITE (LUSAVE) (SMXR(I),RMXR(I),I=1,JMAX)
GO TO 100
END

```

```

DIG4880
DIG4890
DIG4900
DIG4910
DIG4920
DIG4930
DIG4940
DIG4950
DIG4960
DIG4970
DIG4980
DIG4990
DIG5000
DIG5010
DIG5020
DIG5030
DIG5040
DIG5050
DIG5060
DIG5070
DIG5080
DIG5090
DIG5100
DIG5110
DIG5120
DIG5130
DIG5140
DIG5150
DIG5160
DIG5170
DIG5180
DIG5190
DIG5200
DIG5210
DIG5220
DIG5230
DIG5240
DIG5250
DIG5260
DIG5270
DIG5280
DIG5290
DIG5300
DIG5310
DIG5320
DIG5330
DIG5340-

```

	SUBROUTINE STRTNO	STR0000
		STR0010
	COMMON ABCD(202,4),XX(202),C(202),SMALLM(202),BIGM(202),	STR0020
1	DX(201),ALPHA(200),BETA(200)	STR0030
	COMMON /ARRAYS/ JMAX,NR(10),XR(10),D(10),B4LIF(10),TRPLIF(10),	STR0040
1	CAPK(10),GAMMA(10),ETA(10),ZETA(10),SMXR(10),BMXR(10)	STR0050
	COMMON /EXTRAP/ NOPTS,	STR0060
1	OLDC(202),OLDSM(202),OLDBM(202),OLDSMR(10),OLDBMR(10),	STR0070
2	C00 (202),SM00 (202),RM00 (202),SMXR00(10),BMXR00(10),	STR0080
3	C10 (202),SM10 (202),BM10 (202),SMXR10(10),BMXR10(10),	STR0090
4	C20 (202),SM20 (202),BM20 (202),SMXR20(10),BMXR20(10),	STR0100
5	C11 (202),SM11 (202),BM11 (202),SMXR11(10),BMXR11(10),	STR0110
6	C21 (202),SM21 (202),BM21 (202),SMXR21(10),BMXR21(10)	STR0120
	COMMON /OTHER / NDXSMF,SMALLF(501)	STR0130
		STR0140
	K=2	STR0150
	IJ=0	STR0160
	EX=0.	STR0170
	DO 12 J=1,JMAX	STR0180
	IMAX=NR(J)	STR0190
	DO 11 I=1,IMAX	STR0200
	IJ=IJ+1	STR0210
1	IF(EX-C00(K+1)) 2,4,4	STR0220
2	IF(EX-C00(K)) 3,7,7	STR0230
3	K=K+1	STR0240
	IF(K.GT.1) GO TO 2	STR0250
	K=1	STR0260
	GO TO 7	STR0270
4	K=K+1	STR0280
	IF(K-NDXSMF) 1,5,5	STR0290
5	K=NDXSMF-1	STR0300
7	ID=C10(K)+.05	STR0310
	ID=MAX0(ID,0)+1	STR0320
	ID=MIN0(ID,NDXSMF)	STR0330
	IL=K-(ID-1)/2	STR0340
	IL=MAX0(IL,1)	STR0350
	IU=IL+ID-1	STR0360
	IU=MIN0(IU,NDXSMF)	STR0370
	ID=IU-IL+1	STR0380
	DO 8 N=1,ID	STR0390
	ABCD(N,1)=C00 (IL)	STR0400
	ABCD(N,2)=OLDC(IL)	STR0410
8	IL=IL+1	STR0420
	C(IJ)=PLIF(EX,ID,ABCD(1,1),ABCD(1,2))	STR0430
	ID=SM10(K)+.05	STR0440
	ID=MAX0(ID,0)+1	STR0450
	ID=MIN0(ID,NDXSMF)	STR0460
	IL=K-(ID-1)/2	STR0470
	IL=MAX0(IL,1)	STR0480
	IU=IL+ID-1	STR0490
	IU=MIN0(IU,NDXSMF)	STR0500
	ID=IU-IL+1	STR0510
	DO 9 N=1,ID	STR0520
	ABCD(N,1)=C00 (IL)	STR0530
	ABCD(N,2)=OLDSM(IL)	STR0540
9	IL=IL+1	STR0550
	SMALLM(IJ)=PLIF(EX,ID,ABCD(1,1),ABCD(1,2))	STR0560
	ID=BM10(K)+.05	STR0570
	ID=MAX0(ID,0)+1	STR0580
	ID=MIN0(ID,NDXSMF)	STR0590
	IL=K-(ID-1)/2	STR0600

```

      IL=MAX0(IL,1)
      IU=IL+ID-1
      IU=MIN0(IU,NDXSMF)
      ID=IU-IL+1
      DO 10 N=1,ID
      ABCD(N,1)=C00 (IL)
      ABCD(N,2)=OLDBM(IL)
10  IL=IL+1
      BIGM(IJ)=PLIF(EX,ID,ABCD(1,1),ABCD(1,2))
11  EX=EX+DX(IJ)
      SMXR(J)=SMALLM(IJ)
      BMXR(J)=BIGM (IJ)
12  CONTINUE
      C(IJ+1)=0.
      RETURN
      END

```

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STR0610
STR0620
STR0630
STR0640
STR0650
STR0660
STR0670
STR0680
STR0690
STR0700
STR0710
STR0720
STR0730
STR0740
STR0750
STR0760-

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C	SUBROUTINE EXTRA(I)	EXT0000
C	THIS ROUTINE PERFORMS THE FIRST TWO LEVELS OF AN EXTRAPOLATION	EXT0010
C	TO THE LIMIT PROCEDURE. THE RATIO OF SUCCESSIVE VALUES OF	EXT0020
C	DELTA-T IS 1/2.	EXT0030
C	REFERENCE PETER HENRICI, ELEMENTS OF NUMERICAL ANALYSIS,	EXT0040
C	WILEY (1964) PP.239-241.	EXT0050
C		EXT0060
	COMMON ABCD(202,4),XX(202),C(202),SMALLM(202),BIGM(202),	EXT0070
1	DX(201),ALPHA(200),BETA(200)	EXT0080
	COMMON /ARRAYS/ JMAX,NR(10),XR(10),D(10),B4LIF(10),TRPLIF(10),	EXT0090
1	CAPK(10),GAMMA(10),ETA(10),ZETA(10),SMXR(10),BMXR(10)	EXT0100
	COMMON /EXTRAP/ NOPTS,	EXT0110
1	OLDC(202),OLDSM(202),OLDBM(202),OLDSMR(10),OLDBMR(10),	EXT0120
2	C00 (202),SM00 (202),BM00 (202),SMXR00(10),BMXR00(10),	EXT0130
3	C10 (202),SM10 (202),BM10 (202),SMXR10(10),BMXR10(10),	EXT0140
4	C20 (202),SM20 (202),BM20 (202),SMXR20(10),BMXR20(10),	EXT0150
5	C11 (202),SM11 (202),BM11 (202),SMXR11(10),BMXR11(10),	EXT0160
6	C21 (202),SM21 (202),BM21 (202),SMXR21(10),BMXR21(10)	EXT0170
C		EXT0180
	IF(I.GT.2) GO TO 11	EXT0190
	IF(I.GT.0) GO TO 3	EXT0200
	DO 1 N=1,NOPTS	EXT0210
	C00 (N)=C (N)	EXT0220
	SM00(N)=SMALLM(N)	EXT0230
1	BM00(N)=BIGM (N)	EXT0240
	DO 2 N=1,JMAX	EXT0250
	SMXR00(N)=SMXR(N)	EXT0260
2	BMXR00(N)=BMXR(N)	EXT0270
	GO TO 10	EXT0280
3	IF(I.GT.1) GO TO 7	EXT0290
	DO 4 N=1,NOPTS	EXT0300
	C10 (N)=C (N)	EXT0310
	C11 (N)=2.*C10 (N)-C00 (N)	EXT0320
	C (N)=C11 (N)	EXT0330
	SM10(N)=SMALLM(N)	EXT0340
	SM11(N)=2.*SM10(N)-SM00(N)	EXT0350
	SMALLM(N)=SM11(N)	EXT0360
	BM10(N)=BIGM (N)	EXT0370
	BM11(N)=2.*BM10(N)-BM00(N)	EXT0380
4	BIGM (N)=BM11(N)	EXT0390
	DO 5 N=1,JMAX	EXT0400
	SMXR10(N)=SMXR(N)	EXT0410
	SMXR11(N)=2.*SMXR10(N)-SMXR00(N)	EXT0420
	SMXR (N)=SMXR11(N)	EXT0430
	BMXR10(N)=BMXR(N)	EXT0440
	BMXR11(N)=2.*BMXR10(N)-BMXR00(N)	EXT0450
5	BMXR (N)=BMXR11(N)	EXT0460
	GO TO 10	EXT0470
7	DO 8 N=1,NOPTS	EXT0480
	C20 (N)=C (N)	EXT0490
	C21 (N)= 2.*C20 (N)-C10 (N)	EXT0500
	C (N)=(4.*C21 (N)-C11 (N))/3.	EXT0510
	SM20(N)= SMALLM(N)	EXT0520
	SM21(N)= 2.*SM20(N)-SM10(N)	EXT0530
	SMALLM(N)=(4.*SM21(N)-SM11(N))/3.	EXT0540
	BM20(N)=BIGM (N)	EXT0550
	BM21(N)= 2.*BM20(N)-BM10(N)	EXT0560
8	BIGM (N)=(4.*BM21(N)-BM11(N))/3.	EXT0570
	DO 9 N=1,JMAX	EXT0580
	SMXR20(N)=SMXR(N)	EXT0590
	SMXR21(N)= 2.*SMXR20(N)-SMXR10(N)	EXT0600

```

      SMXR (N)=(4.*SMXR21(N)-SMXR11(N))/3.
      BMXR20(N)=BMXR(N)
      BMXR21(N)= 2.*BMXR20(N)-BMXR10(N)
