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CHAINT Computer Code: Users Guide

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ABSTRACT

CHAINT is a two-dimensional numerical model for the analysis of contaminant transport in a fractured porous medium. The physical processes accounted for include advection, dispersion, diffusion, retardation, radionuclide chain decay coupling, and mass injection. The computational scheme employed by CHAINT is based on a Galerkin finite-element method and block-diagonal frontal solution technique. Continuum portions of the medium may be modeled with two-dimensional isoparametric elements. Discrete features are modeled with one-dimensional elements that are embedded along the sides of the continuum elements. Principal input to this model consists of files from a predecessor MAGNUM-2D simulation of bouyancy driven fluid flow. Output from CHAINT includes a printed report of contaminant concentrations along with postprocessor graphics files. This report contains information relevant to general usage of the CHAINT code.

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1.0 INTRODUCTION

1.1 BACKGROUND

A suite of numerical models (i.e., computer codes) has been developed and interfaced for use in assessing the long-term performance of a repository in basalt (DOE-RL 1982). These models are based primarily on deterministic approaches (Runchal et al. 1985, Estey et al. 1985, England et al. 1985); however, certain codes are formulated on a probabilistic framework (Sagar and Clifton 1983, Clifton et al. 1983, Eslinger et al. 1985). The numerical models are grouped by space scale into three categories:

1. Waste package-scale (very near-field) models
2. Repository-scale (near-field) models
3. Regional-scale (far-field) models.

The waste package-scale models provide predictions of the temperature and flow field around the waste package and radionuclide release rates from the waste package and/or emplacement horizon. The repository-scale models are designed to calculate groundwater flow paths and traveltimes, the large-scale temperature field around the repository, and radionuclide concentrations and releases. Results from the repository-scale analysis provide boundary conditions for regional-scale predictions of groundwater traveltimes to and cumulative releases at the boundary of the accessible environment.

This report introduces one of the deterministic waste package-scale models designated as CHAINT. The CHAINT code embodies a two-dimensional finite-element model applicable to transport of a dissolved radionuclide in a fractured porous medium along with radioactive chain decay and subsequent transport of the dissolved daughters. The conceptual modeling approach is based on representing the space domain by a vertical cross section. Three-dimensional systems with axial symmetry can also be modeled with CHAINT. A set of support codes and graphics software has been developed and interfaced with the CHAINT code to (1) generate, manipulate, and display the finite-element grid, (2) compute and plot the mass flux across selected boundaries, and (3) plot contours, spatial cross sections, and time histories of concentrations. CHAINT and MAGNUM-2D (England et al. 1985) are arranged such that the hydraulic head data file and geometry file from MAGNUM-2D can be used directly as input to CHAINT.

This users guide provides detailed instructions regarding the use of the CHAINT computer code for general solute transport analysis in a fractured porous medium. It also contains descriptions of input data requirements as well as sample input and output for test cases.

1.2 PURPOSE AND SCOPE

The CHAINT computer code was developed by the Basalt Waste Isolation Project (BWIP) at Rockwell Hanford Operations (Rockwell) for use in studies of nuclear waste disposal in deep geologic repositories (Baca et al. 1984a, 1984b; Baca et al. 1981). Subsequent enhancements as well as ongoing maintenance are provided by Boeing Computer Services Richland, Inc., Richland, Washington. This document is intended to serve as a users guide for version 2.1 of the code as it exists at the BWIP computing facility. It is noteworthy that earlier versions of CHAINT have been implemented on a UNIVAC 1100/44 and a CRAY 1, as well as PRIME minicomputers. The current version is installed on a PRIME 750 minicomputer network. Although the BWIP version of CHAINT is maintained and used in a PRIME operating environment, transportability of the code has been given high priority. Features of the current version of the CHAINT computer code as described herein are machine independent except for the isolated service subroutines noted in appendix A.

The format and content of this users guide are with respect to guidance given by the U.S. Nuclear Regulatory Commission (Silling 1983). The partial differential equations solved by CHAINT and the numerical method are summarized in section 2.0 for the purpose of defining nomenclature. The general usage considerations and capabilities are discussed in section 3.0, while detailed instructions for inputting an example problem are given in section 4.0. The output obtainable from CHAINT is described in section 5.0. The possible machine/environment dependencies are discussed in appendix A. Included as appendixes B and C are descriptions and short discussions of several preprocessors and postprocessors that may be used to assist in preparation of the input data for CHAINT and the interpretation of the output data. The input data and output listings for some example problems, along with examples of plots generated by preprocessor and postprocessor graphics programs, are given in appendix D. Diagnostic messages generated by CHAINT are tabulated in appendix F.

2.0 MATHEMATICAL FRAMEWORK

2.1 GOVERNING EQUATIONS

The CHAINT computer code is designed to simulate transient migration of dissolved radionuclide mass in a saturated, fractured porous medium. The code is applicable to problems that can be formulated in two dimensions using rectangular coordinates or axisymmetric radial coordinates. The mathematical model embodied by CHAINT is based on the physical law of conservation of mass. Physical processes accounted for in the model include advection, diffusion, dispersion, and retardation, along with mass decay and production/injection.

The governing mass balance equation for concentration of the jth component of a decay chain containing n total daughters as written for Cartesian coordinates using the summation convention for the space coordinate indices i and k (Huyakorn and Pinder 1983) is

$$R_{d_j}\phi\frac{\partial C_j}{\partial t} + \frac{\partial}{\partial x_i}(q_i C_j) = \frac{\partial}{\partial x_i}\left(D_{m_{ik}}\phi\frac{\partial C_j}{\partial x_k}\right) - \lambda_j R_{d_j}\phi C_j + \dot{m}_j \qquad (1)$$

where

R_d = retardation factor

ϕ = porosity of medium

C = concentration of radionuclide mass in fluid

t = time

x_i = space coordinates (x and y)

q_i = Darcy velocity vector

$D_{m_{ik}}$ = hydrodynamic dispersion tensor

λ = radioactive decay constant

$\dot{m}$ = mass source term.

The principal components of the dispersion tensor are computed according to Scheidegger's relations

$$D_{mx} = D + (\alpha_L U^2 + \alpha_T V^2)/(\bar{q}\phi) \qquad (2a)$$

$$D_{my} = D + (\alpha_T U^2 + \alpha_L V^2)/(\bar{q}\phi) \qquad (2b)$$

where

D = molecular diffusion coefficient

α_L = longitudinal dispersivity

α_T = transverse dispersivity

U = horizontal component of Darcy velocity

V = vertical component of Darcy velocity

$\bar{q} = (U^2 + V^2)^{1/2}$ is the groundwater speed.

It is assumed that the principal axes of the dispersion tensor are coincident with the coordinate system axes and hence the off-diagonal dispersion terms in equation (1) are not treated computationally.

The retardation and decay factors are given by

$$R_{d_j} = 1 + \frac{\rho_s K_{d_j}}{\phi} \tag{3}$$

and

$$\lambda_j = \frac{\ln 2}{T_{\frac{1}{2}j}} \tag{4}$$

where

ρ_s = bulk density

K_d = sorption coefficient

$T_{\frac{1}{2}}$ = half life.

For the original parent radionuclide (i.e., the oth component of the decay chain), $\dot{m}_o$ is the rate at which mass is being released into the system. For the jth daughter in the chain, the source term is given by

$$\dot{m}_j = S_j + \phi \sum_{k=o}^{j-1} R_{d_k} \lambda_k P_{jk} C_k \tag{5}$$

where P denotes the rate of production of the jth component by virtue of decay of the kth component, and S is the rate of mass injection.

The CHAINT computer code is programmed to solve the governing transport equation (1) subject to initial and boundary conditions using a Galerkin finite-element method. The units of the constants, coefficients, and variables are given in the nomenclature table comprising section 6.0.

2.2 SPATIAL DISCRETIZATION

The finite-element method employed by CHAINT in solution of the transport equation (1) is implemented in a fashion that affords substantial flexibility in discretization of the spatial domain. An arbitrarily shaped planar domain may be discretized over a Cartesian global coordinate system as long as the domain is topologically connected and has a continuous

specification of an appropriate angle of revolution. Note that in a radial coordinate system, a line element superimposed on a vertical cross section of a cylinder defines a plane surface intersecting the cylinder.

Quadratic Lagrangian one-dimensional elements (Huyakorn and Pinder, 1983) may be used to represent a one-dimensional domain. Isoparametric triangular and/or serendipity elements (Huyakorn and Pinder 1983) with quadratic shape functions may be used in combination with the quadratic line elements for discretization of a two-dimensional domain. Typical one- and two-dimensional elements show the ordering of nodes (denoted by Latin numerals) and Gauss points (denoted by Arabic numerals) in figure 1. Note that the concentration, C, is defined at the nodes, and the Darcy velocities, U and V, are defined at the Gauss points. The Gauss point locatons in local (η,ψ) coordinates are shown in figure 2. Note also the arrows showing positive coordinate directions.

Guidance for selection of element types is provided in sections 3.1 and 3.2. Detailed descriptions of CHAINT input options and formulas are given in section 4.0. Automated construction of a complete finite-element grid system is outlined in appendix B. Two-dimensional plots of the grid systems used for some example problems may be found in appendix D.

2.3 INITIAL CONDITIONS

A solution of the governing transport equation (1) is dependent on the initial distribution of concentration. To facilitate the present as well as later discussions, let C^{ℓ}_{jk} denote the concentration of the jth component of a decay chain at the kth node at time t^{ℓ}. Then, the initial values of concentration are simply

$$C^{o}_{jk} = C_j\,(x_k,\ y_k,\ t^o) \tag{6}$$

for $0 \leq j \leq n$ and $1 \leq k \leq NP$, where $n + 1$ is the total number of components in the chain, and NP is the total number of nodes in the spatial domain. In general, manual setup of the input corresponding to equation 6 is tedious. Hence, there exists a preprocessor that provides automated generation of an initial condition file for each of the n+1 radionuclides in the chain (appendix B). In the event that an initial concentration distribution is spatially constant, the corresponding input is simplified (sec. 4.0).