9    BMXR (N)=(4.*BMXR21(N)-BMXR11(N))/3.
10   RETURN
11   DO 12 N=1,NOPTS
      C00 (N)=C10 (N)
      C10 (N)=C20 (N)
      C11 (N)=C21 (N)
      SM00(N)=SM10(N)
      SM10(N)=SM20(N)
      SM11(N)=SM21(N)
      BM00(N)=BM10(N)
      BM10(N)=BM20(N)
12   BM11(N)=BM21(N)
      DO 13 N=1,JMAX
      SMXR00(N)=SMXR10(N)
      SMXR10(N)=SMXR20(N)
      SMXR11(N)=SMXR21(N)
      BMXR00(N)=BMXR10(N)
      BMXR10(N)=BMXR20(N)
13   BMXR11(N)=BMXR21(N)
      GO TO 7
      END

```

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EXT0610
EXT0620
EXT0630
EXT0640
EXT0650
EXT0660
EXT0670
EXT0680
EXT0690
EXT0700
EXT0710
EXT0720
EXT0730
EXT0740
EXT0750
EXT0760
EXT0770
EXT0780
EXT0790
EXT0800
EXT0810
EXT0820
EXT0830
EXT0840-

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	SUBROUTINE PRINT	PRI0000
C	COMMON ABCD(202,4),XX(202),C(202),SMALLM(202),BIGM(202),	PRI0010
	1 DX(201),ALPHA(200),BETA(200)	PRI0020
	COMMON /ARRAYS/ JMAX,NR(10),XR(10),D(10),B4LIF(10),TRPLIF(10),	PRI0030
	1 CAPK(10),GAMMA(10),ETA(10),ZETA(10),SMXR(10),BMXR(10)	PRI0040
	COMMON /OTHER / NDXSMF,SMALLF(501)	PRI0050
	COMMON /COM / T	PRI0060
	COMMON /ERRR /ERRR(10)	PRI0070
	COMMON /LUIO / LUIN,LUOUT	PRI0080
	COMMON /TITLE / TITLE(80)	PRI0090
C	INTEGER TITLE	PRI0100
C	DATA MAXLIN/59/	PRI0110
C	99 FORMAT(8H0TIME = F15.4,5X19HRELEASE FRACTION = F10.6)	PRI0120
	98 FORMAT(1H04X1H1,8X1HX13X1HC,10X7HSMALL M11X5HCAP M/)	PRI0130
	97 FORMAT(1X15,1P4E15.7)	PRI0140
	95 FORMAT(1X15,1PE15.7)	PRI0150
	94 FORMAT(6H0 RMS ,1PF15.7)	PRI0160
	93 FORMAT(1H0/33H0INTEGRATION ERROR ESTIMATE TABLE//23H REGION ERROR	PRI0170
	1 ESTIMATE/)	PRI0180
	92 FORMAT(1H1,80A1)	PRI0190
C	SMALF=SMALLF(NDXSMF)	PRI0200
	XRJ=0.	PRI0210
	IJ=0	PRI0220
	LINO=MAXLIN	PRI0230
	DO 13 J=1,JMAX	PRI0240
	IMAX=NR(J)	PRI0250
	SMXRJ=SMXR(J)	PRI0260
	BMXRJ=BMXR(J)	PRI0270
	DO 10 I=1,IMAX	PRI0280
	IJ=IJ+1	PRI0290
	IF(LINO.LT.MAXLIN) GO TO 8	PRI0300
	WRITE (LUOUT,92) TITLE	PRI0310
	WRITE (LUOUT,99) T,SMALF	PRI0320
	WRITE (LUOUT,98)	PRI0330
	LINO=6	PRI0340
	8 LINO=LINO+1	PRI0350
	IF(I .NE.1) GO TO 9	PRI0360
	IF(IJ.EQ.1) GO TO 9	PRI0370
	WRITE (LUOUT,97)	PRI0380
	LINO=LINO+1	PRI0390
	9 WRITE (LUOUT,97) IJ,XRJ,C(IJ),SMALLM(IJ),BIGM(IJ)	PRI0400
	XRJ=XRJ+DX(IJ)	PRI0410
	10 CONTINUE	PRI0420
	11 IJ=IJ+1	PRI0430
	IF(LINO.LT.MAXLIN) GO TO 12	PRI0440
	WRITE (LUOUT,92) TITLE	PRI0450
	WRITE (LUOUT,99) T,SMALF	PRI0460
	WRITE (LUOUT,98)	PRI0470
	LINO=6	PRI0480
	12 LINO=LINO+1	PRI0490
	WRITE (LUOUT,97) IJ,XRJ,C(IJ),SMXRJ,BMXRJ	PRI0500
	IJ=IJ-1	PRI0510
	13 CONTINUE	PRI0520
	WRITE (LUOUT,93)	PRI0530
	RMS=0.	PRI0540
	DO 14 J=1,JMAX	PRI0550
		PRI0560
		PRI0570
		PRI0580
		PRI0590
		PRI0600

```
RMS=RMS+ERRR(J)**2
WRITE (LUOUT,95) J,ERRR(J)
14 CONTINUE
RMS=SQRT(RMS/FLOAT(JMAX))
WRITE (LUOUT,94) RMS
RETURN
END
```

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PRI0610
PRI0620
PRI0630
PRI0640
PRI0650
PRI0660
PRI0670-
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	FUNCTION TRAPZR(TT)		TRA0000
C-----		INTEGRATE C, SMALLM AND BIGM	TRA0010
C			TRA0020
	COMMON	ABCD(202,4),XX(202),C(202),SMALLM(202),BIGM(202),	TRA0030
1	DX(201),ALPHA(200),BETA(200)		TRA0040
	COMMON /ARRAYS/	JMAX,NR(10),XR(10),D(10),B4LIF(10),TRPLIF(10),	TRA0050
1	CAPK(10),GAMMA(10),FTA(10),ZETA(10),SMXR(10),BMXR(10)		TRA0060
	COMMON /CZERO/ R		TRA0070
	COMMON /ERRR /ERRR(10)		TRA0080
C			TRA0090
	TOT=0.		TRA0100
	IJ=0		TRA0110
	EX=0.		TRA0120
	DO 10 J=1,JMAX		TRA0130
	IK=0		TRA0140
	IMAX=NR(J)		TRA0150
	SMXRJ=SMXR(J)		TRA0160
	BMXRJ=BMXR(J)		TRA0170
	DO 5 I=1,IMAX		TRA0180
	IJ=IJ+1		TRA0190
	VAL=C(IJ)+SMALLM(IJ)+BIGM(IJ)		TRA0200
	IF(TT.GT.0.) GO TO 2		TRA0210
	IF(ABS((EX-R)/R).LE..5E-5) VAL=VAL-C(IJ)		TRA0220
2	IK=IK+1		TRA0230
	ABCD(IK,1)=EX		TRA0240
	ABCD(IK,2)=VAL		TRA0250
	EX=EX+DX(IJ)		TRA0260
5	CONTINUE		TRA0270
7	IJ=IJ+1		TRA0280
	VAL=C(IJ)+SMXRJ+BMXRJ		TRA0290
	IK=IK+1		TRA0300
	ABCD(IK,1)=EX		TRA0310
	ABCD(IK,2)=VAL		TRA0320
	CALL INT4PT(ABCD(1,1),ABCD(1,2),IK,1,IK,DTOT,ER,IFLAG)		TRA0330
	TOT=TOT+DTOT		TRA0340
	ERRR(J)=ER		TRA0350
	IJ=IJ-1		TRA0360
10	CONTINUE		TRA0370
	TRAPZR=TOT		TRA0380
	RETURN		TRA0390
	END		TRA0400-

	FUNCTION PLIF(X,N,XJ,FJ)	PLI0000
C----	PLIF . . . P(OLYNOMIAL), L(AGRANGE) I(INTERPOLATION) F(ORMULA).	PLI0010
C	THIS FUNCTION COMPUTES AN INTERPOLATED VALUE OF FJ(.) AT THE POINT	PLI0020
C	X USING A LAGRANGE INTERPOLATION FORMULA DEFINED ON THE N POINTS	PLI0030
C	(XJ(.),FJ(.)).	PLI0040
C		PLI0050
	DIMENSION XJ(N),FJ(N)	PLI0060
C		PLI0070
	POX=0.	PLI0080
	DO 2 I=1,N	PLI0090
	XJI=XJ(I)	PLI0100
	TERM=FJ(I)	PLI0110
	DO 1 J=1,N	PLI0120
	IF(J.NE.I) TERM=((X-XJ(J))/(XJI-XJ(J)))*TERM	PLI0130
1	CONTINUE	PLI0140
2	POX=POX+TERM	PLI0150
	PLIF=POX	PLI0160
	RETURN	PLI0170
	END	PLI0180-

	SUBROUTINE INT4PT(X,F,NN,IAA,IBB,INTEG,ER,IFLAG)	INT0000
C		INT0010
C----	THIS PROCEDURE EVALUATES THE INTEGRAL FROM X(IAA) TO X(IBB) OF A	INT0020
C	FUNCTION WHOSE VALUES AT POINTS X(I), I=1(1)NN ARE STORED IN	INT0030
C	F(I), I=1(1)NN. THE POINTS X(I), WHICH NEED NOT BE EQUALLY SPACED,	INT0040
C	ARE ASSUMED TO BE DISTINCT AND ARRANGED IN ASCENDING OR	INT0050
C	DESCENDING ORDER. THE INTEGRATION IS PERFORMED USING A 4-POINT	INT0060
C	RULE OVER EACH INTERVAL. IF ANY OF THE RELATIONS, NN.LT.4,	INT0070
C	IBB.GT.NN, IAA.LE.0, IAA.GT.IBB ARE TRUE, IFLAG IS SET TO 1	INT0080
C	AND RETURN EXECUTED. ELSE IFLAG = 0. IF NN.GT.4 AN	INT0090
C	ESTIMATE OF THE ERROR IS ASSIGNED TO ER. IF NN.EQ.4 NO INDICATION	INT0100
C	OF THE ERROR IS OBTAINABLE AND ER=0.	INT0110
C		INT0120
C----	REFERENCE P.E. GILL AND B.F. MILLER, AN ALGORITHM FOR THE	INT0130
C	INTEGRATION OF UNEQUALLY SPACED DATA, THE COMPUTER JOURNAL	INT0140
C	VOL. 15, NO. 1, JUNE 1972 PP. 80-83	INT0150
C		INT0160
	REAL INTEG	INT0170
	DIMENSION X(1),F(1)	INT0180
	N=NN	INT0190
	IA=IAA	INT0200
	IB=IBB	INT0210
	IF(N.LT.4) GO TO 16	INT0220
	IF(IA.GT.IB) GO TO 16	INT0230
	IF(IA.LE.0) GO TO 16	INT0240
	IF(IB.GT.N) GO TO 16	INT0250
	TOTAL=0.	INT0260
	E=0.	INT0270
	IF(IA.EQ.IB) GO TO 14	INT0280
C----	BEGIN INTEGRATION ROUTINE	INT0290
	NM1=N-1	INT0300
	NM2=N-2	INT0310
	S=0.	INT0320
	C=0.	INT0330
	R4=0.	INT0340
	J=IA	INT0350
	IF(IA.EQ.NM1) GO TO 2	INT0360
1	IF(IA.GT.3) GO TO 3	INT0370
	J=3	INT0380
	GO TO 3	INT0390
2	IF(N.LE.4) GO TO 1	INT0400
	J=NM2	INT0410
3	K=NM1	INT0420
	IF(IB.EQ.2) GO TO 5	INT0430
4	IF(N.LE.(IB+2)) GO TO 6	INT0440
	K=IB+1	INT0450
	GO TO 6	INT0460
5	IF(N.LE.4) GO TO 4	INT0470
	K=4	INT0480
6	DO 13 I=J,K	INT0490
	IF(I.GT.J) GO TO 7	INT0500
	H2=X(I-1)-X(I-2)	INT0510
	D3=(F(I-1)-F(I-2))/H2	INT0520
	H3=X(I)-X(I-1)	INT0530
	D1=(F(I)-F(I-1))/H3	INT0540
	H1=H2+H3	INT0550
	D2=(D1-D3)/H1	INT0560
	H4=X(I+1)-X(I)	INT0570
	R1=(F(I+1)-F(I))/H4	INT0580
	R2=(R1-D1)/(H4+H3)	INT0590
	H1=H1+H4	INT0600

R3=(R2-D2)/H1	INT0610
IF(IA.GT.1) GO TO 7	INT0620
TOTAL=H2*(F(1)+H2*(D3/2.-H2*(D2/6.-(H2+2.*H3)*R3/12.)))	INT0630
S=-H2**3*(H2*(3.*H2+5.*H4)+10.*H3*H1)/60.	INT0640
GO TO 8	INT0650
7 H4=X(I+1)-X(I)	INT0660
R1=(F(I+1)-F(I))/H4	INT0670
R4=H4+H3	INT0680
R2=(R1-D1)/R4	INT0690
R4=R4+H2	INT0700
R3=(R2-D2)/R4	INT0710
R4=R4+H1	INT0720
R4=(R3-D3)/R4	INT0730
8 IF(I.GT.IB) GO TO 9	INT0740
IF(I.LE.IA) GO TO 9	INT0750
TOTAL=TOTAL+H3*((F(I)+F(I-1))/2.-H3*H3*(D2+R2+(H2-H4)*R3)/12.)	INT0760
C=H3**3*(2.*H3*H3+5.*(H3*(H4+H2)+2.*H4*H2))/120.	INT0770
E=E+(C+S)*R4	INT0780
S=C	INT0790
IF(I.EQ.J) S=C+S	INT0800
GO TO 10	INT0810
9 E=E+R4*S	INT0820
10 IF(I.NE.K) GO TO 12	INT0830
IF(IR.NE.N) GO TO 11	INT0840
TOTAL=TOTAL+H4*(F(N)-H4*(R1/2.+H4*(R2/6.+(2.*H3+H4)*R3/12.)))	INT0850
F=F-H4**3*R4*(H4*(3.*H4+5.*H2)+10.*H3*(H2+H3+H4))/60.	INT0860
11 IF(IB.GE.NM1) E=E+S*R4	INT0870
GO TO 13	INT0880
12 H1=H2	INT0890
H2=H3	INT0900
H3=H4	INT0910
D1=R1	INT0920
D2=R2	INT0930
D3=R3	INT0940
13 CONTINUE	INT0950
14 INTEG=TOTAL	INT0960
ER=E	INT0970
IFLAG=0	INT0980
15 RETURN	INT0990
C---- ERROR RETURN	INT1000
16 IFLAG=1	INT1010
GO TO 15	INT1020
END	INT1030-

```

SUBROUTINE TOLP(TDATA,QDATA,NTS,NQS,NMAX)
C----- THIS ROUTINE PLOTS THE DEPENDENT VARIABLE QDATA(.,.) AGAINST THE
C INDEPENDENT VARIABLE TDATA(.). NTS IS THE NUMBER OF SETS OF POINTS
C TO BE PLOTTED, NQS IS THE NUMBER OF COLUMNS OF QDATA(.,.) AND
C NMAX IS THE LENGTH OF EACH COLUMN OF QDATA. THE DATA ARE
C ASSUMED TO BE UNIFORMLY SPACED.
C NOTE..... NTS .LE. NMAX AND NQS .LE. 5.