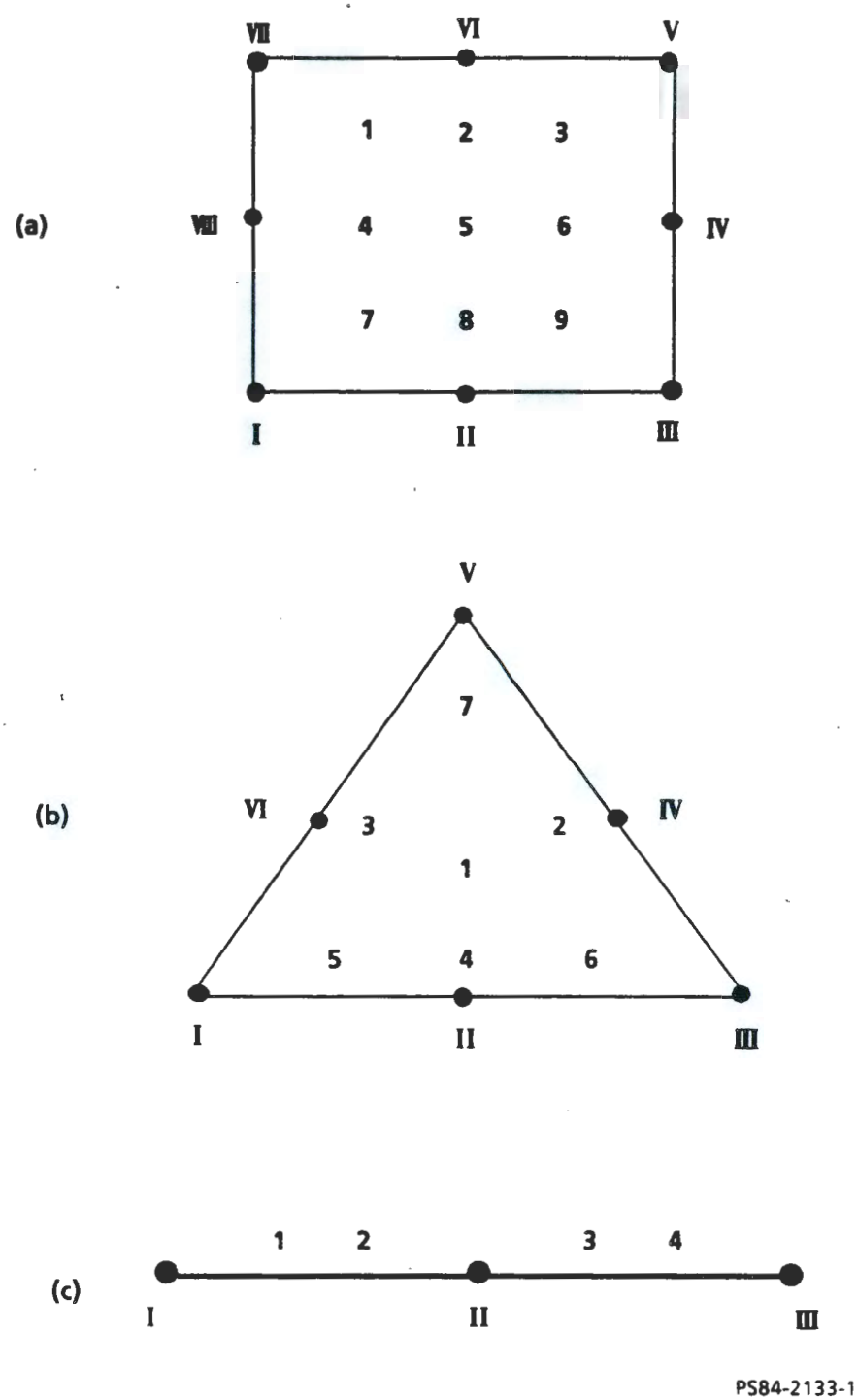

Figure 1. Locations of Nodes and Gauss Points for Quadratic Shape Functions (a) Quadrilateral Element, (b) Triangular Element, and (c) Line Element.

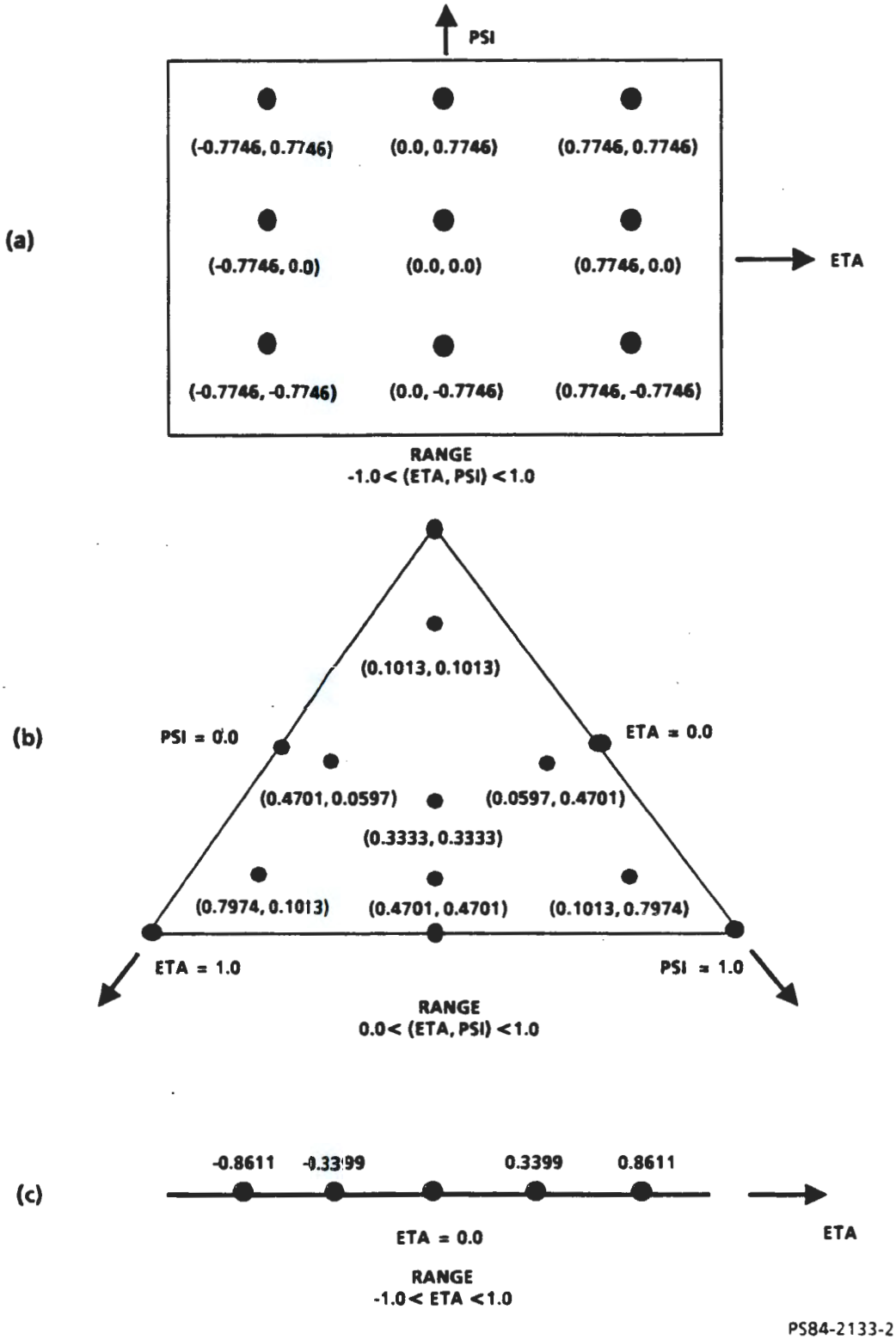

Figure 2. Gauss Points in Local Coordinates for (a) Quadratic Quadrilateral, (b) Quadratic Triangle, and (c) Quadratic Line Element.

2.4 BOUNDARY CONDITIONS

The CHAINT computer code is generally applicable to problems involving solution of the transport equation (1) over a domain meeting the requirements of section 2.2. However, typical usage dictates that the duration and spatial boundaries for a simulation be such that, at all times,

$$\left.\frac{\partial C_j}{\partial z}\right|_{x=x_B,\ y=y_B} = 0 \tag{7a}$$

for each component, where (x_B, y_B) denotes a boundary node, and z is a coordinate normal to the boundary at that point. Hence, the default boundary condition is zero diffusive flux. Optionally, one may specify a Dirichlet boundary condition for any decay chain component at any boundary node,

$$C_j(x_B, y_B) = \text{constant}. \tag{7b}$$

Formatting of input for optional boundary conditions can prove to be tedious. Thus, to further facilitate the setup of a CHAINT simulation, a preprocessor is available to generate boundary condition files (appendix B).

2.5 NUMERICAL SOLUTION METHOD

The finite-element method employed by CHAINT in solution of the governing equation (1) is based on the Galerkin approach (Huyakorn and Pinder 1983). A substantial derivation of the method for the current problem is given by Baca et al. (1984a). A summary, along with complementary details, is provided in the following paragraphs.

Consider an arbitrarily selected element containing m nodes. Then an approximation to C for some component over the element is written

$$C(x,y,t) \doteq \sum_{k=1}^{m} \omega_k(x,y)\ C_k(t) \tag{8}$$

where ω denotes a shape function. Let ε denote the error due to the approximation (8). Then the Galerkin approach to weighted residuals is based on minimization of the error, ε, through the functional

$$\chi = \sum \int_E \omega_k \varepsilon dE \tag{9}$$

where E is the current element and the summation is over all elements. The finite-element equations are formulated in terms of incremental change in C by using a Newton-Raphson algorithm for ε in equation 9 (Baca et al. 1978, 1984a). Communication between fractures and the porous continuum is achieved by superposition which amounts to summing the functionals for concentration in a continuum element and concentration in adjacent fractures.

Expansion of terms for the system of finite-element equations derived for a single element is illustrated by Baca et al. (1984a). Derivatives of C with respect to time as occur in the element equations are approximated by linear combinations of differences over incremental times written

$$\frac{\partial C^{\ell+1}}{\partial t} \equiv \frac{\partial C}{\partial t}\bigg|_{t=t^{\ell+1}} \doteq \theta \frac{C^{\ell+1} - C^{\ell}}{t^{\ell+1} - t^{\ell}} + (1-\theta) \frac{\partial C^{\ell}}{\partial t} . \tag{10}$$

The value of $C^{\ell+1}$ as used in equation 10 is calculated from a non-iterated Hermite-Milne predictor-corrector method characterized by the two stages

$$C^{\ell+1} = -4C^{\ell} + 5C^{\ell-1} + (t^{\ell+1} - t^{\ell}) \left(4 \frac{\partial C^{\ell}}{\partial t} + 2 \frac{\partial C^{\ell-1}}{\partial t}\right) \tag{11}$$

and

$$C^{\ell+1^*} = C^{\ell-1} + \frac{t^{\ell+1} - t^{\ell}}{3} \left(\frac{\partial C^{\ell+1}}{\partial t} + 4 \frac{\partial C^{\ell}}{\partial t} + \frac{\partial C^{\ell-1}}{\partial t}\right) \tag{12}$$

where $C^{\ell+1^*}$ is the corrected value of $C^{\ell+1}$.

The weighting factor, θ, in equation 10 may be specified by the user. Suggested values range between one and two; a value of one corresponds to a first order backward difference approximation, whereas a value of two corresponds to a second-order backward-difference approximation.

Assembly of the blocks of element equations yields a banded system of linear algebraic equations that is solved using a Gaussian frontal-solution technique. The frontwidth of the system is a factor in the amount of memory and processing time needed to solve the system of equations (Irons and Ahmad 1980). In turn, the frontwidth is dependent upon element numbering (King 1970). Hence, as described in appendix B, there is a preprocessor available to optimize the element numbering in the respect that the frontwidth is minimized.

2.6 NUMERICAL ACCURACY AND STABILITY

The Galerkin finite-element method used in both MAGNUM-2D (England et al. 1985) and CHAINT is generally accurate as well as efficient. For the mass transport problem solved by CHAINT, accuracy of the solution at a node is dependent on the local value of the Peclet number

$$Pe \equiv \frac{q\Delta}{2D_m\phi}, \tag{13}$$

where Δ represents an internodal distance in the direction of q. As long as Pe <1/2, mass transport is said to be diffusion-dominated and one should expect good accuracy. For Pe >1/2, upwinding (artificial dispersion) is invoked automatically for line elements to combat numerical diffusion; no other upwinding features are currently in the code. Reasonable accuracy can be expected for Peclet numbers up to about 10.

Stability of the solution is loosely influenced by the weighting factor, θ. The solution is fully implicit if $\theta = 1$ and becomes a Crank-Nicholson procedure for $\theta = 2$. In either case the solution is unconditionally stable in theory. In practice, for any value of θ between 1 and 2 inclusive, the step size guidelines found in section 3.6 should lead to stable results for a well-posed problem. Optimization of time steps and fine-tuning the value of θ beyond the empirical guidelines given herein has been found to be application specific.