C
INTEGER P(53),SYMBOL,SAVE(5)
C----- PLOT DATA
C COMMON /SYMB/SYMBOL(5)
C DIMENSION SYMBOL(5)
C----- INPUT/OUTPUT UNITS
COMMON /LUIO / LUIN,LUOUT
DIMENSION TDATA(NMAX),QDATA(NMAX,NQS)
DIMENSION RANG(5),QMIN(5),QMAX(5),RANGS(5),IWORDS(5)
DATA SYMBOL(1),SYMBOL(2),SYMBOL(3),SYMBOL(4),SYMBOL(5)
1/ 1HF ,1HB ,1HC ,1HD ,1HE /
DATA P( 1),P( 2),P( 3),P( 4),P( 5),P( 6),P( 7),P( 8),P( 9),P(10),
1 P(11),P(12),P(13),P(14),P(15),P(16),P(17),P(18),P(19),P(20),
2 P(21),P(22),P(23),P(24),P(25),P(26),P(27),P(28),P(29),P(30),
3 P(31),P(32),P(33),P(34),P(35),P(36),P(37),P(38),P(39),P(40),
4 P(41),P(42),P(43),P(44),P(45),P(46),P(47),P(48),P(49),P(50),
5 P(51),P(52),P(53)/ 1H*,1H ,1H ,1H ,1H ,1H ,1H,1H,1H ,1H ,
61H ,1H,1H ,1H ,1H ,1H ,1H,1H ,1H ,1H ,1H,1H ,1H ,1H ,1H ,
71H,1H ,1H ,1H ,1H ,1H,1H ,1H ,1H ,1H ,1H,1H ,1H ,1H ,1H,
81H ,1H ,1H ,1H ,1H,1H ,1H ,1H ,1H ,1H ,1H*/
C
99 FORMAT(1X13H SQRT(T) 53H*0****1****2****3****4****5****6****7*
1****8****9****10,6XA1,4(12XA1))
98 FORMAT(1PE13.5,1X,53A1,5E13.5)
97 FORMAT(14X53H*0****1****2****3****4****5****6****7****8****9****10
1)
96 FORMAT(60X7HMAXIMUM1P5E13.5)
95 FORMAT(60X7HMINIMUM1P5E13.5)
94 FORMAT(60X7HRANGE 1P5E13.5)
C
MSIZ=MIN0(NQS,5)
IF(MSIZ.LE.0) GO TO 6
NSIZ=NTS
IF(NSIZ.LE.0) GO TO 6
MSIZP1=MSIZ+1
DO 2 M=1,MSIZ
QMIN=1.E38
QMAX=-QMIN
DO 1 N=1,NSIZ
QMIN=AMIN1(QMIN,QDATA(N,M))
1 QMAX=AMAX1(QMAX,QDATA(N,M))
QMAXS(M)=QMAX
QMIN(5)=QMIN
RANGS(M)=QMAX-QMIN
2 RANG (M)=RANGS(M)/50.
WRITE (LUOUT,99) (SYMBOL(M),M=1,MSIZ)
DO 5 N=1,NSIZ
DO 3 M=1,MSIZ
RANGE=RANG(M)
IF(RANGE.EQ.0.) GO TO 3
QMIN=QMIN(5)
ICHAR=(QDATA(N,M)-QMIN)/RANGE+2.5
SAVE(M)=P(ICHAR)
IWORDS(M)=ICHAR

```

P(ICHAR)=SYMBOL(M)	TOL0610
3 CONTINUE	TOL0620
WRITE (LUOUT,98) TDATA(N),P,(QDATA(N,M),M=1,MSIZ)	TOL0630
M=MSIZP1	TOL0640
DO 4 MM=1,MSIZ	TOL0650
M=M-1	TOL0660
ICHAR=IWORDS(M)	TOL0670
4 P(ICHAR)=SAVE(M)	TOL0680
5 CONTINUE	TOL0690
WRITE (LUOUT,97)	TOL0700
WRITE (LUOUT,96) (QMAXS(M),M=1,MSIZ)	TOL0710
WRITE (LUOUT,95) (QMINS(M),M=1,MSIZ)	TOL0720
WRITE (LUOUT,94) (RANGS(M),M=1,MSIZ)	TOL0730
6 RETURN	TOL0740
END	TOL0750-

SUBROUTINE DIAG3(A,N,X)	DIA0000
C----- THIS ROUTINE SOLVES THE SYSTEM OF N LINEAR EQUATIONS WHERE THE	DIA0010
C COEFFICIENT MATRIX IS TRIDIAGONAL. THE EQUATIONS ARE DEFINED	DIA0020
C AS FOLLOWS	DIA0030
C A(1,2)*X(1) +A(1,3)*X(2) = A(1,4)	DIA0040
C A(I,1)*X(I-1) + A(I,2)*X(I) +A(I,3)*X(I+1) = A(I,4)	DIA0050
C FOR 1 .GT. I .LT. N	DIA0060
C A(N,1)*X(N-1) + A(N,2)*X(N) = A(N,4)	DIA0070
C PARAMETER NMAX=200,NMAXM1=NMAX-1	DIA0080
C DIMENSION A(NMAX,4),X(NMAX),G(NMAX),B(NMAXM1)	DIA0090
C DIMENSION A(202,4),X(202),G(202),B(201)	DIA0100
C----- DIAGONALIZATION PROCESS	DIA0110
W =A(1,2)	DIA0120
G(1)=A(1,4)/W	DIA0130
IF(N.LE.1) GO TO 4	DIA0140
DO 1 I=2,N	DIA0150
B(I-1)= A(I-1,3)/W	DIA0160
W = A(I,2)-A(I,1)*B(I-1)	DIA0170
G(I) =(A(I,4)-A(I,1)*G(I-1))/W	DIA0180
1 CONTINUE	DIA0190
C----- BACK SOLUTION	DIA0200
X(N)=G(N)	DIA0210
NP1=N+1	DIA0220
DO 2 I=2,N	DIA0230
J=NP1-I	DIA0240
X(J)=G(J)-B(J)*X(J+1)	DIA0250
2 CONTINUE	DIA0260
3 RETURN	DIA0270
4 X(1)=G(1)	DIA0280
GO TO 3	DIA0290
END	DIA0300-

APPENDIX B

PROBLEM DATA SET

TEST CASE I - TWO REGIONS		DATA SAVED FOR RESTART AT 1600 SECONDS.						IDENT
1.E-10	.001	1.E-4	1.E-7					R- 1
0.0001								R- 1.1
-1.	1.	.0020						R- 1.2
0.								R- 1.3
5.E-10	1.E-4	1.E-7	0.					R- 2
.0021								R- 2.1
-1.	1.	.01						R- 2.1.1
-1.	1.25	0.1						R- 2.2
0.								R- 2.3
	50.00	1600.	500.	100000.			1.	TIMES
0.	1.	1	0.	0		0.	0	INIT VAL
.002	1.	0	0.	0		0.	0	INIT VAL
.002000001	0.	0	0.	0		0.	0	INIT VAL
1.	0.	0	0.	0		0.	0	INIT VAL
-10.								END INIT
								STOPPER

TEST CASE I - TWO REGIONS		RESTARTED FROM DATA SAVED AT 1600 SECS.						IDENT
1.E-09	.001	1.E-4	1.E-7					R- 1
0.0001								R- 1.1
-1.	1.	.0020						R- 1.2
0.								R- 1.3
1.E-10	1.E-4	1.E-7	1.E-9					R- 2
.0021								R- 2.1
-1.	1.	.01						R- 2.1.1
-1.	1.25	0.1						R- 2.2
0.								R- 2.3
	50.00	2500.	500.	100000.	1600.			TIMES
								STOPPER

APPENDIX C

SOLUTION OF APPENDIX B. DATA

TEST CASE I • TWO REGIONS DATA SAVED FOR RESTART AT 1600 SECONDS, IDENT

J	NR	XR	D	K	K-PRIME	CAP K
1	20	2.0000E-03	1.0000E-10	1.0000E-03	1.0000E-04	1.0000E-07
2	104	1.0000E-01	5.0000E-10	1.0000E-04	1.0000E-07	0.

COMPUTATIONAL TIME STEP	5.0000E-01
MAXIMUM TIME	1.0000E+03
PRINT OUT TIME INTERVAL	5.0000E+02
EXTRAPOLATION TIME LIMIT	1.0000E+05
RESTART	-0.
SAVE	1.0000E+00

TEST CASE I - TWO REGIONS

DATA SAVED FOR RESTART AT 1600 SECONDS,

IDENT

TIME :

0,0000

RELEASE FRACTION = 0,000000

I	X	C	SMALL M	CAP M
1	0,0000000E+00	1,0000000E+00	0,0	0,0
2	1,0000000E+04	1,0000000E+00	0,0	0,0
3	2,0000000E+04	1,0000000E+00	0,0	0,0
4	3,0000000E+04	1,0000000E+00	0,0	0,0
5	4,0000000E+04	1,0000000E+00	0,0	0,0
6	5,0000000E+04	1,0000000E+00	0,0	0,0
7	6,0000000E+04	1,0000000E+00	0,0	0,0
8	7,0000000E+04	1,0000000E+00	0,0	0,0
9	8,0000000E+04	1,0000000E+00	0,0	0,0
10	9,0000000E+04	1,0000000E+00	0,0	0,0
11	1,0000000E+03	1,0000000E+00	0,0	0,0
12	1,1000000E+03	1,0000000E+00	0,0	0,0
13	1,2000000E+03	1,0000000E+00	0,0	0,0
14	1,3000000E+03	1,0000000E+00	0,0	0,0
15	1,4000000E+03	1,0000000E+00	0,0	0,0
16	1,5000000E+03	1,0000000E+00	0,0	0,0
17	1,6000000E+03	1,0000000E+00	0,0	0,0
18	1,7000000E+03	1,0000000E+00	0,0	0,0
19	1,8000000E+03	1,0000000E+00	0,0	0,0
20	1,9000000E+03	1,0000000E+00	0,0	0,0
21	2,0000000E+03	1,0000000E+00	0,0	0,0
21	2,0000000E+03	1,0000000E+00	0,0	0,0
22	2,1000000E+03	0,0	0,0	0,0
23	2,2000000E+03	0,0	0,0	0,0
24	2,3000000E+03	0,0	0,0	0,0
25	2,4000000E+03	0,0	0,0	0,0
26	2,5000000E+03	0,0	0,0	0,0
27	2,6000000E+03	0,0	0,0	0,0
28	2,7000000E+03	0,0	0,0	0,0
29	2,8000000E+03	0,0	0,0	0,0
30	2,9000000E+03	0,0	0,0	0,0
31	3,0000000E+03	0,0	0,0	0,0
32	3,1000000E+03	0,0	0,0	0,0
33	3,2000000E+03	0,0	0,0	0,0
34	3,3000000E+03	0,0	0,0	0,0
35	3,4000000E+03	0,0	0,0	0,0
36	3,5000000E+03	0,0	0,0	0,0
37	3,6000000E+03	0,0	0,0	0,0
38	3,7000000E+03	0,0	0,0	0,0
39	3,8000000E+03	0,0	0,0	0,0
40	3,9000000E+03	0,0	0,0	0,0
41	4,0000000E+03	0,0	0,0	0,0
42	4,1000000E+03	0,0	0,0	0,0
43	4,2000000E+03	0,0	0,0	0,0
44	4,3000000E+03	0,0	0,0	0,0
45	4,4000000E+03	0,0	0,0	0,0
46	4,5000000E+03	0,0	0,0	0,0
47	4,6000000E+03	0,0	0,0	0,0
48	4,7000000E+03	0,0	0,0	0,0
49	4,8000000E+03	0,0	0,0	0,0
50	4,9000000E+03	0,0	0,0	0,0
51	5,0000000E+03	0,0	0,0	0,0

TEST CASE I - TWO REGIONS

DATA SAVED FOR RESTART AT 1600 SECONDS,

IDENT

TIME = 0.0000

RELEASE FRACTION = 0.000000

I	X	C	SMALL M	CAP M
52	5.1000000E+03	0.	0.	0.
53	5.2000000E+03	0.	0.	0.
54	5.3000000E+03	0.	0.	0.
55	5.4000000E+03	0.	0.	0.
56	5.5000000E+03	0.	0.	0.
57	5.6000000E+03	0.	0.	0.
58	5.7000000E+03	0.	0.	0.
59	5.8000000E+03	0.	0.	0.
60	5.9000000E+03	0.	0.	0.
61	6.0000000E+03	0.	0.	0.
62	6.1000000E+03	0.	0.	0.
63	6.2000000E+03	0.	0.	0.
64	6.3000000E+03	0.	0.	0.
65	6.4000000E+03	0.	0.	0.
66	6.5000000E+03	0.	0.	0.
67	6.6000000E+03	0.	0.	0.
68	6.7000000E+03	0.	0.	0.
69	6.8000000E+03	0.	0.	0.
70	6.9000000E+03	0.	0.	0.
71	7.0000000E+03	0.	0.	0.
72	7.1000000E+03	0.	0.	0.
73	7.2000000E+03	0.	0.	0.
74	7.3000000E+03	0.	0.	0.
75	7.4000000E+03	0.	0.	0.
76	7.5000000E+03	0.	0.	0.
77	7.6000000E+03	0.	0.	0.
78	7.7000000E+03	0.	0.	0.
79	7.8000000E+03	0.	0.	0.
80	7.9000000E+03	0.	0.	0.
81	8.0000000E+03	0.	0.	0.
82	8.1000000E+03	0.	0.	0.
83	8.2000000E+03	0.	0.	0.
84	8.3000000E+03	0.	0.	0.
85	8.4000000E+03	0.	0.	0.
86	8.5000000E+03	0.	0.	0.
87	8.6000000E+03	0.	0.	0.
88	8.7000000E+03	0.	0.	0.
89	8.8000000E+03	0.	0.	0.
90	8.9000000E+03	0.	0.	0.
91	9.0000000E+03	0.	0.	0.
92	9.1000000E+03	0.	0.	0.
93	9.2000000E+03	0.	0.	0.
94	9.3000000E+03	0.	0.	0.
95	9.4000000E+03	0.	0.	0.
96	9.5000000E+03	0.	0.	0.
97	9.6000000E+03	0.	0.	0.
98	9.7000000E+03	0.	0.	0.
99	9.8000000E+03	0.	0.	0.
100	9.9000000E+03	0.	0.	0.
101	1.0000000E+02	0.	0.	0.
102	1.0100000E+02	0.	0.	0.
103	1.0225428E+02	0.	0.	0.
104	1.0382749E+02	0.	0.	0.

TEST CASE I - TWO REGIONS

DATA SAVED FOR RESTART AT 1600 SECONDS,

IDENT

TIME =

0.0000

RELEASE FRACTION =

0.000000

I	X	C	SMALL M	CAP M
105	1.0580073E+02	0.	0.	0.
106	1.0827572E+02	0.	0.	0.
107	1.1138005E+02	0.	0.	0.
108	1.1527373E+02	0.	0.	0.
109	1.2018749E+02	0.	0.	0.
110	1.2628308E+02	0.	0.	0.
111	1.3396626E+02	0.	0.	0.
112	1.4360310E+02	0.	0.	0.
113	1.5569037E+02	0.	0.	0.
114	1.7085115E+02	0.	0.	0.
115	1.8986697E+02	0.	0.	0.
116	2.1371808E+02	0.	0.	0.
117	2.4385348E+02	0.	0.	0.
118	2.8115680E+02	0.	0.	0.
119	3.2822081E+02	0.	0.	0.
120	3.8725212E+02	0.	0.	0.
121	4.6129373E+02	0.	0.	0.
122	5.5416242E+02	0.	0.	0.
123	6.7064549E+02	0.	0.	0.
124	8.1674753E+02	0.	0.	0.
125	1.0000000E+01	0.	0.	0.

INTEGRATION ERROR ESTIMATE TABLE

REGION ERROR ESTIMATE

1 0.

2 0.

RMS 0.

TEST CASE I - TWO REGIONS

DATA SAVED FOR RESTART AT 1600 SECONDS,

IDENT

TIMEI =

500,0000

RELEASE FRACTION =

.119544

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	1.5416838E+01	1.5566077E-01	1.7107865E+05
3	2.0000000E+04	2.9291953E+01	2.5599510E-01	2.7414193E+05
4	3.0000000E+04	4.0571042E+01	3.2364083E-01	3.3309943E+05
5	4.0000000E+04	4.8879639E+01	3.5493648E-01	3.6499538E+05
6	5.0000000E+04	5.4443327E+01	3.7094770E-01	3.8126767E+05
7	6.0000000E+04	5.7844280E+01	3.7865415E-01	3.8908187E+05
8	7.0000000E+04	5.9747048E+01	3.8213975E-01	3.9260962E+05
9	8.0000000E+04	6.0720512E+01	3.8361686E-01	3.9410232E+05
10	9.0000000E+04	6.1163890E+01	3.8419033E-01	3.9468116E+05
11	1.0000000E+03	6.1307718E+01	3.8435465E-01	3.9484688E+05
12	1.1000000E+03	6.1241377E+01	3.8426829E-01	3.9475972E+05
13	1.2000000E+03	6.0934077E+01	3.8385721E-01	3.9434472E+05
14	1.3000000E+03	6.0237630E+01	3.8277749E-01	3.9325346E+05
15	1.4000000E+03	5.8880515E+01	3.8023672E-01	3.9068156E+05
16	1.5000000E+03	5.6478730E+01	3.7465209E-01	3.8501775E+05
17	1.6000000E+03	5.2600936E+01	3.6312706E-01	3.7330179E+05
18	1.7000000E+03	4.6908669E+01	3.4076533E-01	3.5050325E+05
19	1.8000000E+03	3.9353816E+01	2.9990490E-01	3.0869341E+05
20	1.9000000E+03	3.0353536E+01	2.2940663E-01	2.3623097E+05
21	2.0000000E+03	2.0832438E+01	1.1411778E-01	1.1706509E+05
21	2.0000000E+03	2.0832438E+01	1.1706209E-02	0.
22	2.1000000E+03	1.8928219E+01	9.3229708E-03	0.
23	2.2000000E+03	1.6904892E+01	7.3369235E-03	0.
24	2.3000000E+03	1.4840517E+01	5.7036328E-03	0.
25	2.4000000E+03	1.2805952E+01	4.3785482E-03	0.
26	2.5000000E+03	1.0861455E+01	3.3183308E-03	0.
27	2.6000000E+03	9.0544431E+02	2.4819723E-03	0.
28	2.7000000E+03	7.4185216E+02	1.8316618E-03	0.
29	2.8000000E+03	5.9736257E+02	1.3333813E-03	0.
30	2.9000000E+03	4.7272499E+02	9.5723735E-04	0.
31	3.0000000E+03	3.6763322E+02	6.7755094E-04	0.
32	3.1000000E+03	2.8095929E+02	4.7274491E-04	0.
33	3.2000000E+03	2.1099987E+02	3.2507327E-04	0.
34	3.3000000E+03	1.5571101E+02	2.2025510E-04	0.
35	3.4000000E+03	1.1291275E+02	1.4701720E-04	0.
36	3.5000000E+03	8.0452755E+03	9.6655577E-05	0.
37	3.6000000E+03	5.6324791E+03	6.2577627E-05	0.
38	3.7000000E+03	3.8743918E+03	3.9889663E-05	0.
39	3.8000000E+03	2.6183910E+03	2.5030182E-05	0.
40	3.9000000E+03	1.7384831E+03	1.5457493E-05	0.
41	4.0000000E+03	1.1339257E+03	9.3926541E-06	0.
42	4.1000000E+03	7.2651374E+04	5.6144330E-06	0.
43	4.2000000E+03	4.5720123E+04	3.3004570E-06	0.
44	4.3000000E+03	2.8236921E+04	1.9074777E-06	0.
45	4.4000000E+03	1.7148801E+04	1.0834479E-06	0.
46	4.5000000E+03	1.0217782E+04	6.0455889E-07	0.
47	4.6000000E+03	5.9758153E+05	3.123341E-07	0.
48	4.7000000E+03	3.4295333E+05	1.7808604E-07	0.
49	4.8000000E+03	1.9307200E+05	9.3885143E-08	0.
50	4.9000000E+03	1.0657600E+05	4.8486232E-08	0.
51	5.0000000E+03	5.7651783E+06	2.4499396E-08	0.

TEST CASE I - TWO REGIONS

DATA SAVED FOR RESTART AT 1600 SECONDS,

IDENT

TIME:

1000.0000

RELEASE FRACTION =

.146341

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	7.1558101E+02	2.084267E-01	2.2359313E+05
3	2.0000000E+04	1.3904661E+01	3.5130109E-01	3.7320888E+05
4	3.0000000E+04	1.9941828E+01	4.4670122E-01	4.7386255E+05
5	4.0000000E+04	2.5075934E+01	5.0895895E-01	5.4113322E+05
6	5.0000000E+04	2.9228595E+01	5.4861989E-01	5.8238114E+05
7	6.0000000E+04	3.2418779E+01	5.7293346E-01	6.0771547E+05
8	7.0000000E+04	3.4734533E+01	5.8749732E-01	6.2276799E+05
9	8.0000000E+04	3.6298738E+01	5.9579102E-01	6.3131105E+05
10	9.0000000E+04	3.7233847E+01	6.0010021E-01	6.3573827E+05
11	1.0000000E+03	3.7646026E+01	6.0173850E-01	6.3741770E+05
12	1.1000000E+03	3.7589244E+01	6.0125949E-01	6.3692339E+05
13	1.2000000E+03	3.7080731E+01	5.9856477E-01	6.3415064E+05
14	1.3000000E+03	3.6097469E+01	5.9291096E-01	6.2832146E+05
15	1.4000000E+03	3.4594155E+01	5.8282304E-01	6.1788713E+05
16	1.5000000E+03	3.2527338E+01	5.692351E-01	6.0033388E+05
17	1.6000000E+03	2.9883867E+01	5.5386880E-01	5.7190948E+05
18	1.7000000E+03	2.6709353E+01	4.9613740E-01	5.2724181E+05
19	1.8000000E+03	2.3131175E+01	4.3147245E-01	4.5890286E+05
20	1.9000000E+03	1.9371468E+01	3.3564974E-01	3.5684682E+05
21	2.0000000E+03	1.5748523E+01	1.9688519E-01	2.0773009E+05
21	2.0000000E+03	1.5748523E+01	2.0771887E+02	0.
22	2.1000000E+03	1.5023934E+01	1.7789778E+02	0.
23	2.2000000E+03	1.4187824E+01	1.5143690E+02	0.
24	2.3000000E+03	1.3265036E+01	1.2841614E+02	0.
25	2.4000000E+03	1.2280804E+01	1.0770436E+02	0.
26	2.5000000E+03	1.1259402E+01	8.9963927E+01	0.
27	2.6000000E+03	1.0223885E+01	7.0655114E+01	0.
28	2.7000000E+03	9.1952113E+00	6.1540233E+01	0.
29	2.8000000E+03	8.1918055E+00	5.0387348E+01	0.
30	2.9000000E+03	7.2292270E+00	4.0973484E+01	0.
31	3.0000000E+03	6.3199927E+00	3.3087347E+01	0.
32	3.1000000E+03	5.4735482E+00	2.6851306E+01	0.
33	3.2000000E+03	4.6963515E+00	2.1122982E+01	0.
34	3.3000000E+03	3.9921097E+00	1.6696130E+01	0.
35	3.4000000E+03	3.3620403E+00	1.3101058E+01	0.
36	3.5000000E+03	2.8052388E+00	1.0204370E+01	0.
37	3.6000000E+03	2.3190370E+00	7.8898171E+00	0.
38	3.7000000E+03	1.8994323E+00	6.0540343E+00	0.
39	3.8000000E+03	1.5414260E+00	4.6105337E+00	0.
40	3.9000000E+03	1.2393927E+00	3.4845300E+00	0.
41	4.0000000E+03	9.8738628E+00	2.6133667E+00	0.
42	4.1000000E+03	7.7940200E+00	1.9449021E+00	0.
43	4.2000000E+03	6.0958839E+00	1.4362038E+00	0.
44	4.3000000E+03	4.7240793E+00	1.0522926E+00	0.
45	4.4000000E+03	3.6275029E+00	7.6496348E+00	0.
46	4.5000000E+03	2.7600281E+00	5.5171677E+00	0.
47	4.6000000E+03	2.0808450E+00	3.9477093E+00	0.
48	4.7000000E+03	1.5545052E+00	2.8023073E+00	0.
49	4.8000000E+03	1.1507393E+00	1.9734053E+00	0.
50	4.9000000E+03	8.4411301E+00	1.3785980E+00	0.
51	5.0000000E+03	6.1357838E+00	9.5535964E+00	0.

TEST CASE I - TWO REGIONS

DATA SAVED FOR RESTART AT 1600 SECONDS,

IDENT

TIME = 1500.0000

RELEASE FRACTION = .160124

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	4.1215819E+02	2.2487506E-01	2.5072847E+05
3	2.0000000E+04	8.0411031E+02	3.8561192E-01	4.2806853E+05
4	3.0000000E+04	1.1620392E+01	4.9903036E-01	5.5201517E+05
5	4.0000000E+04	1.4771382E+01	5.7792021E-01	6.3749076E+05
6	5.0000000E+04	1.7446441E+01	6.3190643E-01	6.9553612E+05
7	6.0000000E+04	1.9630063E+01	6.6813960E-01	7.3422553E+05
8	7.0000000E+04	2.1330562E+01	6.9181652E-01	7.5936590E+05
9	8.0000000E+04	2.2571553E+01	7.0664091E-01	7.7502607E+05
10	9.0000000E+04	2.3383957E+01	7.1510357E-01	7.8392968E+05
11	1.0000000E+03	2.3799041E-01	7.1873605E-01	7.8773546E+05
12	1.1000000E+03	2.3843860E+01	7.1826357E-01	7.8722177E+05
13	1.2000000E+03	2.3539725E+01	7.1369240E-01	7.8238616E+05
14	1.3000000E+03	2.2903485E+01	7.0433242E-01	7.7286735E+05
15	1.4000000E+03	2.1951789E+01	6.8875873E-01	7.5589299E+05
16	1.5000000E+03	2.0707480E+01	6.6471394E-01	7.3015384E+05
17	1.6000000E+03	1.9207090E+01	6.3895173E-01	6.9160085E+05
18	1.7000000E+03	1.7509136E+01	5.9770191E-01	6.3515703E+05
19	1.8000000E+03	1.5701635E+01	5.0297289E-01	5.5393062E+05
20	1.9000000E+03	1.3909871E+01	3.9902052E-01	4.3870867E+05
21	2.0000000E+03	1.2304633E+01	2.5507626E-01	2.7730303E+05
21	2.0000000E+03	1.2304633E+01	2.7727961E-02	0.
22	2.1000000E+03	1.1983585E+01	2.4900220E-02	0.
23	2.2000000E+03	1.1583848E+01	2.1561098E-02	0.
24	2.3000000E+03	1.1115561E+01	1.8896728E-02	0.
25	2.4000000E+03	1.0589573E+01	1.6492423E-02	0.
26	2.5000000E+03	1.0017124E+01	1.4332859E-02	0.
27	2.6000000E+03	9.4095293E+02	1.2402273E-02	0.
28	2.7000000E+03	3.7775948E+02	1.0684655E-02	0.
29	2.8000000E+03	3.1328582E+02	9.1639420E-03	0.
30	2.9000000E+03	7.4843667E+02	7.8241945E-03	0.
31	3.0000000E+03	6.8414967E+02	6.6497662E-03	0.
32	3.1000000E+03	6.2123155E+02	5.6254534E-03	0.
33	3.2000000E+03	5.6037876E+02	4.7366260E-03	0.
34	3.3000000E+03	5.0217231E+02	3.9693377E-03	0.
35	3.4000000E+03	4.4707660E+02	3.3104142E-03	0.
36	3.5000000E+03	3.9544183E+02	2.7475200E-03	0.
37	3.6000000E+03	3.4780949E+02	2.2692034E-03	0.
38	3.7000000E+03	3.0342035E+02	1.8649224E-03	0.
39	3.8000000E+03	2.6322443E+02	1.5250514E-03	0.
40	3.9000000E+03	2.2689224E+02	1.2408723E-03	0.
41	4.0000000E+03	1.9432681E+02	1.0045508E-03	0.
42	4.1000000E+03	1.6537597E+02	8.0910164E-04	0.
43	4.2000000E+03	1.3994440E+02	6.4834423E-04	0.
44	4.3000000E+03	1.1750509E+02	5.1685105E-04	0.
45	4.4000000E+03	9.8109857E+03	4.0989133E-04	0.