2.7 FLUX CALCULATIONS

The computations performed by CHAINT are directed toward solving for the state variable, concentration. Frequently, it is also of interest to have fractional mass release rates and cumulative mass fluxes as outputs. To this end, there exists a postprocessor, CHTFLX, which computes the total instantaneous flux, say Q, of some radionuclide across some surface S. The surface S must be a subset of the spatial domain and must be topologically closed and connected. Spatial concentration distributions are passed through a file from CHAINT to CHTFLX (see section 4 and appendix C). Interactively the CHTFLX user can then approximate the flux

$$Q_j = \int_S \left(\frac{\partial C_j}{\partial z} + q\, C_j \right) ds$$

and display it as a function of time in the form of either fractional mass release rate, $\frac{Q}{M_0}$, or cumulative flux, $\int_0^T Q(t)dt$, for some arbitrarily chosen end time T.

3.0 GENERAL MODEL CONSIDERATIONS

3.1 MODEL GENERATION

The majority of the time required in formulation and generation of a finite-element-based simulation is spent in developing the grid that represents the physical domain. This consists of determining the global nodal coordinates and specifying the elemental connectivity in terms of node numbers.

One of the advantages of the finite-element approach used in CHAINT is that it permits the use of a "graded" mesh. A graded mesh is a variable computational grid that is coarse in areas of low gradients and is fine in areas of high gradients. The significance of the graded mesh is that it permits accurate representation of the spatial domain and its boundaries, and it minimizes the space truncation error thus optimizing the computational problem. Selection of the mesh layout is, therefore, one of the most important steps in applying the code.

Mesh generation for a practical simulation problem is generally an iterative process. The process begins with a trial mesh layout that is selected to conform with the anticipated solution field(s) and system boundaries. A test simulation is performed with CHAINT and the results are analyzed typically through the use of graphics postprocessors. From these initial results the grid is refined as needed, and the process is repeated until the simulation results show convergence to a reasonable solution.

Time may be saved in the geometry definition phase of the problem formulation by making use of the preprocessing utilities described in appendix B (e.g., GEN and FEMESH to generate the mesh, MESHER to optimize it, PURGE to verify it, and BCGEN to identify the boundary nodes). In addition, there is a processor called PLT that displays the geometry on a graphics terminal and a family of postprocessors that assist in the analysis of the output data.

The following guidelines should be considered in generating a two-dimensional finite-element mesh.

- Quadrilateral elements should be used for most of the mesh, and if necessary, triangular elements should be used for transition regions; line elements are used for discrete fractures.
- Element aspect ratios should not exceed roughly 100.
- Midside nodes should be located in the middle third of the element side or length.
- The element numbering sequence should be continuous and should begin along the side of the grid with the fewest elements.

The CHAINT computer code uses a frontal solution algorithm developed by Hood (1976) to solve unsymmetric finite-element matrix equations. This technique is an implementation of Gaussian elimination in which the assembly of equations alternates with their solution. With respect to accuracy, the algorithm is insensitive to node numbering and independent of matrix bandwidth. The numbering of the elements, however, must be assigned in a contiguous and optimal sequence to assure computational efficiency. In general, the optimal element numbering begins along the side of the mesh with the fewest elements. A preprocessor program, designated as MESHER, has been developed to read a finite-element mesh (element-node table and nodal coordinate list), reorder the element numbering sequence according to the algorithm given by King (1970), and output the optimized mesh layout into a file suitable for input to CHAINT.

3.2 ELEMENT TYPES

The CHAINT code uses a grid system composed of quadratic one- and two-dimensional elements. Representative examples are depicted in figure 1. The preceding section sets forth a procedure for constructing a CHAINT grid system under the tacit assumption that the CHAINT code is being operated in a stand-alone capacity. If CHAINT is being utilized in modeling advection in a transient flow field, then the Darcy velocities must come directly from a MAGNUM-2D output file. In this case, CHAINT must use the same geometry as was used by the predecessor MAGNUM-2D simulation and, hence, the predecessor run must have used only quadratic elements as well.

The other consideration pertinent to this section is the correspondence of host properties to elements. Material properties are specified on an elemental basis, thus, material boundaries must coincide with element boundaries. Moreover, the dispersivities, α_L and α_T, for a two-dimensional element are with respect to global coordinates, while the dispersivity along a line element is with respect to the local coordinate. These orientations assumed for dispersion are consistent with the manner in which hydraulic heads and, thus, Darcy velocities are computed by MAGNUM-2D (England et al. 1985).

3.3 INITIAL CONDITIONS

The initial concentration of each component of a decay chain must be specified at each node in the spatial domain. The initial value is summed with incremental concentrations as obtained from time-stepping to yield

$$C_{jk}^{\ell} = C_{jk}^{o} + \sum_{i=1}^{\ell} \Delta C_{jk}^{i} \ . \tag{14}$$

The computing time required to find ΔC_{jk}^{i} is independent of the starting value C_{jk}^{o}.

3.4 BOUNDARY CONDITIONS

The default boundary condition implemented in CHAINT is the zero flux Neumann condition given in equation 7. Use of this boundary condition is computationally advantageous, as may be seen from inspection of the Jacobian matrix, which is detailed by Baca et al. (1983). Furthermore, use of this boundary condition is appropriate in the solution of a given problem for a boundary that either coincides with an axis of symmetry or is sufficiently distant from any source of contaminant mass. In the event that the default boundary condition is not appropriate at some boundary node for some component of a decay chain, the alternative constant concentration may be used as per input instructions in section 4.0 and supplemental preprocessing instructions in appendix B.

3.5 MASS SOURCES

Any two-dimensional element in the spatial domain may be designated as a mass source. Two options are available by which to specify the source strength for any component of a radionuclide decay chain. Regardless of which option is used, the source strength is uniform over the source region. Note that by definition, the source region is simply the union of all designated source elements.

The more general of the two available release rate options allows specification of a piecewise linear volumetric mass injection profile. This first option is implemented analogously to the piecewise linear volumetric thermal energy release rate option in the MAGNUM-2D computer code (England et al. 1985). Under the second option, the mass injection rate, S, for any component of a decay chain is computed internally, and has the value

$$M_o e^{-\ln 2 \left(\frac{1}{T_{\frac{1}{2}}} + \frac{1}{T_L}\right) t}$$

where M_o is the initial volumetric inventory and T_L is the leaching period. The leaching period is defined to be the duration required to release half of the original inventory, neglecting decay. Details of the input format for these two injection rate options are found in section 4.0.

An important special case, constant injection, is easily simulated using the general piecewise linear rate option with two points. Under the assumption of negligible decay, the release interval (i.e., the duration required to deplete the inventory) is the reciprocal of the constant fractional mass injection rate. If in this case decay is also significant, an effective time interval of injection can be determined as in appendix A of Kline et al. (1983).

3.6 TIME STEPPING

The time steps used to drive a CHAINT simulation are divided into groups of equally sized steps. The number of steps of any given size is arbitrary. The user need only specify the step size and number of steps for each group of time steps as described in section 4.0.

For each time interval (i.e., group of time steps) so defined, the user may also define an active node zone. All nodes within this zone are considered to be active computational nodes, while those outside it take no part in the calculations. The boundary condition for this zone is the zero flux Neumann condition. This feature allows the user to dynamically expand and contract the spatial domain. The active node zone is defined by providing the top, bottom, left, and right dimensions of the zone on the time-step records. The active node zone is therefore modifiable only at the beginning of a time interval.

Apart from the procedural task of inputting time-step data is the need for a criterion to gage time-step size. As a rule of thumb, a step size for any interval of steps should be of the magnitude of

$$\Delta t = \frac{T_{ch}}{20} \cdot \tag{15a}$$

where the characteristic time, T_{ch}, is empirically related to a critical pathlength, L, (e.g., the linear distance through a subset of an active node zone) by

$$T_{ch} = \frac{4R_d L^2}{D_m} \cdot \tag{15b}$$

The interval length given by equation 15b is roughly the time to steady state for the distribution of concentration of a nondecaying radionuclide mass following from constant saturation-limited dissolution into a finite volume. During the course of a simulation, it is typical for the time steps to grow. An upper bound is for the maximum step size to satisfy

$$\max \Delta t \leq 1.3 \min_j T_{\frac{1}{2}j} \cdot \tag{16}$$

The step-size criteria given by equations 15 and 16 are based on attributes of a single contaminating species, but the step size so chosen applies for all components of decay chains under consideration in a CHAINT simulation. If the half lives of the components differ radically (i.e., by

more than three orders of magnitude), the step size may not be appropriate for all members. In particular, if for the jth daughter in a chain at some step of size Δt

$$T_{\frac{1}{2}j} < \frac{\ln\frac{1}{2}}{0.8}\,\Delta t\ , \tag{17}$$

then this component might be in secular equilibrium with its parents. The numerical criterion used to determine the applicability of the equilibrium assumption given that equation 17 holds is

$$T_{\frac{1}{2}j} < \frac{T_{\frac{1}{2}k}}{300P_{jk}}\ . \tag{18}$$

where the subscript k represents the parent component. In the case that both equations 17 and 18 hold for the jth daughter, then numerically the daughter is simply replaced by the $j + 1^{st}$ daughter and the total number, n, of daughter product is reduced by 1. If for the jth daughter equation 17 holds but equation 18 does not, the decay chain remains intact. However, in this latter case one should be watchful for signs of instability in the solution for concentration of the jth daughter and its subordinates. Finally, if a species for which no parents are specified satisfies equation 17 at some step, it is assumed that the species quickly decays to zero concentration and is ignored in any further computations. In practice, it is found that these automatic disenchainment features are not overly stringent and are rarely invoked because the user has sufficient information (Rd, Dm, Δt, $T_{\frac{1}{2}}$, and P) to avoid inputting a stiff problem.

3.7 SIMULATION RESTART

Restart capabilities are particularly useful in simulations that span long time periods relative to the time-step size. The first interval of time steps can be checked for errors before continuing an extensive run. After a given time period, perturbations in the system can be simulated by changing values in the input data file and restarting the run.

The user flags the initial run to generate the restart output file by using parameter IS4 to specify a logical unit number (LUN). The file so generated will contain data from the last time step completed. When the restart run is started, the LUN formerly entered as IS4 is specified as the input restart file using parameter IS3 (see card type C).

Note that the primary input file must be provided in its entirety for the restart run, but modifications may be made to some parameters such as material properties and boundary conditions. No modifications may be made to the geometry.

3.8 EXECUTION CONTROL

Execution control parameters make up most of the parameters on the second and third input records. These two cards specify the items such as the temporal nature of the velocity field, number and type of boundary conditions, number of constituents, type of initial conditions, output options, and all of the logical unit numbers (LUNs) used for files. In several cases, values entered in these records are used later during input to control the number of values to be entered (e.g., the numbers of nodes and elements). Note that not all the controlling parameters are located in these records. In some cases, they may immediately precede the table of values to be entered.

The LUN or file numbers entered on the third card often serve a dual capacity (e.g., the parameter IS3 for restart). If this value is blank or indicates zero, no restart is performed. When IS3 is a positive number, it indicates that a restart run is being made and also specifies the LUN to be read for restart data.

Details of all the user input data may be found in section 4.0 broken down by card type and parameter. Any interaction between control values and input data is explained in context.

3.9 DATA INPUT RECORDS

The input for a CHAINT simulation is a sequence of 80-character "card images." All the input is entered in fixed-length fields as defined in the following sections and consists of numeric or alphanumeric (character) data. It is entered in a manner consistent with the conventions of the FORTRAN programming language, of which an abbreviated description is the substance of this section.

The input records are divided into series of fields, each field being a fixed, predetermined number of characters in length. These fields may be used to enter either numeric or alphanumeric data. In the case of numeric data, there are two types: integer and real.