46	4.5000000E+03	8.1398833E+03	3.2337292E-04	0.
47	4.6000000E+03	6.7108603E+03	2.5378016E-04	0.
48	4.7000000E+03	5.4979076E+03	1.9811615E-04	0.
49	4.8000000E+03	4.4759011E+03	1.5384379E-04	0.
50	4.9000000E+03	3.6210278E+03	1.1883060E-04	0.
51	5.0000000E+03	2.9110928E+03	9.1296885E-05	0.

TEST CASE I - TWO REGIONS

DATA SAVED FOR RESTART AT 1600 SECONDS,

IDENTY

TIME =

1600.0000

RELEASE FRACTION =

.162116

I	X	C	SMALL M	CAP. M
1	0.	0.	0.	0.
2	1.0000000E+04	3.7606382E+02	2.2655530E+01	2.5466610E+05
3	2.0000000E+04	7.3370689E+02	3.8941869E+01	4.3575092E+05
4	3.0000000E+04	1.0606243E+01	5.0511283E+01	5.6511903E+05
5	4.0000000E+04	1.3490946E+01	5.8621820E+01	6.5161030E+05
6	5.0000000E+04	1.5949325E+01	6.4221953E+01	7.1222085E+05
7	6.0000000E+04	1.7966698E+01	6.8017720E+01	7.5500960E+05
8	7.0000000E+04	1.9548224E+01	7.0525477E+01	7.7979070E+05
9	8.0000000E+04	2.0711965E+01	7.2112784E+01	7.9665310E+05
10	9.0000000E+04	2.1482539E+01	7.3029385E+01	8.0634822E+05
11	1.0000000E+03	2.1855904E+01	7.3429785E+01	8.1056332E+05
12	1.1000000E+03	2.1945900E+01	7.3388197E+01	8.1010218E+05
13	1.2000000E+03	2.1682971E+01	7.2907438E+01	8.0498328E+05
14	1.3000000E+03	2.1115254E+01	7.1920841E+01	7.9446275E+05
15	1.4000000E+03	2.0261838E+01	7.0289269E+01	7.7608636E+05
16	1.5000000E+03	1.9147728E+01	6.7791473E+01	7.5006884E+05
17	1.6000000E+03	1.7809939E+01	6.4109771E+01	7.1009602E+05
18	1.7000000E+03	1.6304127E+01	5.8808980E+01	6.5205401E+05
19	1.8000000E+03	1.4711498E+01	5.1309091E+01	5.6412964E+05
20	1.9000000E+03	1.3146173E+01	4.0850523E+01	4.5223158E+05
21	2.0000000E+03	1.1763839E+01	2.6450957E+01	2.8933466E+05
21	2.0000000E+03	1.1763889E+01	2.5930841E+02	0.
22	2.1000000E+03	1.1487432E+01	2.5673307E+02	0.
23	2.2000000E+03	1.1138083E+01	2.5696813E+02	0.
24	2.3000000E+03	1.0724400E+01	1.9988425E+02	0.
25	2.4000000E+03	1.0255647E+01	1.7534459E+02	0.
26	2.5000000E+03	9.7415229E+02	1.5320637E+02	0.
27	2.6000000E+03	9.1918978E+02	1.3332254E+02	0.
28	2.7000000E+03	8.6165635E+02	1.1554345E+02	0.
29	2.8000000E+03	8.0250066E+02	9.0718510E+01	0.
30	2.9000000E+03	7.4262106E+02	8.5697799E+01	0.
31	3.0000000E+03	6.8284890E+02	7.3333943E+01	0.
32	3.1000000E+03	6.2393527E+02	6.2481497E+01	0.
33	3.2000000E+03	5.6634137E+02	5.3002152E+01	0.
34	3.3000000E+03	5.1123231E+02	4.4761784E+01	0.
35	3.4000000E+03	4.5847433E+02	3.7633309E+01	0.
36	3.5000000E+03	4.0868505E+02	3.1496971E+01	0.
37	3.6000000E+03	3.6198650E+02	2.6240830E+01	0.
38	3.7000000E+03	3.1871049E+02	2.1761090E+01	0.
39	3.8000000E+03	2.7890574E+02	1.7962248E+01	0.
40	3.9000000E+03	2.4239653E+02	1.4757104E+01	0.
41	4.0000000E+03	2.0974221E+02	1.2066656E+01	0.
42	4.1000000E+03	1.8024720E+02	9.8197616E+00	0.
43	4.2000000E+03	1.5397116E+02	7.9530005E+00	0.
44	4.3000000E+03	1.3073882E+02	6.4100713E+00	0.
45	4.4000000E+03	1.1034934E+02	5.1414265E+00	0.
46	4.5000000E+03	9.2584935E+01	4.1037527E+00	0.
47	4.6000000E+03	7.7218486E+01	3.2894478E+00	0.
48	4.7000000E+03	6.4020284E+01	2.5760920E+00	0.
49	4.8000000E+03	5.2763436E+01	2.0259237E+00	0.
50	4.9000000E+03	4.3228805E+01	1.5853299E+00	0.
51	5.0000000E+03	3.5208028E+01	1.2343612E+00	0.

TEST CASE I - TWO REGIONS DATA SAVED FOR RESTART AT 1600 SECONDS, IDENT

TIME = 1600.0000 RELEASE FRACTION = .162116

I	X	C	SMALL M	CAP M
52	5.1000000E+03	2.8506436E+03	9.5627467E-05	0.
53	5.2000000E+03	2.2944634E+03	7.3711162E-05	0.
54	5.3000000E+03	1.8359489E+03	5.6531056E-05	0.
55	5.4000000E+03	1.4604463E+03	4.3135793E-05	0.
56	5.5000000E+03	1.1549428E+03	3.2747607E-05	0.
57	5.6000000E+03	9.0800820E+02	2.4734735E-05	0.
58	5.7000000E+03	7.0970524E+02	1.8507298E-05	0.
59	5.8000000E+03	5.5148024E+02	1.3896408E-05	0.
60	5.9000000E+03	4.2604010E+02	1.0336243E-05	0.
61	6.0000000E+03	3.2722365E+02	7.6488094E-06	0.
62	6.1000000E+03	2.4987214E+02	5.6311053E-06	0.
63	6.2000000E+03	1.8970353E+02	4.1243963E-06	0.
64	6.3000000E+03	1.4319346E+02	3.0053348E-06	0.
65	6.4000000E+03	1.0746501E+02	2.1786647E-06	0.
66	6.5000000E+03	8.0188727E+01	1.5712775E-06	0.
67	6.6000000E+03	5.9493351E+01	1.1274071E-06	0.
68	6.7000000E+03	4.3887331E+01	8.0477601E-07	0.
69	6.8000000E+03	3.2190861E+01	5.7152746E-07	0.
70	6.9000000E+03	2.3477727E+01	4.0380252E-07	0.
71	7.0000000E+03	1.7026179E+01	2.8383982E-07	0.
72	7.1000000E+03	1.2277898E+01	1.9849658E-07	0.
73	7.2000000E+03	8.8040970E+00	1.3810573E-07	0.
74	7.3000000E+03	6.2778100E+00	9.5599010E-08	0.
75	7.4000000E+03	4.4514655E+00	6.5838911E-08	0.
76	7.5000000E+03	3.1389093E+00	4.5113287E-08	0.
77	7.6000000E+03	2.2011245E+00	3.0755616E-08	0.
78	7.7000000E+03	1.5350089E+00	2.0861642E-08	0.
79	7.8000000E+03	1.0646032E+00	1.4079367E-08	0.
80	7.9000000E+03	7.3432674E-01	9.4544285E-09	0.
81	8.0000000E+03	5.0375106E-01	6.3170213E-09	0.
82	8.1000000E+03	3.4370795E-01	4.1997374E-09	0.
83	8.2000000E+03	2.3324816E-01	2.7782605E-09	0.
84	8.3000000E+03	1.5743957E-01	1.8288308E-09	0.
85	8.4000000E+03	1.0570337E-01	1.1979342E-09	0.
86	8.5000000E+03	7.0592039E-02	7.8083774E-10	0.
87	8.6000000E+03	4.6895099E-02	5.0648551E-10	0.
88	8.7000000E+03	3.0989695E-02	3.2693542E-10	0.
89	8.8000000E+03	2.0372243E-02	2.1001793E-10	0.
90	8.9000000E+03	1.3323119E-02	1.3426454E-10	0.
91	9.0000000E+03	8.6682756E-03	8.5425649E-11	0.
92	9.1000000E+03	5.6109136E-03	5.4093986E-11	0.
93	9.2000000E+03	3.6134585E-03	3.4092230E-11	0.
94	9.3000000E+03	2.3153444E-03	2.1385505E-11	0.
95	9.4000000E+03	1.4761309E-03	1.3352198E-11	0.
96	9.5000000E+03	9.3640193E-04	8.2978296E-12	0.
97	9.6000000E+03	5.9106166E-04	5.1328442E-12	0.
98	9.7000000E+03	3.7121361E-04	3.1602374E-12	0.
99	9.8000000E+03	2.3194085E-04	1.9363719E-12	0.
100	9.9000000E+03	1.4411651E-04	1.1802570E-12	0.
101	1.0000000E+02	8.8948017E-05	7.1473321E-13	0.
102	1.0100000E+02	5.4362990E-05	4.2853349E-13	0.
103	1.0225428E+02	2.9149177E-05	2.2448091E-13	0.
104	1.0382749E+02	1.3246713E-05	9.9202364E-14	0.

TEST CASE I - TWO REGIONS DATA SAVED FOR RESTART AT 1600 SECONDS, IDENT

TIME: 1600.0000 RELEASE FRACTION = .162116

I	X	C	SMALL M	CAP M
105	1.0580073E+02	4.8931646E+12	3.5462324E+14	0.
106	1.0827572E+02	1.4000888E+12	9.7756797E+13	0.
107	1.1138005E+02	2.9478833E+13	1.9759772E+13	0.
108	1.1527373E+02	4.3473729E+14	2.7918391E+16	0.
109	1.2015749E+02	4.3032464E+15	2.6475926E+17	0.
110	1.2628308E+02	2.7725524E+16	1.6341051E+18	0.
111	1.3396626E+02	1.1337200E+17	6.8239540E+20	0.
112	1.4360310E+02	2.9181607E+19	1.5883310E+21	0.
113	1.5569037E+02	4.6650831E+21	2.4480032E+23	0.
114	1.7085115E+02	4.6201241E+23	2.3424058E+25	0.
115	1.8986607E+02	2.8291487E+25	1.3886629E+27	0.
116	2.1371808E+02	1.0706323E+27	3.0970134E+30	0.
117	2.4363398E+02	2.5045283E+30	1.1583991E+32	0.
118	2.8115680E+02	3.6241985E+33	1.6309693E+35	0.
119	3.2822081E+02	3.2469898E+36	1.4235968E+38	0.
120	3.8725212E+02	1.8027714E+39	7.7093950E+42	0.
121	4.6129373E+02	6.2085621E+43	2.5922699E+45	0.
122	5.5416242E+02	1.3274034E+46	5.24159802E+49	0.
123	6.7064549E+02	1.7632530E+50	7.0353285E+53	0.
124	8.1674753E+02	1.4561660E+54	3.6849986E+57	0.
125	1.0000000E+01	0.	0.	0.

INTEGRATION ERROR ESTIMATE TABLE

REGION ERROR ESTIMATE

1 = 3.5264367E+08
2 = 1.0614055E+10

RMS 2.4933665E+08

THE ABOVE CONCENTRATION DISTRIBUTIONS HAVE BEEN SAVED FOR RESTARTING.

TEST CASE I - TWO REGIONS DATA SAVED FOR RESTART AT 1600 SECONDS, IDENT
TIME HISTORY OF RELEASE FRACTION

SORT(T)	707777177772777377747775777677777778777977710	F
0.07107E+00	7	0.503687E+02
1.00000E+01	7	6.56484E+02
1.22474E+01	7	7.69012E+02
1.41421E+01	7	8.59175E+02
1.58114E+01	7	9.34782E+02
1.73205E+01	7	1.00006E+01
1.87083E+01	7	1.05739E+01
2.00000E+01	7	1.10836E+01
2.12132E+01	7	1.15409E+01
2.23007E+01	7	1.19544E+01
2.34521E+01	7	1.23303E+01
2.44949E+01	7	1.26739E+01
2.54951E+01	7	1.29892E+01
2.64575E+01	7	1.32797E+01
2.73861E+01	7	1.35484E+01
2.82843E+01	7	1.37975E+01
2.91548E+01	7	1.40289E+01
3.00000E+01	7	1.42445E+01
3.08221E+01	7	1.44457E+01
3.16228E+01	7	1.46341E+01
3.24037E+01	7	1.48107E+01
3.31662E+01	7	1.49766E+01
3.39116E+01	7	1.51327E+01
3.46410E+01	7	1.52799E+01
3.53553E+01	7	1.54189E+01
3.60555E+01	7	1.55504E+01
3.67423E+01	7	1.56750E+01
3.74166E+01	7	1.57932E+01
3.80789E+01	7	1.59055E+01
3.87298E+01	7	1.60124E+01
3.93700E+01	7	1.61143E+01
4.00000E+01	7	1.62116E+01
707777177772777377747775777677777778777977710		MAXIMUM 1.62116E+01
		MINIMUM 0.
		RANGE 1.62116E+01

TEST CASE I - TWO REGIONS RESTARTED FROM DATA SAVED AT 1600 SECS. IDENT

J	NR	KR	D	K	K+PRIME	CAP K
1	20	2.0000E+03	1.0000E-09	1.0000E-03	1.0000E+04	1.0000E+07
2	104	1.0000E-01	1.0000E-10	1.0000E-04	1.0000E+07	1.0000E+09

RESTART DATA TITLE IS., TEST CASE I - TWO REGIONS. DATA SAVED FOR RESTART.

COMPUTATIONAL TIME STEP	5.0000E+01
MAXIMUM TIME	2.5000E+03
PRINT OUT TIME INTERVAL	5.0000E+02
EXTRAPOLATION TIME LIMIT	1.0000E+05
RESTART	1.6000E+03
SAVE	0.

AT 1600 SECONDS, IDENT

TEST CASE I - TWO REGIONS

RESTARTED FROM DATA SAVED AT 1500 SECS,

IDENT

TIME =

0.0000

RELEASE FRACTION = 0.000000

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	3.7606382E+02	2.2655530E+01	2.5466610E+05
3	2.0000000E+04	7.3370689E+02	3.8941869E+01	4.3575092E+05
4	3.0000000E+04	1.0606243E+01	5.0511283E+01	5.6311903E+05
5	4.0000000E+04	1.3490946E+01	5.8621820E+01	6.5161030E+05
6	5.0000000E+04	1.5949325E+01	6.4221953E+01	7.1222085E+05
7	6.0000000E+04	1.7966698E+01	6.8017720E+01	7.5300980E+05
8	7.0000000E+04	1.9548224E+01	7.0525477E+01	7.7979070E+05
9	8.0000000E+04	2.0711965E+01	7.2112784E+01	7.9665310E+05
10	9.0000000E+04	2.1482539E+01	7.3029385E+01	8.0634822E+05
11	1.0000000E+03	2.1885904E+01	7.3429745E+01	8.1056332E+05
12	1.1000000E+03	2.1945900E+01	7.3388197E+01	8.1010218E+05
13	1.2000000E+03	2.1682971E+01	7.2907438E+01	8.0498324E+05
14	1.3000000E+03	2.1115254E+01	7.1920891E+01	7.9446275E+05
15	1.4000000E+03	2.0261838E+01	7.0289269E+01	7.7698636E+05
16	1.5000000E+03	1.9147728E+01	6.7791473E+01	7.5006884E+05
17	1.6000000E+03	1.7809939E+01	6.4109771E+01	7.1009802E+05
18	1.7000000E+03	1.6304127E+01	5.8808980E+01	6.5205401E+05
19	1.8000000E+03	1.4711498E+01	5.1309091E+01	5.6912964E+05
20	1.9000000E+03	1.3146173E+01	4.0850523E+01	4.5223154E+05
21	2.0000000E+03	1.1763899E+01	2.6450957E+01	2.8933466E+05
21	2.0000000E+03	1.1763889E+01	2.8930841E+02	0.
22	2.1000000E+03	1.1487432E+01	2.5673307E+02	0.
23	2.2000000E+03	1.1135093E+01	2.2696813E+02	0.
24	2.3000000E+03	1.0724400E+01	1.9988425E+02	0.
25	2.4000000E+03	1.0255647E+01	1.7534459E+02	0.
26	2.5000000E+03	9.7415229E+02	1.5320637E+02	0.
27	2.6000000E+03	9.1918978E+02	1.3332254E+02	0.
28	2.7000000E+03	8.6165635E+02	1.1554345E+02	0.
29	2.8000000E+03	8.0250066E+02	9.9718510E+03	0.
30	2.9000000E+03	7.4262106E+02	8.5697749E+03	0.
31	3.0000000E+03	6.8284890E+02	7.333543E+03	0.
32	3.1000000E+03	6.2393527E+02	6.2481497E+03	0.
33	3.2000000E+03	5.6654137E+02	5.3002152E+03	0.
34	3.3000000E+03	5.1123231E+02	4.4761784E+03	0.
35	3.4000000E+03	4.5847433E+02	3.7633309E+03	0.
36	3.5000000E+03	4.0863505E+02	3.1496971E+03	0.
37	3.6000000E+03	3.6198650E+02	2.6240830E+03	0.
38	3.7000000E+03	3.1871049E+02	2.1761090E+03	0.
39	3.8000000E+03	2.7890574E+02	1.7962248E+03	0.
40	3.9000000E+03	2.4259653E+02	1.4757104E+03	0.
41	4.0000000E+03	2.0974221E+02	1.2066636E+03	0.
42	4.1000000E+03	1.8024720E+02	9.8197616E+04	0.
43	4.2000000E+03	1.5397116E+02	7.9530005E+04	0.
44	4.3000000E+03	1.3073882E+02	6.4100713E+04	0.
45	4.4000000E+03	1.1034934E+02	5.1414265E+04	0.
46	4.5000000E+03	9.2584935E+03	4.1037527E+04	0.
47	4.6000000E+03	7.7218486E+03	3.2594478E+04	0.
48	4.7000000E+03	6.4020254E+03	2.5760920E+04	0.
49	4.8000000E+03	5.2763456E+03	2.0259237E+04	0.
50	4.9000000E+03	4.3228805E+03	1.5853299E+04	0.
51	5.0000000E+03	3.5208028E+03	1.2343612E+04	0.

TEST CASE I - TWO REGIONS RESTARTED FROM DATA SAVED AT 1600 SECS, IDENT

TIME = 0.0000 RELEASE FRACTION = 0.000000

I	X	C	SMALL M	CAP M
105	1.0580073E+02	4.8931646E+12	3.3962524E+14	0.
106	1.0827572E+02	1.4000888E+12	9.7756797E+15	0.
107	1.1138005E+02	2.9478833E+13	1.9759772E+15	0.
108	1.1527373E+02	4.3473729E+14	2.7918391E+16	0.
109	1.2015749E+02	4.3052464E+15	2.6475926E+17	0.
110	1.2628308E+02	2.7725524E+16	1.6341051E+18	0.
111	1.3396626E+02	1.1357209E+17	6.4259340E+20	0.
112	1.4360310E+02	2.9181607E+19	1.5883310E+21	0.
113	1.5569037E+02	4.6650831E+21	2.4480032E+23	0.
114	1.7085115E+02	4.6201241E+23	2.3424058E+25	0.
115	1.9986697E+02	2.8291487E+25	1.3886629E+27	0.
116	2.1371808E+02	1.0700323E+27	5.0970134E+30	0.
117	2.4363398E+02	2.5045283E+30	1.1583991E+32	0.
118	2.8115680E+02	3.6241985E+33	1.8309693E+35	0.
119	3.2822081E+02	3.2469898E+36	1.4235968E+38	0.
120	3.8725212E+02	1.8027714E+39	7.7093950E+42	0.
121	4.6129373E+02	6.2085621E+43	2.5922699E+45	0.
122	5.5416242E+02	1.3274094E+46	5.4159802E+49	0.
123	6.7064549E+02	1.7632550E+50	7.0353285E+53	0.
124	8.1674753E+02	1.4561660E+54	5.6849986E+57	0.
125	1.0000000E+01	0.	0.	0.

INTEGRATION ERROR ESTIMATE TABLE

REGION ERROR ESTIMATE

1 = 3.5261367E+08
2 = 1.0614055E+10

RMS 2.4933665E+08

TEST CASE I - TWO REGIONS

RESTARTED FROM DATA SAVED AT 1500 SECS.

IDENT

TIME = 500,0000

RELEASE FRACTION = ,058281

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	1.2255310E+02	2.2526634E-01	2.6471834E+05
3	2.0000000E+04	2.4260047E+02	3.8968912E-01	4.5558901E+05
4	3.0000000E+04	3.5825293E+02	5.0877032E-01	5.9225459E+05
5	4.0000000E+04	4.6809279E+02	5.9430315E-01	6.8937756E+05
6	5.0000000E+04	5.7107228E+02	6.5518568E-01	7.5781972E+05
7	6.0000000E+04	6.6643551E+02	6.9803679E-01	8.0554612E+05
8	7.0000000E+04	7.5366566E+02	7.2771443E-01	8.3831289E+05
9	8.0000000E+04	8.3244458E+02	7.4769060E-01	8.6018466E+05
10	9.0000000E+04	9.0262366E+02	7.6034409E-01	8.7391608E+05
11	1.0000000E+03	9.6420117E+02	7.6717115E-01	8.8122243E+05
12	1.1000000E+03	1.0173045E+01	7.6892602E-01	8.8295695E+05
13	1.2000000E+03	1.0621767E+01	7.6570264E-01	8.7920690E+05
14	1.3000000E+03	1.0991643E+01	7.5695006E-01	8.6931555E+05
15	1.4000000E+03	1.1287096E+01	7.4144532E-01	8.5183341E+05
16	1.5000000E+03	1.1513603E+01	7.1720409E-01	8.2439828E+05
17	1.6000000E+03	1.1677399E+01	6.8134054E-01	7.8353940E+05
18	1.7000000E+03	1.1786328E+01	6.2986910E-01	7.2439658E+05
19	1.8000000E+03	1.1849034E+01	5.5744294E-01	6.4033948E+05
20	1.9000000E+03	1.1876744E+01	4.5702084E-01	5.2246600E+05
21	2.0000000E+03	1.1882661E+01	3.1945205E-01	3.5895202E+05
21	2.0000000E+03	1.1882661E+01	3.5890950E-02	6.9617359E+08
22	2.1000000E+03	1.1941829E+01	3.2016501E-02	6.3446364E+08
23	2.2000000E+03	1.1508066E+01	2.8531943E-02	5.8364092E+08
24	2.3000000E+03	1.0846205E+01	2.5410823E-02	5.4235322E+08
25	2.4000000E+03	1.0129255E+01	2.2610516E-02	5.0770603E+08
26	2.5000000E+03	9.4400957E+02	2.0088462E-02	4.7687102E+08
27	2.6000000E+03	8.8003930E+02	1.7809371E-02	4.4778961E+08
28	2.7000000E+03	8.2025292E+02	1.5746365E-02	4.1927032E+08
29	2.8000000E+03	7.6317862E+02	1.3879281E-02	3.9080273E+08
30	2.9000000E+03	7.0769292E+02	1.2192364E-02	3.6231042E+08
31	3.0000000E+03	6.5327525E+02	1.0672383E-02	3.3394790E+08
32	3.1000000E+03	5.9989199E+02	9.3074311E-03	3.0596709E+08
33	3.2000000E+03	5.4779192E+02	8.0862926E-03	2.7864124E+08
34	3.3000000E+03	4.9734029E+02	6.9981568E-03	2.5222656E+08
35	3.4000000E+03	4.4891402E+02	6.0325325E-03	2.2694467E+08
36	3.5000000E+03	4.0284857E+02	5.1792486E-03	2.0297549E+08
37	3.6000000E+03	3.5941471E+02	4.4264889E-03	1.8045822E+08
38	3.7000000E+03	3.1881171E+02	3.7708373E-03	1.5948770E+08
39	3.8000000E+03	2.8116840E+02	3.1973204E-03	1.4012204E+08
40	3.9000000E+03	2.4654804E+02	2.6994437E-03	1.2238376E+08
41	4.0000000E+03	2.1475507E+02	2.2692207E-03	1.0686438E+08
42	4.1000000E+03	1.8634275E+02	1.8991928E-03	9.1728851E+07
43	4.2000000E+03	1.6062123E+02	1.5824418E-03	7.8720101E+07
44	4.3000000E+03	1.3766559E+02	1.3125935E-03	6.7163508E+07
45	4.4000000E+03	1.1732370E+02	1.0838147E-03	5.6971186E+07
46	4.5000000E+03	9.9423559E+01	8.9080265E-04	4.8045976E+07
47	4.6000000E+03	8.3780234E+01	7.2876920E-04	4.0285065E+07
48	4.7000000E+03	7.0201597E+01	5.9341962E-04	3.3583156E+07
49	4.8000000E+03	5.8493831E+01	4.8092735E-04	2.7855195E+07
50	4.9000000E+03	4.8465791E+01	3.8796553E-04	2.2938609E+07
51	5.0000000E+03	3.9932528E+01	3.1137631E-04	1.8795096E+07

TEST CASE I - TWO REGIONS

RESTARTED FROM DATA SAVED AT 1600 SECS,

IDENT

TIMEI =

1000,0000

RELEASE FRACTION =

,088512

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	8.1573046E-03	2.1905317E-01	2.6462008E+05
3	2.0000000E+04	1.6132767E-02	3.8012971E-01	4.6528958E+05
4	3.0000000E+04	2.3801206E-02	4.9790376E-01	6.0657673E+05
5	4.0000000E+04	3.1078784E-02	5.8394460E-01	7.0809258E+05
6	5.0000000E+04	3.7911267E-02	6.4547562E-01	7.8066273E+05
7	6.0000000E+04	4.4265599E-02	6.997913E-01	8.3222808E+05
8	7.0000000E+04	5.0123493E-02	7.464735E-01	8.6852948E+05
9	8.0000000E+04	5.5477016E-02	7.8378653E-01	8.9362271E+05
10	9.0000000E+04	6.0325400E-02	7.5865193E-01	9.1025896E+05
11	1.0000000E+03	6.4672974E-02	7.6766727E-01	9.2015368E+05
12	1.1000000E+03	6.8527951E-02	7.7155425E-01	9.2416480E+05
13	1.2000000E+03	7.1901838E-02	7.7040711E-01	9.2258485E+05
14	1.3000000E+03	7.4809340E-02	7.6371283E-01	9.1416782E+05