Integer numbers are entered as a string of numerals (0 through 9) with no decimal points. They may be preceded by an algebraic sign (+ or -), if required, and should not have any commas or blanks embedded in them. Examples are as follows:

- 100
- -53
- 0
- +1025

In the descriptions that follow, an integer value is specified by using the FORTRAN editing code of Ixx, where the I stands for integer, and the xx is a number indicating the length of the field that will contain the integer number. Examples are as follows:

- I5 - Integer field 5 digits long
- I10 - Integer field 10 digits long.

All integers must be right-justified within their respective fields or erroneous results will occur.

Real numbers can be entered in two forms. The first is called a real fixed-point number and is entered as a string of numerals with a decimal point. If required, they may be preceded by an algebraic sign and should not have any commas or blanks embedded in them. Examples are as follows:

- 3.14159
- 2034.
- -1.0
- +2.57

In the descriptions that follow, a real fixed-point value is specified by using the FORTRAN editing code of Fxx.xx, where the F stands for real fixed, and the xx is a number indicating the length of the field that will contain the real number. The xx that follows the decimal point indicates the number of decimal places that will be assumed if no decimal point is entered. Examples are as follows:

- F10.2 - Real number in a field 10 digits long with an assumed decimal point two places to the left of the last digit. A number entered as 1024 will be interpreted as the value 10.24
- F10.0 - Real number in a field 10 digits long with no assumed decimal point. A number entered as 1024 will be interpreted as the value 1024.

All numbers entered must fit within the field specified, or erroneous results will occur.

A real floating-point number consists of a string of numerals with a decimal point and may be preceded by a sign (as in the real fixed-point number). However, the real floating-point number is followed by an E and up to a two-digit number (three digits on some machines) which indicate the

power of 10 by which the preceding real fixed-point number should be multiplied to produce the correct order of magnitude. The power of 10 value, called the exponent, may be a signed number as well. Examples are as follows:

- 1.24E2 = 124.0
- -10.45E4 = -104500.0
- -45.63E-4 = -0.004563
- 3141592E-6 = 3.141592

In the descriptions that follow, a real floating-point value is specified by using the FORTRAN editing code of Exx.xx, where the E stands for floating point, and the xx is a number indicating the length of the field that will contain the number. The xx that follows the decimal point indicates the number of decimal places that will be assumed if no decimal point is entered as follows.

- E10.2 - Real number in a field 10 digits long with an assumed decimal point two places from the right of the last digit. A number entered as 1024 or as 1.024E1 will be interpreted as the value 10.24.
- E10.0 - Real number in a field 10 digits long with no assumed decimal point. A number entered as 1024 will be interpreted as the value 1024.

All numbers entered must fit within the field specified, or erroneous results will occur.

Alphanumeric (character) data are often entered for titling purposes. These data consist of a string of characters of the users choice, not exceeding the input field length in number. Examples are as follows:

- THIS IS AN EXAMPLE TITLE 24 character string
- ANOTHER LINE 12 character string.

In the descriptions that follow, an alphanumeric value is specified by using the FORTRAN editing code of Axx, where the A stands for alphanumeric, and the xx is a number indicating the length of the field that will contain the characters. Examples are as follows:

- A10 - A field of 10 is available for character input. The characters may be entered anywhere within the field.

All characters entered must fit within the field specified, or erroneous results will occur.

4.0 INPUT PREPARATION

4.1 INTRODUCTION

Preparation of input for a CHAINT simulation consists of a series of interrelated but identifiable steps. These steps are as follows:

1. Construction of a suitably discretized geometric model that takes into account the materials comprising the various regions of the spatial domain

2. Specification of the initial and boundary conditions

3. Specification of the material properties and radionuclide decay paths

4. Specification of the program control parameters and time-step sequences.

While the following input data descriptions will not follow these points in the order given, each item should be kept in mind to ensure completeness of the data set representing the problem.

The input data for CHAINT are entered in a very definite, controlled order. In some cases, data entered early in a data set control the type and quantity of other data entered later. Care should be taken to ensure that the values entered in these cases are consistent.

All the card types available to the user for input are presented in the following two subsections. The parameters that are entered on each card are described in section 4.2. Section 4.3 is a summary of the card types giving column numbers, FORTRAN variable names, editing codes, and short field descriptions for easy reference during setup of simulation input. In both instances, the card types are given in the order of their occurrence in an input stream.

4.2 INPUT DATA DESCRIPTION

An in-depth description of each input parameter is found in this section. Numbers appearing in parentheses represent allowable values for some parameters that have a limited range of choices.

<u>Card Type A</u> Title Card

<u>TITLE</u> - This parameter is a character string of up to 80 characters that may be input to describe the analysis. It is limited to one card. This title field will be output as part of the header on the CHAINT printout.

Card Type B — Control Parameters

NOAL - This parameter is the total number of decay chain constituents to be input to CHAINT. This value should include all the daughters that may be generated during radioactive decay of the original components. All these components need not be active at the same time, but if data is to be input for them, they must be included in the count.

NE - This parameter is the number of elements needed to define the model used for the current simulation. It is used to control the geometry input later. This value should be entered properly even if the geometry is to be entered from a binary geometry file. The element count on the binary file is checked against it.

NP - This parameter is the number of node points needed to define the model used for the current simulation. It is used to control the geometry input later. This value should be entered properly even if the geometry is to be entered from a binary geometry file. The nodal point count on the binary file is checked against it.

NENT - This parameter is the number of specified boundary conditions that will be input. The actual boundary conditions are not input until card type N. If this parameter is left blank or set to zero, it indicates that the active node zone feature is activated and that the zone definition on card type E will be used.

NMAT - This parameter indicates the number of different material or rock types that will be used in the model. It is used to control the material data input later.

IECHO - This parameter controls the input echo.

If IECHO=0, the principal problem specifications, nuclide decay tables, rock properties, initial and boundary conditions, and mass loading history will be printed in tabular form. If IECHO=1, the input geometry and element connectivity will be printed as well.

ISKO - This parameter controls the problem solution printout. A full printout is given if ISKO=1, while an abbreviated listing is given if ISKO=2.

If ISKO=2, certain headings and labels are not generated. In addition, the initial concentrations for the nuclides at each node point are not listed. If ISKO=1, a more expansive version of the same output is generated.

NVEL - This parameter controls the type of velocity field that will be used to drive the mass transport. Four options are available: 0, 1, 2, 3.

If NVEL=0, a uniform velocity field is defined by a single input record. If NVEL=1, the velocity will be input by material type on input cards. This means that NMAT records will be input, each representing the velocity in a specified material. The velocity is uniform over the elements comprising a material type. If NVEL=2, the velocity field will be calculated from the head data read in from file IS2. The data expected on this file is a history data set. This file would typically contain all the head data generated at all the time steps from a MAGNUM-2D run. If NVEL=3, the velocity field is again calculated from the head data on file IS2, but this file is only read for a single set of head values (the assumption being that the head field is constant).

Summary: NVEL=0 determines when card type 01 is used; NVEL=1 determines when card type 02 is used; and NVEL=2 or 3 determines how the data from file IS2 is interpreted.

NCFLX - This parameter specifies the number of constituents (contaminants, either original or decay daughters) that will be included in the flux output file. With the aid of a postprocessor, this file is used to calculate the mass flux across a boundary (defined by card type P2) and controls the amount of data input using card type P1. The data file generated for this analysis is written to the logical unit specified by IS7.

NSYS - This parameter controls the type of coordinate system to be used in defining the simulation model. The choices are Cartesian (0) or axisymmetric radial about the Y axis (1).

NSUMS - NSUMS=1 invokes an appication debugging option. The output from this option is the total contaminant released into the domain from all boundary conditions.

Card Type C File Assignments

CHAINT is designed to allow data to be read from or written to a mass storage device. The user must provide LUNs for optional files that are being used. Each system will have a slightly different way of associating LUNs with files so the system documentation should be consulted for advice on how to accomplish this. The default input unit (defined internally) is IIN=5 and the output unit is IIOUT=6.

IS1 - This field is a dual-purpose indicator with the following interpretation:

IS1=0 implies that a global initial condition is to be read for each constituent from the primary input file. Otherwise there must be an initial condition card for each node for each constituent. Moreover, in this latter case, IS1<0 implies that the entries are in the primary input file; otherwise the entries are read from logical unit IS1.

If IS1=0, NQAL entries are needed. The order of those entries is arbitrary since the concentrations are entered with the constituent number. If IS1≠0, however, there must be NQAL sets of NP entries. The first set of NP entries must be the concentrations at each node corresponding to the first constituent entered on card type H1; the second set of NP entries must correspond to the second constituent entered; and so on.

Initial conditions also may be created by the preprocessor program ICGEN. See card type H2 for a description of the use of such a preprocessor file and appendix B for a description of ICGEN.

IS2 - This logical unit is used for the input file of velocities generated by MAGNUM-2D. The contents and use of this file are discussed in the paragraph covering the parameter NVEL. It contains the head values at each node in the model, either for single or multiple time steps.

IS3 - This logical unit is used as the input file for restarting a simulation started at an early time. The file should be the file specified as IS4 in the previous run. Note that for restarting a simulation, all the data must be re-input, but some may not be used. This parameter is used as a switch to indicate whether a restart run is being made (IS3>0) or not (IS3=0).

IS4 - This logical unit is used to save the data necessary to restart the simulation at a later time. It is the file that is used as IS3 when restarting. Note that this parameter is used as a switch to indicate whether this file is to be generated (IS4>0) or not (IS4=0).

IS5 - This logical unit is used to save the concentration data for eventual plotting or further analysis by the postprocessing programs. See appendix C for a description of these programs.

IS6 - This logical unit is used as input for the geometry that has been created using a preprocessor, or has been saved (see below) from a previous simulation using the same model. This file may be a binary or coded file. If the initial attempt to read as a coded file fails, a binary read is used. Binary files are recommended to reduce I/O time.

IS7 - This logical unit is used to save the data necessary for mass flux calculations. This file may be used as input to the postprocessor CHTFLX, which will generate two-dimensional plots of fractional release and total release.

Card Type D — Constants/Scale Factors

SSF - This parameter specifies the starting time for the simulation. It is typically set to 0.0. Restarted simulations will automatically start at the ending time of the previous run.

ALFA - This parameter specifies the weighting factor, θ, to be used by the solver. It must be a value between 1 and 2, i.e., $1 < \theta < 2$. The time derivatives of the dependent variables are approximated by the finite-difference equation (see section 2.0). When $\theta = 1$, the expression is backward difference or the fully implicit method with maximum damping. The Crank-Nicolson approximation is invoked when $\theta = 2$. A commonly used value for θ is 1.8.

XSCALE - This parameter allows the user to apply a uniform scale factor to the x-dimensions of a model without having to modify the input data. This is a multiplicative factor.

YSCALE - This parameter allows the user to apply a uniform scale factor to the y-dimensions of a model without having to modify the input data. This is a multiplicative factor.

USCALE - This parameter allows the user to apply a uniform scale factor to the x-component of Darcy velocities entered in card type 01 or 02. It has no affect on velocities calculated from head data.

VSCALE - This parameter allows the user to apply a uniform scale factor to the y-component of Darcy velocities entered in card type 01 or 02. It has no affect on velocities calculated from head data.

Card Type E — Dynamic Control Card

This card type is used to specify the time-step information for the simulation. The total time for the simulation is broken into intervals that are arbitrary in length and is broken further into equally sized time steps. Three data items are required for each interval, as described in the following paragraphs. A limit on the number of intervals is imposed by parameter NTT (see appendix A). The variable time-step size allows the user to tailor CHAINT to each problem. After a perturbation occurs in the model, small time steps capture rapid changes. Larger time steps are adequate when the model response is slow. Note the step size guidelines of section 3.6.

NTS - This parameter specifies the number of time steps to be used in a specific time interval. Typically the user would specify more time steps of shorter duration for those time intervals expected to have more variation in the concentrations (perhaps in regions of higher velocity gradients).

NTSG - This parameter specifies the frequency at which the results of the simulation will be printed, i.e., at intervals of NTSG steps, the current results will be written to the print file. As an example, consider NTS=25 and NTSG=4. The results will be six printouts corresponding to the time steps 4, 8, 12, 16, 20, and 24.

DLT - This parameter specifies the time-step size in years. As an example, consider the previous example of NTS=25 and NTSG=4. If DLT=10.0, then the time interval will be 250 yr (25 time steps of 10.0 yr each) and will have printout corresponding to 40, 80, 120, 160, 200, and 240 yr.

CHAINT allows the user to define a computational zone around an area that will be active in the simulation. This zone is defined by the following four parameters. Elements outside the zone will not be included in computations, while those inside the defined zone will be included. The boundary condition used for this zone is the default boundary condition of section 2.4. Moreover, if the default boundary condition is used everywhere, an active node zone must be specified. The zone may be redefined for each time interval and will be active for all time steps in that interval.

ZONEL - This parameter defines the left boundary for the active node zone, and its value is in units of meters.

ZONER - This parameter defines the right boundary for the active node zone, and its value is in units of meters.

ZONET - This parameter defines the top boundary for the active node zone, and its value is in units of meters.

ZONEB - This parameter defines the bottom boundary for the active node zone, and its value is in units of meters.

Card Type F — Material Properties

J - This parameter specifies the material type number. It is the number referred to in the element definition as IMAT.

ORT(J,1) - This parameter specifies the longitudinal dispersivity, α_L, of this material type in meters (m).

ORT(J,2) - This parameter specifies the transverse dispersivity, α_T, of this material type in meters (m).

RHO(J) - This parameter specifies the bulk density of this material type in kg/m^3.

POR(J) - This parameter specifies the effective porosity, ϕ, of the rock for this material type as a volume percentage.

WIDTH - This parameter specifies the fracture aperture for a line element in meters (m).

NME - This parameter may be used to assign a name to this rock type. It is optional and may be up to eight characters in length. It is printed with the input echo.

Card Type G — Constituent Activation

ISLT - This parameter is used to indicate the contaminant or decay daughter to be considered for calculation during the analysis. The data input will consist of a series of zeros (or blanks) and ones. Each number one indicates that a constituent is active. There is a one-to-one correlation between the entries on this card type and the entries on card type H. The left-most entry on this card type corresponds to the first entry in H.

Card Type H — Decay Coefficients

This card type and the next card type define the contaminant characteristics and the characteristics of its daughters, if any. Each of the constituent types must be defined here. This card type also defines the nuclide decay chain.

L - This parameter specifies the constituent number. Since this parameter is used as an index to an array, it is recommended that the user select constituent numbers that start with the number one and are contiguous. This is not strictly required, but the arrays used by the program are typically small and choice of a number outside the array range will result in an error. The maximum number of constituents is in turn controlled by FORTRAN parameter MQL (see appendix A).

AMU - This parameter specifies the mass number for the current constituent.

DIAG - This parameter specifies the atomic half-life of the current constituent in years.

ISU(L,1) - This parameter specifies the first daughter constituent number. That is, it tells which of the constituents defined on an H1 card type results from the decay of the current constituent.

FRAC(L,1) - This parameter specifies the splitting fraction of the first daughter whose number was specified in ISU(L,1). It tells what percent of the parent becomes daughter.

ISU(L,2) - This parameter specifies the second daughter constituent number. Only two daughters may be defined.

FRAC(L,2) - This parameter specifies the splitting fraction of the second daughter whose number was specified in ISU(L,2). It determines what percent of the parent becomes daughter.

CNAM - This parameter specifies an optional name which may be associated with this constituent. It may be a maximum of six characters long and will be printed in the output table of concentrations.

ESPN - This parameter specifies a positive numerical threshold for concentrations below which the constituent concentration will be considered zero.

Card Type H1 Molecular Diffusivities

This card type is used to specify a value of molecular diffusivity for each decay chain component for each material type. The first NMAT values are diffusivities of component one in material types one through NMAT. The next NMAT values begin on a new card and are for component two in materials one through NMAT, and so forth. Up to eight values may be entered on each card. In all there should be NMAT times NQAL entries on NQAL sets of cards.

DML(J,I) - This parameter specifies the molecular diffusivity for constituent J in rock type I in m^2/yr.

Card Type H2 Sorption Coefficients

This card defines the sorption coefficient in each material type for each constituent. The first NMAT entries are sorption coefficients corresponding to constituent number one in materials one through NMAT. The second NMAT entries begin on a new card and are for constituent number two in materials one through NMAT, and so on. Up to eight values may be entered on each card. All total, there must be NMAT times NQAL entries.

XKDI(J,I) - This parameter specifies the sorption coefficient for the Jth constituent in the Ith material type in mL/g.

Card Type I Element (Connectivity) Definition

This card type should be omitted if a data file is being used for geometry input, i.e., if IS6 is nonzero on card type C. The number of sets of the following parameters should correspond to the value entered for the number of elements (NE) on card type B.

J - This parameter specifies the element number being entered. While it is not necessary to enter the element data in sequence, it would be a good idea. The element numbers are used as indices to arrays so they must be contiguous starting with the number one but need not be entered in any specific order.

NOP - This parameter specifies the node numbers that define the element. There are up to eight nodes per element, as in figure 1, and they must be entered counterclockwise. All eight nodes must be entered for a quadrilateral element. If a triangular element is needed, it may be specified by entering six nodes counterclockwise. Three nodes determine a line element.

IMAT - This parameter specifies the material type used for this element. It must correspond to one of the material types defined on the type F cards.

NFIXH - This parameter specifies the order in which this element will be considered during the solution phase of the simulation. These values may be input by the user but are typically modified by one of the preprocessors that optimizes the model geometry.

Card Type J — Coordinate (Geometry) Definition

This card type should be omitted if a data file is being used for geometry input, i.e., if IS6 is nonzero on card type C. The number of sets of the following parameters should correspond to the value entered for the number of node points (NP) on card type B.

N - This parameter specifies the number of the node being entered. Like the elements, the nodes need not be entered sequentially, although this makes the entry less prone to error, but node numbers must be contiguous and start with the number one.

CORD(N,1) - This parameter specifies the x coordinate of the node point.

CORD(N,2) - This parameter specifies the y coordinate of the node point.

Card Type L1 — Initial Condition Definition by Constituent Type

The use of this card type is controlled by the value of variable IS1 entered on card type C. If IS1=0, a single card of this type is used to specify the global initial value of concentration for each constituent. A total of NQAL of these cards is needed.

LK - This parameter specifies the constituent for which the initial condition is being entered.

TOLD(N,LK) - This parameter specifies the concentration to be used initially for all node(s) in the model for the constituent LK. It is entered in milligrams per liter (mg/L).

Note that if a restart simulation is being performed, the initial condition specification must be present for the restart run to be valid.

Card Type L2 — Initial Condition Definition by Node Points

The use of this card type is controlled by the value of IS1 that was entered on card type C. If IS1≠0, NP cards of this type are used to define the initial conditions for concentrations for every node in the model, and NQAL sets are generated to cover all the constituents. A total of NQAL times NP cards is needed.

N - This parameter specifies the node number for which the initial condition is being entered.

TOLD(N,L) - This parameter specifies the concentration to be used initially for node N in the model for the constituent L. It is entered in milligrams per liter (mg/L)

These values are repeated for each node point. The set is then repeated for each constituent.

Note that if a restart simulation is being performed, the initial condition specification must be present for the restart run to be valid.

Initial conditions may also be created by the preprocessor program ICGEN. The ICGEN initial condition file must be inserted into the data deck at this location.

Card Type N — Boundary Condition Values

The number of records of this type is controlled by the value entered for NENT on card type B. One set is entered for each node at which a boundary condition is to be specified.

A zero flux Neumann condition is assumed at all unspecified boundary nodes. This is a feature inherent to finite-element basis functions.

L - This parameter specifies the node number at which the boundary condition is being specified.

BCS(N) - This parameter specifies the actual boundary condition value to be used for concentration of constituent number one at the node in question. It is specified in milligrams per liter (mg/L). There must be NQAL entries (N ranges from one to NQAL) for each node specified. As many cards as necessary are used with eight fields per card.

Card Type 01 — Initial Darcy Velocities: Uniform Field Defined by a Single Card

The use of this card type is controlled by the parameter NVEL entered on card type B. If NVEL=0, this card type is used to describe the constant and uniform velocity field to be used. Only one card is input, and the velocities are used for all elements in the model.

UL - This parameter specifies the x-component of flow, U, in meters per year (m/yr).

VL - This parameter specifies the y-component of flow, V, in meters per year (m/yr).

Card Type 02 — Initial Darcy Velocities: Varying Field Defined by Material Type

The use of this card type is controlled by the parameter NVEL entered on card type B. If NVEL=1, this card type is used to describe the constant and uniform velocity field to be used. One card is input for each material type, and the velocities are used for all elements in the model with the corresponding material types. The NMAT records of this card type are required.

N - This parameter specifies the material type (entered as parameter J on card type F) for which the following velocities will be entered.

UL - This parameter specifies the x-component of flow, U, in meters per year (m/yr).

VL - This parameter specifies the y-component of flow, V, in meters per year (m/yr).

Card Type P1 — Mass Flux Constituents

The use of this card type is controlled by the parameter NCFLX on card type B and by parameter IS7 on card type C. It is used to specify the constituents for which the mass flux across a boundary can be determined. It is omitted if either NCFLX<1 or IS7<1.

ICFLX(N) - This parameter specifies a constituent number, as entered on card type H1. It may be repeated for as many constituents as needed. Up to 16 values may be entered on each record. The NCFLX values (see card type B) are required.

Card Type P2 — Number of Flux Surface Elements

The use of this card type is controlled by the parameter NCFLX on card type B and by parameter IS7 on card type C. It is omitted if either NCFLX<1 or IS7<1.

NEFLX - This parameter specifies the number of elements that define the flux surface. There are up to MAXSF entries on this card type, or for each flux surface.

Card Type P3 Flux Surface Elements

The use of this card type is controlled by the parameter NCFLX on card type B and by parameter IS7 on card type C. It is omitted if either NCFLX<1 or IS7<1.

IEFLX - This parameter specifies the element number (as entered on card type I) for an element through which the flux surface passes. The number of values entered is controlled by the parameter entered on card type P2. These elements must be connected (i.e., they must have a common side, and must be listed in a clockwise direction around the region containing the source). As many cards as are necessary are used. Each new surface element list is started as in a new card.

Card Type Q Loading Control (Mass Release)

This card type must be present for every simulation. If no mass release is to be specified, this is indicated using the parameter NLD in the following description.

NLD - The absolute value of this parameter specifies the number of elements in the model that will be considered as mass release source elements. If no release is to be applied to the model, this parameter should be entered as a zero or a blank record. If NLD>0, then the release rate will be specified as a piecewise-linear function on card type S. NLD<0 indicates that the data will be given as an initial inventory, and the rates will be determined using the release period specified on this card type.

SCF - This parameter specifies a scale factor which is applied to the mass release data entered on card type S. This parameter is ignored if NLD=0 above.

RELZ - This parameter specifies the release period in years. It is ignored if NLD>0 or NLD=0. This period is used to determine the release rates used by CHAINT when the initial inventory is specified, i.e., when NLD<0.

Card Type R Source Elements

This card type is omitted if NLD=0 on card type Q.