15	1.4000000E+03	7.7269930E-02	7.5031986E-01	8.9807661E+05
16	1.5000000E+03	7.9306486E-02	7.2835636E-01	8.7176519E+05
17	1.6000000E+03	8.0952944E-02	6.9509719E-01	8.3178329E+05
18	1.7000000E+03	8.2247740E-02	6.4677657E-01	7.7329686E+05
19	1.8000000E+03	8.3250908E-02	5.7834113E-01	6.8970911E+05
20	1.9000000E+03	8.4034609E-02	4.8313558E-01	5.7216163E+05
21	2.0000000E+03	8.4703662E-02	3.3251123E-01	4.0888751E+05
22	2.1000000E+03	8.51394197E-02	4.0882573E-02	1.1935285E+07
23	2.2000000E+03	9.1441645E-02	3.7248176E-02	1.1578048E+07
24	2.3000000E+03	9.4451722E-02	3.3775732E-02	1.1081760E+07
25	2.4000000E+03	9.2191316E-02	3.0512761E-02	1.0526871E+07
26	2.5000000E+03	8.8409133E-02	2.7481504E-02	9.9495028E+06
27	2.6000000E+03	8.3726051E-02	2.4686186E-02	9.3675547E+06
28	2.7000000E+03	7.8594137E-02	2.2119878E-02	8.7894021E+06
29	2.8000000E+03	7.3305975E-02	1.9769970E-02	8.2171973E+06
30	2.9000000E+03	6.8030576E-02	1.7621900E-02	7.6514346E+06
31	3.0000000E+03	6.2855669E-02	1.5661295E-02	7.0927323E+06
32	3.1000000E+03	5.7823805E-02	1.3874920E-02	6.5426505E+06
33	3.2000000E+03	5.2957265E-02	1.2250874E-02	6.0036528E+06
34	3.3000000E+03	4.8272068E-02	1.0778414E-02	5.4790057E+06
35	3.4000000E+03	4.3783895E-02	9.4476522E-03	4.9721725E+06
36	3.5000000E+03	3.9509210E-02	8.2492713E-03	4.4865828E+06
37	3.6000000E+03	3.5464196E-02	7.1743174E-03	4.0251377E+06
38	3.7000000E+03	3.1663146E-02	6.2140767E-03	3.5904362E+06
39	3.8000000E+03	2.8117136E-02	5.3600224E-03	3.1842904E+06
40	3.9000000E+03	2.4853223E-02	4.6038100E-03	2.8079051E+06
41	4.0000000E+03	2.1814179E-02	3.9373017E-03	2.4618618E+06
42	4.1000000E+03	1.9058596E-02	3.3526001E-03	2.1461698E+06
43	4.2000000E+03	1.6561270E-02	2.8421231E-03	1.8603373E+06
44	4.3000000E+03	1.4313711E-02	2.3985865E-03	1.6034482E+06
45	4.4000000E+03	1.2304732E-02	2.0151030E-03	1.3742277E+06
46	4.5000000E+03	1.0521038E-02	1.6851833E-03	1.1711495E+06
47	4.6000000E+03	8.9478081E-03	1.4027656E-03	9.9247989E+05
48	4.7000000E+03	7.5692203E-03	1.1622311E-03	8.3635970E+05
49	4.8000000E+03	6.3689315E-03	9.5841143E-04	7.0086206E+05
50	4.9000000E+03	5.3304917E-03	7.8658827E-04	5.8404448E+05
51	5.0000000E+03	4.4376937E-03	6.4248651E-04	4.8599272E+05

TEST CASE 1 - TWO REGIONS

RESTARTED FROM DATA SAVED AT 1600 SECS,

IDENT

TIME:

1500.0000

RELEASE FRACTION =

.110760

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	6.6853960E+03	2.1193653E-01	2.7327970E+05
3	2.0000000E+04	1.3206686E-02	3.6864024E-01	4.7252273E+05
4	3.0000000E+04	1.9453583E-02	4.8401282E-01	6.1723967E+05
5	4.0000000E+04	2.5354826E-02	5.8664155E-01	7.2200273E+05
6	5.0000000E+04	3.0866996E-02	6.3051572E-01	7.9761384E+05
7	6.0000000E+04	3.5966231E-02	6.7559404E-01	8.5200012E+05
8	7.0000000E+04	4.0642109E-02	7.0824961E-01	8.9089562E+05
9	8.0000000E+04	4.4893251E-02	7.3161408E-01	9.1835427E+05
10	9.0000000E+04	4.8724239E-02	7.4783774E-01	9.3712836E+05
11	1.0000000E+05	5.2143558E-02	7.5827820E-01	9.4893700E+05
12	1.1000000E+05	5.5162364E-02	7.6362684E-01	9.5464218E+05
13	1.2000000E+05	5.7793946E-02	7.6397939E-01	9.5434419E+05
14	1.3000000E+05	6.0053715E-02	7.5885525E-01	9.4740349E+05
15	1.4000000E+05	6.1960042E-02	7.4716802E-01	9.3239252E+05
16	1.5000000E+05	6.3535074E-02	7.2714840E-01	9.0697674E+05
17	1.6000000E+05	6.4807533E-02	6.9621859E-01	8.6772074E+05
18	1.7000000E+05	6.5814265E-02	6.5081555E-01	8.0981000E+05
19	1.8000000E+05	6.6605783E-02	5.8615799E-01	7.2667403E+05
20	1.9000000E+05	6.7249668E-02	4.9594998E-01	6.0949008E+05
21	2.0000000E+05	6.7838998E-02	3.7201200E-01	4.4653963E+05
22	2.1000000E+05	6.7838998E-02	4.4645663E-02	1.5720517E+07
23	2.2000000E+05	7.3732300E-02	4.1335307E-02	1.5667148E+07
24	2.3000000E+05	7.7697910E-02	3.8051152E-02	1.5358980E+07
25	2.4000000E+05	7.9712909E-02	3.4851780E-02	1.4867527E+07
26	2.5000000E+05	7.9936117E-02	3.1780116E-02	1.4249399E+07
27	2.6000000E+05	7.8640741E-02	2.8864815E-02	1.3547525E+07
28	2.7000000E+05	7.6150308E-02	2.6122617E-02	1.2793350E+07
29	2.8000000E+05	7.2787516E-02	2.3561081E-02	1.2009392E+07
30	2.9000000E+05	6.8840296E-02	2.1181217E-02	1.1211722E+07
31	3.0000000E+05	6.4544794E-02	1.8979746E-02	1.0412049E+07
32	3.1000000E+05	6.0081873E-02	1.6950822E-02	9.6193038E+06
33	3.2000000E+05	5.5582488E-02	1.5087241E-02	8.8407039E+06
34	3.3000000E+05	5.1137411E-02	1.3381189E-02	8.0823854E+06
35	3.4000000E+05	4.6807824E-02	1.1824658E-02	7.3497102E+06
36	3.5000000E+05	4.2634626E-02	1.0409628E-02	6.6473664E+06
37	3.6000000E+05	3.8645499E-02	9.1281302E-03	5.9793583E+06
38	3.7000000E+05	3.4859655E-02	7.9722407E-03	5.3489549E+06
39	3.8000000E+05	3.1290663E-02	6.9340684E-03	4.7586438E+06
40	3.9000000E+05	2.7947925E-02	6.0057485E-03	4.2101089E+06
41	4.0000000E+05	2.4837347E-02	5.1794553E-03	3.7042831E+06
42	4.1000000E+05	2.1961614E-02	4.4474335E-03	3.2411921E+06
43	4.2000000E+05	1.9320340E-02	3.8020428E-03	2.8204230E+06
44	4.3000000E+05	1.6910236E-02	3.2358116E-03	2.4408111E+06
45	4.4000000E+05	1.4725359E-02	2.7414922E-03	2.1007357E+06
46	4.5000000E+05	1.2757428E-02	2.3121141E-03	1.7981802E+06
47	4.6000000E+05	1.0996208E-02	1.9410317E-03	1.5308295E+06
48	4.7000000E+05	9.4299227E-03	1.6219646E-03	1.2961627E+06
49	4.8000000E+05	8.0456685E-03	1.3490287E-03	1.0915369E+06
50	4.9000000E+05	6.8298110E-03	1.1167582E-03	9.1426189E+05
51	5.0000000E+05	5.7683504E-03	9.2011807E-04	7.6166327E+05
52	5.1000000E+05	4.8472432E-03	7.3450803E-04	6.3113527E+05

TEST CASE I - TWO REGIONS

RESTARTED FROM DATA SAVED AT 1600 SECS.

IDENT

TIME :

2000,0000

RELEASE FRACTION :

.129714

I	X	C	SMALL M	CAP. M
1	0	0	0	0
2	1.0000000E+04	5.9979632E+03	2.0467356E-01	2.7643189E+05
3	2.0000000E+04	1.1841388E+02	3.5673052E-01	4.7874761E+05
4	3.0000000E+04	1.7426963E+02	4.6934264E-01	6.2640440E+05
5	4.0000000E+04	2.2688515E+02	5.5254751E-01	7.3394058E+05
6	5.0000000E+04	2.7586371E+02	6.1392464E-01	8.1213704E+05
7	6.0000000E+04	3.2099438E+02	6.5913131E-01	8.6891002E+05
8	7.0000000E+04	3.6219362E+02	6.9232287E-01	9.0998895E+05
9	8.0000000E+04	3.9946303E+02	7.1647805E-01	9.3942752E+05
10	9.0000000E+04	4.3285971E+02	7.3364487E-01	9.5998078E+05
11	1.0000000E+03	4.6247638E+02	7.4511916E-01	9.7337222E+05
12	1.1000000E+03	4.8842931E+02	7.5156418E-01	9.8046971E+05
13	1.2000000E+03	5.1083290E+02	7.5507737E-01	9.8138028E+05
14	1.3000000E+03	5.2989975E+02	7.5692096E-01	9.7547199E+05
15	1.4000000E+03	5.4574699E+02	7.5693391E-01	9.6132639E+05
16	1.5000000E+03	5.5860741E+02	7.5208838E-01	9.3661985E+05
17	1.6000000E+03	5.6874926E+02	6.9171495E-01	8.9793872E+05
18	1.7000000E+03	5.7652130E+02	6.4895744E-01	8.4046252E+05
19	1.8000000E+03	5.8239173E+02	5.8778682E-01	7.5766892E+05
20	1.9000000E+03	5.8699528E+02	5.0224680E-01	6.4075999E+05
21	2.0000000E+03	5.9120024E+02	3.8459872E-01	4.7806226E+05
21	2.0000000E+03	5.9120024E+02	4.7795593E-02	1.8872760E+07
22	2.1000000E+03	6.3324987E+02	4.7737910E-02	1.9071905E+07
23	2.2000000E+03	6.6555455E+02	4.1636382E-02	1.8946804E+07
24	2.3000000E+03	6.8651662E+02	3.8544063E-02	1.8561647E+07
25	2.4000000E+03	6.9569547E+02	3.5505758E-02	1.7976725E+07
26	2.5000000E+03	6.9359909E+02	3.2557401E-02	1.7241649E+07
27	2.6000000E+03	6.8142012E+02	2.9726259E-02	1.6398389E+07
28	2.7000000E+03	6.6076359E+02	2.7031723E-02	1.5481301E+07
29	2.8000000E+03	6.3340357E+02	2.4486447E-02	1.4518095E+07
30	2.9000000E+03	6.0109172E+02	2.2097608E-02	1.3530940E+07
31	3.0000000E+03	5.6542658E+02	1.9868131E-02	1.2537535E+07
32	3.1000000E+03	5.2778668E+02	1.7797770E-02	1.1532056E+07
33	3.2000000E+03	4.8927533E+02	1.5883992E-02	1.0585921E+07
34	3.3000000E+03	4.5078917E+02	1.4122656E-02	9.6483579E+06
35	3.4000000E+03	4.1298670E+02	1.2508500E-02	8.7468177E+06
36	3.5000000E+03	3.7635541E+02	1.1035510E-02	7.8872425E+06
37	3.6000000E+03	3.4124319E+02	9.6970905E-03	7.0742467E+06
38	3.7000000E+03	3.0789123E+02	8.4862772E-03	6.3112382E+06
39	3.8000000E+03	2.7646033E+02	7.3958174E-03	5.6008128E+06
40	3.9000000E+03	2.4705051E+02	6.4182609E-03	4.9433386E+06
41	4.0000000E+03	2.1971493E+02	5.5460358E-03	4.3400442E+06
42	4.1000000E+03	1.9446946E+02	4.7715222E-03	3.7901168E+06
43	4.2000000E+03	1.7129943E+02	4.0871250E-03	3.2923078E+06
44	4.3000000E+03	1.5016488E+02	3.4853439E-03	2.8447840E+06
45	4.4000000E+03	1.3100300E+02	2.9588581E-03	2.4450519E+06
46	4.5000000E+03	1.1373522E+02	2.5005511E-03	2.0904599E+06
47	4.6000000E+03	9.8266674E+01	2.1036290E-03	1.7779202E+06
48	4.7000000E+03	8.4491933E+01	1.7616198E-03	1.5042087E+06
49	4.8000000E+03	7.2297439E+01	1.4684349E-03	1.2660031E+06
50	4.9000000E+03	6.1564600E+01	1.2183945E-03	1.0599931E+06
51	5.0000000E+03	5.2172550E+01	1.0062464E-03	8.8291756E+05

TEST CASE I - TWO REGIONS

RESTARTED FROM DATA SAVED AT 1500 SECS.

IDENT

TIME:

2500.0000

RELEASE FRACTION =

.147030

I	X	C	SMALL M	CAP M
1	0.	0.	0.	0.