NLE(I) - This parameter specifies the element numbers of the elements that are to be considered as the mass sources in the model. The number of these elements is controlled by the parameter NLD on card type Q above. Each record may contain eight fields at most, and the records may be repeated as many times as needed.

Card Type S — Mass Release Rate History

This card type is omitted if NLD=0 on card type Q.

The loading is specified by defining a set of node points in time at which the mass release rate is known. The range of times input must bracket or coincide with the range covered by the simulation. Any times used by the simulation, but not input, are interpolated as long as the input times bracket the time required. This interpolation thus requires that a minimum of two time/load pairs be input.

TLE(I) - This parameter specifies the time of the load being entered for the next parameter. It is given in years (yr).

RLE(I,J) - This parameter specifies the load for the time entered in TLE(I). The NQAL values are entered for each time, one for each constituent specified on card type H1. The interpretation of these values is made based on the value of NLD. If NLD>0, then RLE is the mass loading rate given in grams per cubic meter per year (mg/L-yr.). If NLD<0, then RLE is the initial inventory at this time given in grams per cubic meter (mg/L). If NLD<0, the release rates are calculated internally for each constituent using the release period RELZ from card type Q, and the initial mass is entered here. Finally, if NLD<0, TLE(I) is not used

These time and load value sets are input as many times as needed to define the loading history.

4.3 INPUT DATA FORMAT

Card Type A — Title Card

1-80	TITLE	20A4	Title or description of this analysis, up to 80 characters.

Card Type B — Control Parameters

01-05	NQAL	I5	Number of constituents (dissolved components, including all daughters).
06-10	NE	I5	Number of elements in the model.
11-15	NP	I5	Number of nodes in the model.

16-20	NENT	I5	Number of specified boundary conditions. If NENT = 0, ZONEL, ZONER, etc., must be specified on card type E.
21-25	NMAT	I5	Number of rock types (material types) in the model.
26-30	IECHO	I5	Input data echo option = 0 Echo selected portion of the input data. = 1 Echo all the input data.
31-35	ISKO	I5	Results printout option = 1 Full listing. = 2 Abbreviated listing.
36-40	NVEL	I5	Type of velocity field = 0 Constant velocity field defined by a single card. = 1 Varying velocity field on cards, specified by rock type. = 2 Varying velocity field on file IS2, specified by heads. = 3 Constant velocity field on file IS2, specified by heads (read only once).
41-45	NCFLX	I5	Number of constituents to be included in the mass flux analysis.
46-50	NSYS	I5	Coordinate system control = 0 Cartesian coordinates (x,y). = 1 Radial coordinates (r,z) with symmetry about the line r=0.
51-55	NSUM	I5	= 1 Compute total mass injection/ production.

<u>Card Type C</u> File Assignments

01-05	IS1	I5	Initial condition type = 0 Read only one card per constituent to define ICs at all nodes. ≠ 0 Read one card per node to define ICs. There must be NQAL sets, one for each constituent.
06-10	IS2	I5	Velocity input file from MAGNUM-2D.

11-15	IS3	I5	Restart input data file (generated by an earlier CHAINT run). = 0 No input file.
16-20	IS4	I5	Restart output data file (to be generated for use by a later CHAINT run). = 0 No output file.
21-25	IS5	I5	Plot file logical unit number: = 0 No file produced. > 0 Generate plot records at the end of each group of time steps. < 0 Generate plot records at the end of each individual time step.
26-30	IS6	I5	Geometry input file.
31-35	IS7	I5	Binary mass flux output file.

<u>Card Type D</u> Constants/Scale Factors

01-10	SSF	F10.1	Initial time (year).
11-20	ALFA	F10.1	Weighting factor $1 \leq \theta \leq 2$.
21-30	XSCALE	F10.1	X-coordinate scale factor.
31-40	YSCALE	F10.1	Y-coordinate scale factor.
41-50	USCALE	F10.1	X-velocity scale factor.
51-60	VSCALE	F10.1	Y-velocity scale factor.

Note: USCALE and VSCALE are applied only to velocities input on card types 01 and 02.

<u>Card Type E</u> Dynamic Control Card

(This card is repeated up to NTT times. Terminate this card type set with NTS=9999.)

01-05	NTS(I)	I5	Number of time steps.
06-10	NTSG(I)	I5	Printout frequency.

11-20	DLT(I)	F10.1	Time-step size in years.
21-30	ZONEL(I)	F10.1	Left boundary for active node zone (m).
31-40	ZONER(I)	F10.1	Right boundary for active node zone (m).
41-50	ZONET(I)	F10.1	Top boundary for active node zone (m).
51-60	ZONEB(I)	F10.1	Bottom boundary for active node zone (m).

Card Type F — Material Properties

NMAT cards required.

01-10	J	I10	Rock type numbers.
11-20	ORT(J,1)	F10.1	Longitudinal dispersivity, α_L (m).
21-30	ORT(J,2)	F10.1	Transverse dispersivity, α_T (m).
31-40	RHO(J)	F10.1	Bulk density, ρ_s (kg/m^3).
41-50	POR(J)	F10.1	Effective porosity, ø.
51-60	WIDTH(J)	F10.1	Fracture width (m).
63-70	NME(J)	A8	Rock type identifier.

Card Type G — Constituent Activation

(NQAL entries required, up to 30 entries per card, 30I2).

01-02	ISLT(1)	I2	Activation flag for constituent 1 = 0 Drop out constituent. = 1 Include constituent.
03-04	ISLT(2)	I2	Activation flag for constituent 2.
.	.	.	Note: Constituents defined on card type H below.
.	.	.	
.	.	.	

Card Type H — Decay Coefficients

(One card required for each constituent.)

Note: Components must be numbered sequentially from top to bottom of the decay chain.

01-05	L	I5	Constituent number.
06-10	AMU(L)	F5.1	Atomic number of constituent.
11-20	DIAG(L)	F10.0	Half-life, $T_{\frac{1}{2}}$ (years).
21-25	ISU(L,1)	I5	First daughter constituent number.
26-35	FRAC(L,1)	F10.0	Splitting fraction for first daughter.
36-40	ISU(L,2)	I5	Second daughter constituent number.
41-50	FRAC(L,2)	F10.0	Splitting fraction for second daughter.
51-56	CNAM(L)	A6	Constituent name.
61-70	EPSN(L)	F10.0	Cut-off threshold for concentrations.

Card Type H1

Molecular Diffusivities

At least one card is required for each constituent. Each card contains diffusivity values for up to eight material types.

01-10	J	I10	Constituent Number
11-20	DML(1,1)	E10.1	Diffusion coefficient for constituent number 1 in material number 1 (m^2/yr).
21-30	DML(1,2)	E10.1	Diffusion coefficient for constituent number 1 in material number 2 (m^2/yr).
.	.	.	
.	.	.	
.	.	.	
01-10	J	I10	Constituent Number
11-20	DML(2,1)	E10.1	In general, DML (J,I) is the coefficient of molecular diffusion for the Jth constituent in the Ith rock type.
21-30	DML(2,2)	E10.1	
.	.	.	
.	.	.	
.	.	.	

Card Type H2			Sorption Coefficients
			At least one card is required for each constituent. Each card contains sorption coefficients for up to eight material types.
01-10	J	I10	Constituent number.
11-20	XKDI(1,1)	E10.0	Sorption coefficient for constituent number 1, material number 1 (mL/g).
21-30	XKDI(1,2)	E10.0	Sorption coefficient for constituent number 1, material number 2 (mL/g).
.	.	.	
.	.	.	
.	.	.	
01-10	J	I10	Constituent number.
11-20	XKDI(2,1)	E10.0	Sorption coefficient for constituent number 2, material number 1 (mL/g).
21-30	XKDI(2,2)	E10.0	Sorption coefficient for constituent number 2, material number 2 (mL/g).
.	.	.	
.	.	.	
.	.	.	In general, XKDI(J,I) is the sorption coefficient for the jth component of the decay chain in the ith rock type.
			Note that the units of sorption are mL/g for input, but are converted to m^3/kg internally.

Card Type I			Element (Connectivity) Definition
			The number of cards for this card type set is controlled by the parameter NE defined earlier. OMIT this card type set if a geometry input file is used (i.e., if IS6 is NOT equal to zero).
01-05	J	I5	Element number.
06-45	NOP(J,K)	8I5	Up to eight node numbers for elements listed counterclockwise.
46-50	IMAT(J)	I5	Element type (material type). The number entered must correspond to one of the parameters specified as J under card type F above.

51-55	NFIXH(J)	I5	Element ordering array. This parameter is the number of the Jth element to process and may be used to optimize the solution of the matrix equations by modifying the frontwidth.

<u>Card Type J</u>

Coordinate (Geometry) Definition

The number of cards for this card type set is controlled by the parameter NP defined earlier. OMIT this card type set if a geometry input file is used; i.e., if IS6 is NOT equal to zero.

01-05	N	I5	Node number.
06-15	CORD(N,1)	F12.3	X-coordinate (m).
16-25	CORD(N,2)	F12.3	Y-coordinate (m).

<u>Card Type L1</u>

Spatially Constant Initial Conditions.

Read only if IS1 = 0 in which case NQAL cards are required. Use card type L2 if ISI ≠ 0. See card type C.

01-10	LK	I10	Constituent number.
11-20	TOLD(N,LK)	F10.0	Initial concentration for all nodes for this constituent (mg/L).

<u>Card Type L2</u>

Spatially Varying Initial Conditions.

Read only if IS1 ≠ 0. NQAL sets of NP cards are required.

01-10	N	I10	Node number.
11-20	TOLD(N,L)	F10.0	Initial concentration of constituent L at node N (mg/L).

There must be NQAL sets of cards provided with each set containing NP cards of this type (one for each node). See card type C.

Note: If a restart run is being made, the initial conditions must still be specified.

Card Type N			Boundary Condition Values
			NENT values are required as defined on card type B.
01-10	L	I10	Node number.
11-20	BCS(1)	F10.3	Specified concentration for constituent number 1 (mg/L).
21-30	BCS(2)	F10.3	Specified concentration for constituent number 2 (mg/L).
31-40	BCS(3)	F10.3	Specified concentration for constituent number 3 (mg/L).
.	.	.	
.	.	.	
.	.	.	Continue the concentration cards as needed with up to eight fields per card. Each node must be started on a new card.
Card Type 01			Initial Darcy Velocities Uniform field defined by a single card.
			Read only if NVEL = 0. See card type B.
01-10	N	I10	Dummy index.
11-20	UL(1)	F10.0	X-component of flow, U (m/yr).
21-30	VL(1)	F10.0	Y-component of flow, V (m/yr).
Card Type 02			Initial Darcy Velocities Varying field defined by material type.
			Read only if NVEL = 1. NMAT cards required. See card type B.
01-10	N	I10	Material type index.
11-20	UL(N)	F10.0	X-component of flow, U (m/yr).
21-30	VL(N)	F10.0	Y-component of flow, V (m/yr).
Card Type P1			Mass Flux Constituents
			OMIT this card type if NCFLX <1 on card type B or if IS7 <1 on card type C.
			NCFLX values required.

01-05	ICFLX(1)	I5	Constituent number of the constituent to be used for the calculation of mass flux.
06-10	ICFLX(2)	I5	Constituent number of the second constituent.
11-15	ICFLX(3)	I5	Constituent number of the third constituent.
.	.	.	
.	.	.	
.	.	.	(Repeat as needed up to 16 fields per card.)

<u>Card Type P2</u>

Flux Boundary Definition

OMIT this card type if NCFLX <1 on card type B or if IS7 <1 on card type C. The maximum number of flux boundaries is set by parameter MAXFS (see appendix A).

01-05	NEFLX(1)	I5	Number of elements to be used as mass flux surface number 1.
06-10	NEFLX(2)	I5	Number of elements comprising mass flux surface number 2.
11-15	NEFLX(3)	I5	Number of elements comprising mass flux surface number 3.

<u>Card Type P3</u>

Flux Boundary Elements

OMIT this card type if NCFLX <1 on card type B or if IS7 <1 on card type C.

NEFLX values required.

01-05	IEFLX(1,1)	I5	Element number.
06-10	IEFLX(2,1)	I5	Element number.
11-25	IEFLX(3,1)	I5	Element Number.
.	.	.	
.	.	.	Elements must be connected and listed clockwise as they enclose the area across which the flux of C is of interest. Sixteen elements may be given per card. IEFLX(I,J) is the Ith element in the list of elements for the Jth surface. Each new surface must start on a new card.
.	.	.	

Card Type Q			Loading Control (Mass Release)
			This card type must be entered whether loading is being specified or not.
01-10	NLD	I10	Number of source elements. NLD = 0 indicates that no loading will occur. NLD >0 = >mass loading rate input. NLD <0 = >initial inventory input.
11-20	SCF	D10.0	Scale factor for release rate. Ignore if NLD = 0.
21-30	RELZ	D10.0	Waste form release period (yr), used only when NLD <0.
Card Type R			Source Elements
			OMIT this card type if parameter NLD = 0 on card type Q.
01-80	NLE	I10	Elements at which mass release occurs (eight values may be entered on a single card). There must be NLD total values entered where NLD was defined on the previous card. This card type may be repeated as many times as needed.
Card Type S			Mass Release Rate Histories
			OMIT this card type if parameter NLD = 0 on card type Q. (Repeat this card type as needed and terminate it with a negative time value.)
01-08	TLE(1)	F8.0	Time of loading for first time (yr).
09-16	RLE(1,1)	F8.0	Mass release for constituent 1, time 1. NQAL values are required. NLD >0 mass loading rate (mg/L-yr). NLD <0 initial inventory (mg/L).
17-24	RLE(1,2)	F8.0	Mass release (as above) for time 1 constituent 2.

25-32	RLE(1,3)	F8.0	Mass release (as above) for time 1 constituent 3.
.	.	.	
.	.	.	
.	.	.	(Repeat as many cards as needed to provide NQAL values, leaving the first field (F8.0) blank until next time value is required.)

Continue entering time and load input sets (a time value followed by NQAL release values) until load history is defined. Repeat this card type as many times as needed.

Note: Only a time value may be entered in Columns 1 through 8. On continuation cards, the data values start in Column 9 and enter in fields 8 long. The NQAL release values MUST be provided.

5.0 OUTPUT

5.1 INTRODUCTION

The output from the CHAINT program takes two forms. The first is the printed output that reports on the input data, the parameters that were set, the events that took place during execution, the concentrations that were calculated at the various time steps, the duration of the run (in model time), and so on. The second form of output is composed of the various data files that are created for use by postprocessing programs such as CHTFLX. This section will give an overview and some explanation of the printed output report file and the possible use of each of the other files.

5.2 PRINTED REPORT

The CHAINT program generates a report file suitable for spooling to a printer. The contents of this report may be modified by the input data using the parameters IECHO, ISKO, and NCFLX, which appear on card type B. These parameters are described in section 4.2 and are discussed in section 4.3; therefore, no further explanation will be given here. However, their effects will be pointed out in the following discussion.

For examples of the output report, please consult appendix D, Example Problems.

5.2.1 Banner Page

The generated report begins with a banner page that announces (1) the version and revision of CHAINT, (2) the day, date, and time of the run that generated the printout, and (3) the unique identifier assigned to the run. This identifier is placed on all the mass storage files and is displayed by the graphics postprocessors. It acts as an "audit" trail, that allows the user to ensure a match between printout and graphic results.

5.2.2 Input Verification

The next section of the output is the input verification section that is divided into several tables. Note that in some of the tables, the units are printed with the names of the parameters. However, due to space considerations, not all parameters are printed with units. In general, output units will be consistent with input units unless specified differently on the printout.

The first output table, "PROBLEM CONTROL PARAMETERS," is an echo of the parameters input on card types B, C, and D. The card types are echoed in the order just given, and the parameters on each card type are echoed in the input order (as described in section 4.3).

The second output table, "TIME CONTROL AND RUN SPECIFICATIONS," is an echo of the time-step definition and zones defined on card type E. In addition, it shows the cumulative time covered by the analysis calculated from the time step/interval data.

The third output table, "ROCK CHARACTERISTICS," is an echo of the internal properties input on card type F. The entries in this table are arranged in a two-dimensional matrix. The columns represent the properties (identified by name and units), and the rows represent the various rock or material types (identified by number on the left and by user input name on the far right).

The fourth output table, "INPUT DECAY CHAIN DATA," is an echo of the properties input on card type H. It is displayed much like the material properties, which are arranged in a two-dimensional matrix. The columns represent the actual properties (identified by name and in some case units), and the rows represent the various components (identified by number and name on the left). The constituent activation data input on card type G is reflected in this table. Any nonactive component will be flagged by an asterisk in column one.

The fifth and sixth output tables, "NUCLIDE MOLECULAR DIFFUSION COEFFICIENTS" and "NUCLIDE SORPTION (MLGM)," are echos of the factors entered on card types H1 and H2. They, too, are displayed as two-dimensional matrices with the columns representing the different material types, identified by number and input name, and with the rows representing the contaminant constituents identified by number and name.

The seventh output table graphically portrays the decay chain and the decay rate associated with the contaminates that have been input. It reflects a composite of the previous information.

The eighth output table, "SPECIFIED BOUNDARY NODES AND VALUES," is an echo of the boundary condition concentrations entered for each constituent. It is displayed as a two-dimensional matrix with the nodes represented as the rows and the constituents represented as the columns. The concentrations are given in units of milligrams per liter (mg/L).

The ninth output table, "CONSTANT DARCY VELOCITY SPECIFIED," echos the input from card type 01 or 02, if either is used. It simply lists the x and y velocity components specified.

The tenth output table summarizes the "NODAL CONNECTIONS AND MATERIAL NUMBERS" specified on card type I. It is simply a table of element numbers and the corresponding node numbers that define each element (up to the maximum of eight nodes). These are given in the order that CHAINT encountered them. Note that the table also includes the element type (the material or rock type) and the order used in solving the matrix equations (this may be modified or defined manually or by using a geometry preprocessor such as MESHER). This table is not produced if IECHO=0.

The eleventh output table, "NODE POINT COORDINATES (M)," is an echo of the node point locations as defined for the problem on card type J. It is simply a table of node numbers and corresponding x- and y-coordinates. This table is not produced if IECHO=0. Note that the (M) in the table title refers to the fact that coordinate values are taken to be meters.

The twelfth output table, "ELEMENT SOURCE LOADS," echos the mass loading or release information input on card types Q, R, and S. The card types are echoed in the order just given, and the parameters on each card type are echoed in the input order (see section 4.2). Note that if NLD is zero or blank, card types R and S are not used. In addition, the value for the release period (RELZ) is output only if NLD<0.

The thirteenth output table, "MASS FLUX COMPUTATIONAL DATA," reports the data input on card types P1, P2, and P3, in that order. This data will be printed only when the flux output has been requested (NCFLX>0), and the corresponding data has been input.

The fourteenth output table presents the "INITIAL CONDITIONS." This is an echo of the "INITIAL CONDITIONS" defined by the user or generated by CHAINT, at the request of the user, on card type L1 or L2. It consists of a list of the node numbers at which the initial conditions are defined, and the concentrations are specified at those nodes. This table is not produced if ISKO=0.

5.2.3 Simulation Results

The title entered by the user on card type A is printed in the upper left corner of each page of simulation results, immediately below the CHAINT banner page. The next line announces the results time in years, or that the results are for steady state. The constituent name and number are displayed, and the concentrations are listed in tabular form on a node-by-node basis. This table is repeated for each active constituent in the model. The user will note asterisks occurring beside some of the concentration values. These mark the specified boundary conditions. Note that if the user has asked for the abbreviated listing (ISKO=2), many of the header items and labels will be omitted from this output.

Immediately before the output for each time step, the user is informed of the decay chain that was used for the next time period. Immediately after each step, a small table reporting the maximum and relative change in concentration for each constituent and the approximate maximum Peclet number for each material type is produced. The latter is often useful for determining the progress of the solution process in fine tuning the model.

5.3 OTHER OUTPUT FILES

The input/output file LUNs are all specified on card type C, File Assignments. The parameters associated with these other output files are IS4, IS5, and IS7. The use of some of these files may be clarified by considering the data flow diagrams in appendix A. A discussion of each of these files follows.

IS4 CHAINT Binary Restart Data File. It contains all the necessary data needed to restart the simulation from the time step at which the file was produced. When CHAINT is flagged to produce this file, it will indicate that the restart file was generated by printing a message to that effect after the concentration printout. The time step at which this message is printed is the time step at which the restarted run will commence.

IS5 CHAINT Binary Plot File. It contains the concentration values at each node for each user-specified time step. This data may be gridded using GRIDDER or LEGRID; contour, time history, or spatial profile plots may be produced from it. In addition, the data may be used to generate a single-element results plot using PLOT1.

IS7 CHAINT Binary Mass Flux File. It contains the same results that were printed from calculations. This file may be utilized by the CHTFLX program for graphic display of the fractional release and the total release.

6.0 NOMENCLATURE

Symbol	Interpretation	Typical Units
R_d	Retardation	--
ϕ	Effective porosity	--
C	Concentration	mg/L
t	Time coordinate	yrs
x,y	Global space coordinates	m
η,ψ	Local space coordinates	--
q	Darcy velocity	m/yr
D_m	Hydrodynamic dispersion coefficient	m^2/yr
λ	Decay rate	1/yr
$\dot{m}$	Mass source strength	mg/L-yr
D	Coefficient of molecular diffusion	m^2/yr
α	Dispersivity	m
U	Lateral Darcy velocity	m/yr
V	Vertical Darcy velocity	m/yr
$\bar{q}$	Groundwater speed	m/yr
K_d	Sorption coefficient	m^3/kg
ρ_s	Bulk density	kg/m^3
$T_{\frac{1}{2}}$	Half-life	yr
P	Splitting fraction	--
S	Injection rate	mg/L-yr
NP	Total number of nodes	--
ω	Shape function	--
ε	Residual	--
χ	Galerkin functional	--

θ	Weighting factor	--
Pe	Peclet number	--
Q	Mass flux	mg/m^2-yr
M_o	Total mass	mg
T_L	Leach period	yr
T_{ch}	Characteristic time	yr

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APPENDIX A

PROGRAM INTERNALS

INTRODUCTION

The CHAINT program is written in PRIME FORTRAN 77 and is currently running on the Basalt Waste Isolation Project PRIME 750 computer system. Earlier development work was performed on a UNIVAC 1100/40. Attempts were made to use standard FORTRAN 77, but some PRIME specific functions were used in isolated incidences. These will be pointed out in the following sections.

SUBROUTINES AND THEIR FUNCTIONS

The section will list the subroutines used by the CHAINT program and give a brief explanation of the function of each.

CHAINT — The main program that controls the simulation by calling the appropriate subroutines. The CHAINT subroutine initiates the solution for each time interval. For transient solutions, the dependent variables and their gradients are predicted for the next time step. The flow field is calculated using subroutine VEL, if necessary. The contaminant concentration file, restart data file, and the mass flux file are written in this module.

BANNER — Prints a banner page including the date and time at which the run is initiated. This subroutine also generates the unique run identifier.