2	1.0000000E+04	5.6131690E-03	1.9731460E-01	2.7932694E+05
3	2.0000000E+04	1.1078904E-02	3.4490518E-01	4.8446228E+05
4	3.0000000E+04	1.6298550E-02	4.5465191E-01	6.3481291E+05
5	4.0000000E+04	2.1208848E-02	5.3627134E-01	7.4488452E+05
6	5.0000000E+04	2.5771831E-02	5.9695445E-01	8.2583903E+05
7	6.0000000E+04	2.9967281E-02	6.4207254E-01	8.8438220E+05
8	7.0000000E+04	3.3787162E-02	6.7557437E-01	9.2743939E+05
9	8.0000000E+04	3.7231594E-02	7.0029350E-01	9.5866448E+05
10	9.0000000E+04	4.0306008E-02	7.1818081E-01	9.8081523E+05
11	1.0000000E+03	4.3019240E-02	7.3047335E-01	9.9561981E+05
12	1.1000000E+03	4.5382369E-02	7.3780762E-01	1.0039517E+04
13	1.2000000E+03	4.7408174E-02	7.4028288E-01	1.0059245E+04
14	1.3000000E+03	4.9111146E-02	7.3747871E-01	1.0009137E+04
15	1.4000000E+03	5.0508038E-02	7.2842886E-01	9.8750962E+05
16	1.5000000E+03	5.1618969E-02	7.1155263E-01	9.6339884E+05
17	1.6000000E+03	5.2469199E-02	6.8454300E-01	9.2517277E+05
18	1.7000000E+03	5.3091633E-02	6.4420927E-01	8.6805188E+05
19	1.8000000E+03	5.3530333E-02	5.8626967E-01	7.8551253E+05
20	1.9000000E+03	5.3845157E-02	5.0508794E-01	6.6879562E+05
21	2.0000000E+03	5.4117951E-02	3.9334560E-01	5.0626960E+05
21	2.0000000E+03	5.4117951E-02	5.0613586E-02	2.1693514E+07
22	2.1000000E+03	5.6845891E-02	4.7728269E-02	2.2064577E+07
23	2.2000000E+03	5.9100627E-02	4.4763924E-02	2.2075908E+07
24	2.3000000E+03	6.0716026E-02	4.1765516E-02	2.1785110E+07
25	2.4000000E+03	6.1594748E-02	3.8773979E-02	2.1246805E+07
26	2.5000000E+03	6.1703372E-02	3.5825322E-02	2.0511280E+07
27	2.6000000E+03	6.1062726E-02	3.2949988E-02	1.9623686E+07
28	2.7000000E+03	5.9735397E-02	3.0172699E-02	1.8623708E+07
29	2.8000000E+03	5.7812337E-02	2.7512665E-02	1.7545614E+07
30	2.9000000E+03	5.5400170E-02	2.4984042E-02	1.6418552E+07
31	3.0000000E+03	5.2610335E-02	2.2596549E-02	1.5267015E+07
32	3.1000000E+03	4.9550694E-02	2.0356125E-02	1.4111366E+07
33	3.2000000E+03	4.6319771E-02	1.8265587E-02	1.2968369E+07
34	3.3000000E+03	4.3003413E-02	1.6325221E-02	1.1851684E+07
35	3.4000000E+03	3.9673458E-02	1.4533305E-02	1.0772293E+07
36	3.5000000E+03	3.6387892E-02	1.2886532E-02	9.7388624E+06
37	3.6000000E+03	3.3191899E-02	1.1380362E-02	8.7580451E+06
38	3.7000000E+03	3.0119560E-02	1.0009300E-02	7.8347239E+06
39	3.8000000E+03	2.7195519E-02	8.7671209E-03	6.9722205E+06
40	3.9000000E+03	2.4436731E-02	7.6470469E-03	6.1724763E+06
41	4.0000000E+03	2.1853944E-02	6.6419036E-03	5.4362168E+06
42	4.1000000E+03	1.9452960E-02	5.7442500E-03	4.7681074E+06
43	4.2000000E+03	1.7235644E-02	4.9464954E-03	4.1519037E+06
44	4.3000000E+03	1.5200725E-02	4.2410054E-03	3.6005976E+06
45	4.4000000E+03	1.3344436E-02	3.6201981E-03	3.1065603E+06
46	4.5000000E+03	1.1661021E-02	3.0766307E-03	2.6666789E+06
47	4.6000000E+03	1.0143161E-02	2.6030768E-03	2.2774856E+06
48	4.7000000E+03	8.7823356E-03	2.1925923E-03	1.9352768E+06
49	4.8000000E+03	7.5691365E-03	1.8385706E-03	1.6362214E+06
50	4.9000000E+03	6.4935527E-03	1.5347864E-03	1.3764538E+06
51	5.0000000E+03	5.5452198E-03	1.2754273E-03	1.1521555E+06

TEST CASE I - TWO REGIONS

RESTARTED FROM DATA SAVED AT 1600 SECS,

IDENT

TIME =

2500.0000

RELEASE FRACTION =

.147030

I	X	C	SMALL M	CAP M
52	5.1000000E+03	4.7136427E+03	1.0551148E+03	9.5962142E+09
53	5.2000000E+03	3.9883904E+03	8.6891451E+04	7.9531230E+09
54	5.3000000E+03	3.3592608E+03	7.1233751E+04	6.5589458E+09
55	5.4000000E+03	2.8164176E+03	5.8133295E+04	5.3826810E+09
56	5.5000000E+03	2.3504991E+03	4.7227411E+04	4.3958335E+09
57	5.6000000E+03	1.9526995E+03	3.8193887E+04	3.5724949E+09
58	5.7000000E+03	1.6148252E+03	3.0748590E+04	2.8893861E+09
59	5.8000000E+03	1.3293312E+03	2.4642789E+04	2.3255994E+09
60	5.9000000E+03	1.0893339E+03	1.9660298E+04	1.8628912E+09
61	6.0000000E+03	8.8861113E+04	1.5614521E+04	1.4851393E+09
62	6.1000000E+03	7.2158584E+04	1.2345504E+04	1.1783799E+09
63	6.2000000E+03	5.8330066E+04	9.7170438E+05	9.3056638E+10
64	6.3000000E+03	4.6938350E+04	7.6139279E+05	7.3142128E+10
65	6.4000000E+03	3.7600768E+04	5.9593239E+05	5.7220864E+10
66	6.5000000E+03	2.9984849E+04	4.6123644E+05	4.4557179E+10
67	6.6000000E+03	2.3803781E+04	3.5659361E+05	3.4535620E+10
68	6.7000000E+03	1.8811859E+04	2.7446825E+05	2.6644828E+10
69	6.8000000E+03	1.4800007E+04	2.1032202E+05	2.0462771E+10
70	6.9000000E+03	1.1591492E+04	1.6045643E+05	1.5643816E+10
71	7.0000000E+03	9.0378853E+05	1.2187514E+05	1.1904853E+10
72	7.1000000E+03	7.0153168E+05	9.2164735E+06	9.0188538E+11
73	7.2000000E+03	5.4210532E+05	6.9392442E+06	6.8017884E+11
74	7.3000000E+03	4.1704122E+05	5.2019189E+06	5.1067993E+11
75	7.4000000E+03	3.1940103E+05	3.8826239E+06	3.8171372E+11
76	7.5000000E+03	2.4353356E+05	2.8853854E+06	2.8405296E+11
77	7.6000000E+03	1.8486289E+05	2.1350377E+06	2.1044695E+11
78	7.7000000E+03	1.3970515E+05	1.5730299E+06	1.5523041E+11
79	7.8000000E+03	1.0511149E+05	1.1539969E+06	1.1400155E+11
80	7.9000000E+03	7.8734779E+06	8.4297578E+07	8.3359177E+12
81	8.0000000E+03	5.8717189E+06	6.1316152E+07	6.0689486E+12
82	8.1000000E+03	4.3596318E+06	4.4411001E+07	4.3994614E+12
83	8.2000000E+03	3.2227310E+06	3.2030863E+07	3.1755581E+12
84	8.3000000E+03	2.3718755E+06	2.3004650E+07	2.2823564E+12
85	8.4000000E+03	1.7380302E+06	1.6452733E+07	1.6334282E+12
86	8.5000000E+03	1.2680151E+06	1.1717698E+07	1.1640499E+12
87	8.6000000E+03	9.2108013E+07	8.3106477E+08	8.2606153E+13
88	8.7000000E+03	6.6616318E+07	5.8697838E+08	5.8375182E+13
89	8.8000000E+03	4.7970965E+07	4.1286718E+08	4.1079689E+13
90	8.9000000E+03	3.4395007E+07	2.8920508E+08	2.8788250E+13
91	9.0000000E+03	2.4554776E+07	2.0175066E+08	2.0091037E+13
92	9.1000000E+03	1.7484390E+07	1.4016627E+08	1.3963886E+13
93	9.2000000E+03	1.2353947E+07	9.6983364E+09	9.6648027E+14
94	9.3000000E+03	8.7064804E+08	6.8831488E+09	6.6622026E+14
95	9.4000000E+03	6.1036645E+08	4.5866811E+09	4.5736253E+14
96	9.5000000E+03	4.2690216E+08	3.1350856E+09	3.1269869E+14
97	9.6000000E+03	2.9700674E+08	2.1341544E+09	2.1291548E+14
98	9.7000000E+03	2.0573364E+08	1.4467808E+09	1.4437093E+14
99	9.8000000E+03	1.4186777E+08	9.7059911E+10	9.7472164E+15
100	9.9000000E+03	9.7356094E+09	6.3017043E+10	6.5502908E+15
101	1.0000000E+02	6.6441586E+09	4.3849058E+10	4.3780141E+15
102	1.0100000E+02	4.5024951E+09	2.9091551E+10	2.9030364E+15
103	1.0225428E+02	2.7476646E+09	1.7295821E+10	1.7274342E+15
104	1.0382749E+02	1.4667974E+09	8.9438618E+11	8.9344299E+16

TEST CASE I - TWO REGIONS RESTARTED FROM DATA SAVED AT 1000 SEC8, IDENT

TIME = 2500.0000 RELEASE FRACTION = .147030

I	X	C	SMALL M	CAP M
105	1.0580073E+02	0.6039477E-10	3.8757946E-11	3.8724533E+16
106	1.0827572E+02	2.3981040E-10	1.3457204E-11	1.3448113E+16
107	1.1138005E+02	0.6098626E-11	3.5572003E-12	3.5554037E+17
108	1.1527373E+02	1.3450355E-11	6.7869841E-13	6.7845076E+18
109	1.2015749E+02	1.8673553E-12	8.8946398E-14	8.8924052E+19
110	1.2628308E+02	1.7098463E-13	7.6876631E-15	7.6863519E+20
111	1.3396626E+02	1.0006913E-14	4.2538496E-16	4.2533770E+21
112	1.4360310E+02	3.6672431E-16	1.4777818E-17	1.4776792E+22
113	1.5569037E+02	8.3137095E-18	3.1855657E-19	3.1834368E+24
114	1.7085115E+02	1.1584164E-19	4.2339062E-21	4.2338195E+26
115	1.8986697E+02	9.8925488E-22	3.4592257E-23	3.4592026E+28
116	2.1371808E+02	5.1737892E-24	1.7357619E-25	1.7357669E+30
117	2.4363398E+02	1.6579436E-26	5.3502421E-28	5.3502925E+33
118	2.8115680E+02	3.2588865E-29	1.0139176E-30	1.0139317E+35
119	3.2822081E+02	3.9347316E-32	1.1827387E-33	1.1827589E+38
120	3.8725212E+02	2.9225551E-35	8.5035330E-37	8.5036956E+42
121	4.6129373E+02	1.3374232E-38	3.7732258E-40	3.7733031E+45
122	5.5416242E+02	3.7763093E-42	1.0346496E-43	1.0346718E+48
123	6.7064549E+02	6.5880682E-46	1.7554088E-47	1.7554472E+52
124	8.1674753E+02	7.1104961E-50	1.8448965E-51	1.8449374E+56
125	1.0000000E+01	0.	0.	0.

INTEGRATION ERROR ESTIMATE TABLE

REGION ERROR ESTIMATE

1 = 2.9100717E+08
2 = 2.3528686E+10

RMS 2.0577987E+08

TIME HISTORY OF RELEASE FRACTION

SQRT(T)	707777177772777377747775777677777778777977710	P
0.07107E+00	7	0.32217E+03
1.00000E+01	7	1.03828E+02
1.22474E+01	7	2.35289E+02
1.41421E+01	7	2.99138E+02
1.58114E+01	7	3.56765E+02
1.73205E+01	7	4.09260E+02
1.87083E+01	7	4.57492E+02
2.00000E+01	7	5.02148E+02
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4.30116E+01	7	1.24248E+01
4.35890E+01	7	1.26087E+01
4.41588E+01	7	1.27909E+01
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4.52769E+01	7	1.31504E+01
4.58258E+01	7	1.33279E+01
4.63681E+01	7	1.35040E+01
4.69042E+01	7	1.36787E+01
4.74342E+01	7	1.38522E+01
4.79583E+01	7	1.40245E+01
4.84768E+01	7	1.41957E+01
4.89898E+01	7	1.43658E+01
4.94975E+01	7	1.45349E+01
5.00000E+01	7	1.47030E+01
707777177772777377747775777677777778777977710		1.47030E+01
	MAXIMUM	1.47030E+01
	MINIMUM	0.
	RANGE	1.47030E+01

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