INPUT — Reads in control parameters, file unit assignments, time-step parameters, scale factors, geometry data, initial and boundary conditions, and material properties (both rock material and contaminate).

LOAD — Reads and computes the mass release rate for the (source term) nuclide in the decay chain. Input data includes source load values at specified times. A linear interpolation is used to compute the source loads as a function of time using entry point LOADS.

LOAD1 — Computes the mass loading rate history for an arbitrary decay chain. A closed-form analytical solution is used to take into account initial inventory and release period, as well as banded release.

HEADR — Writes file headers to external files and reads the header record from the velocity file, if required. Note that the header on the Restart Data file is read in the INPUT subroutine.

FRONT Performs a Gauss elimination procedure using a frontal solution method for unsymmetric matrices. Partial pivoting is used in the elimination process.

FLUX Prints the mass flux data to the mass flux output file.

RESOL Performs the back substitution for the updated right-hand sides. The algorithm is based on the frontal solution approach.

RGHTSD Forms the right-hand side load vectors that take into account updated loading rates and source terms from the decay chain.

SELECT Scans the decay chain connectivity and restructures the chain. Components with short half-lives relative to the time step are dropped from the chain and flagged for subsequent computation on the basis of secular equilibrium.

SETUP Sets up a pointer array for the finite element matrix and computes the total storage requirements.

STIFR Forms the coefficient matrices for each finite element. A Gaussian quadrature is used in the numerical integration of the Galerkin finite equations. Quadratic basis functions are used in the approximations of the spatially varying coefficients and the dependent variables over the isoparametric finite elements (triangles and quadrilaterals).

SURFAC Checks connectivity of the flux surface element list. A list of these connections is created along with a list of all nodes connected to flux surface elements.

UPSTRM Calculates the upstream weighting functions for the Petrov-Galerkin modeling. This is used only for line elements and only when the Peclet number exceeds one-half. It is assumed that the velocity gradients are negligible.

UPDATE Transfers data from one internal array to another to update time-step data for velocities before reading the new time-step data.

VEL Computes the Darcian flow velocity at element Gauss points from the hydraulic head and conductivity values. Quadratic-shape functions are used in computing the velocity components on the two-dimensional elements. Permeabilities are given in x and y only (no cross term). Line elements are treated as isotropic.

WRT Performs mass transfer of pivotal row to scratch file according to a flag. Calls subroutine RWND (rewind file), POSIT (position file), and BINOUT (writes file).

RED Reads pivotal row from scratch file for back substitution with mass transfer of data. Calls subroutines POSIT (position file) and BININ (read file).

9 3 1 2 4 1 7 1 7 7 3

RWND A subroutine using PRIMOS calls to rewind the scratch file.

POSIT A subroutine using PRIMOS calls to position the file pointer relative to the current location.

BININ A subroutine using PRIMOS calls to read variable length records from disk.

BINOUT A subroutine using PRIMOS calls to write a binary variable-length record to disk.

PRINT Prints out the tabular results for nuclide concentrations at each nodal point. Specific boundary values are indicated in the output by an asterisk.

RDVEL Reads the input data from the MAGNUM-2D pathline file. This data is used to calculate velocities at element Gauss points.

BLKDAT A block data routine that contains shape function and derivative evaluations at the Gauss points within the isoparametric finite elements (triangles or quadrilaterals). The data statements contain evaluations specific to Gaussian quadrature formulas based on 2x2 Gauss points for linear-shape functions (that are not used for CHAINT) and 3x3 Gauss points for quadratic shape functions. Block data is not executable code.

PARA This is not really a subroutine, but a file containing the parameter statements used to define the program limits. See the next section for details.

PROGRAM LIMITS

All arrays that would need to be changed due to a need to increase the model size are dimensioned using "PARAMETER" statements. If required, the maximum limits can be increased or decreased by changing these parameters within the insert file PARA and recompiling the program. Note that PARA contains images that are included or inserted in a subroutine at compilation time. Most systems have such a facility. In PRIMOS, it is the INSERT FORTRAN directive.

The following parameters are used in CHAINT:

MQL Maximum number of decay chain components

MAXE Maximum number of elements

MAXP Maximum number of node points

MAXMAT Maximum number of material types

NMAX Maximum frontwidth of equation network array

NTT	Maximum number of time intervals
MAXFLX	Maximum number of flux surface definition elements
MAXPF	Maximum number of flux nodes that may be defined
MAXSLT	Maximum number of source load times that may be defined
MAXSF	Maximum number of flux surfaces.

The arrays affected by the parameters listed with the names of the common blocks in which they reside are as follows:

COMMON /BLK1/

EXTLD(MAXE,MQL)	Array holding the element loading at a given time for a specific contaminate
FRAC(MQL,2)	Splitting fraction for the radionuclide daughters
ISLT(MQL)	Activation flag for each constituent
ISU(MQL,2)	Constituent numbers of the daughter nuclide
NBC(MAXP)	Equation number for the nonboundary condition nodes.
NPCLET(MAXMAT)	Element containing the largest Peclet number for each material type.
PECLET(MAXMAT)	Maximum Peclet number for each material type
XKCOEF(MQL,MQL)	Constituent decay rate

COMMON /BLK1A/

CORD(MAXP,2)	X- and y-coordinates for each node
IMAT(MAXE)	Material type of each element
NOP(MAXE,8)	List of element-node connectivity

COMMON /BLK2/

AMU(MQL)	Mass number of each constituent
DIAG(MQL)	Half-life of each constituent
DLT(NTT)	Time-step size for each time interval

DML(MQL)	Molecular diffusion (m^2/yr) for each constituent
NTS(NTT)	Number of time steps taken within each time interval
NTSG(NTT)	Result data print frequency within each time interval
POR(MAXMAT)	Effective porosity
ROD(MAXMAT)	Rock bulk density (kg/m^3)
ZONEB(NTT)	Bottom boundaries for active zones for all time intervals
ZONEL(NTT)	Left boundaries for active zones for all time intervals
ZONER(NTT)	Right boundaries for active zones for all time intervals
ZONET(NTT)	Top boundaries for active zones for all time intervals

COMMON /BLK3/

ORT(MAXMAT,2)	Longitudinal (1) and lateral (2) dispersivity for each material type (m)
UL(MAXMAT)	X-component of flow (m/yr) when defined by material type
VELU(MAXE,9)	X-component of velocity (m/yr) at each Gauss point for each element
VELV(MAXE,9)	Y-component of velocity (m/yr) at each Gauss point for each element
VL(MAXMAT)	Y-component of flow (m/yr) when defined by material type
WIDTH(MAXMAT)	Fracture thickness (m)
XKDI(MQL,MAXMAT)	Retardation factors for each constituent and each material

COMMON /BLK3A/

CNAM(MQL)	Constituent name
NME(MAXMAT)	Material (rock) name

9 2 1 2 4 1 7 1 7 7 6

CUNITS(MQL)	Character label containing units of concentration for each constituent

COMMON /BLK4/

IFL(MQL)	Vector used to track the blocking of the matrix during solution
NFIX(MAXP)	Active node flag (set if node is inside an active node zone
NFIXH(MAXE)	Element ordering array

COMMON /BLK5/

ISUP(MQL,2)	Working array for constituent daughter number
XFRAC(MQL,2)	Working array for splitting fraction

COMMON /BLK7/

NLE(MAXSLT)	Element numbers to which loads are applied
RLE(NTT,MQL)	Mass loading rates or initial inventories
TLE(NTT)	Time of loading

COMMON /BLK9/

LHED(NMAX)	Flags heading vectors
PVKOL(NMAX)	Flags pivot columns
QQ(NMAX)	Solution work vector

COMMON /BLK10/

HKAX(MAXMAT)	Hydraulic conductivity in the x-direction (m/yr)
HKAY(MAXMAT)	Hydraulic conductivity in the y-direction (m/yr)
HKXY(MAXMAT)	Hydraulic conductivity tensor cross terms (read from MAGNUM-2D data file and included for completeness)
THETA1(MAXE)	Temperature correction term to hydraulic conductivity (read from MAGNUM-2D data file)

THETA2(MAXE)	Temperature correction term to hydraulic conductivity (read from MAGNUM-2D data file)

COMMON /BLK10A/

BOUY1(MAXP)	Buoyancy correction to vertical velocity terms (read from MAGNUM-2D data file)
BUOY2(MAXP)	Buoyancy correction to vertical velocity terms (read from MAGNUM-2D data file)

COMMON /BLK10B/

H1(MAXP)	Head at each node (read from MAGNUM-2D data file)
H2(MAXP)	Head at each node (read from MAGNUM-2D data file)

COMMON /BLK11/

ICFLX(MQL)	Constituent numbers of constituents to be used in calculating mass flux
IEFLX (MAXFLX,MAXFS)	Element numbers of elements defining the flux surfaces
IPFLX(MAXPF)	List of nodes used by elements defining the flux boundary surface
NLIST (MAXFLX,2,MAXFS)	Direction pointer indicating if flux is entering or leaving the enclosed areas

COMMON /BLK12/

EPSN(MQL)	Cutoff threshold for concentrations

COMMON /BLK13A/

TDOT(MAXP,MQL)	Time derivatives of concentration for the current time step

COMMON /BLK13B/

TDOTO(MAXP,MQL)	Time derivatives of concentration for the previous time step

COMMON /BLK13C/

TNEW(MAXP,MQL)	Concentration values for the current time step

COMMON /BLK13D/

TOLD(MAX)P,MQL)	Concentration values for previous time step

COMMON /BLK14/

R1(MAXP)	Work array used in solving the matrix equations

COMMON /DUMCOM/

TDOT1(MAXP,MQL)	Concentration derivatives two time steps back
TOLD1(MAXP,MQL)	Concentration values two time steps back
DUMMY(MAXP)	Dummy array used in reading data from MAGNUM-2D data files.

FILE MANIPULATION

All mass storage files used by CHAINT are referenced internally by their logical unit numbers (LUN). Each operating system has its own way of associating the LUN with the files needed or being created by an application program. For this reason, the user should consult the operating system reference publications for the machine being used. The remainder of this section specifically refers to the PRIME operating system (PRIMOS) but contains information that may prove of value for other machines as well. It is recommended for at least a cursory reading.

Preassigned Logical Unit Numbers

All the files except three are associated with, or may be associated with, a file previously generated or which will be generated by CHAINT. The first exception is LUN 16 that is used as the "out-of-core" solution scratch file. This file must be opened but is for scratch purposes only. The second and third exceptions are LUN 5 and LUN 6 (internal variables IIN=5 and IIOUT=6) that are used for the main input file and printed output file, respectively. That is, all the information discussed in section 4.3 enters CHAINT via LUN 5, and all reports of the results of the analyses are printed (written out) via LUN 6. Variables IIN AND IIOUT are set in the main program and are passed through common block INOUT where needed.

PRIMOS Files

In PRIMOS the LUNs are associated with the appropriate files by using the OPEN command. It should be noted that the PRIME version of CHAINT requires special attention to the assignment and use of LUNs. The numbers used in section 4.3 for card type B are the FORTRAN logical unit numbers. These numbers have a range starting with one and going to a maximum value (consult the current PRIME FORTRAN manual). These are decimal numbers.

The PRIMOS LUNs, however, are octal numbers and have an offset of four relative to their FORTRAN counterparts. The following table shows the arrangement:

FORTRAN (decimal)	PRIMOS (octal)
1	user terminal
2	paper tape
3	card reader
4	serial printer
5	1
6	2
7	3
8	4
9	5
10	6
11	7
12	10
13	11
.	.
.	.
.	.

Note that the arrangement shown means the FORTRAN I/O LUN 5 and LUN 6 correspond to the PRIMOS LUN 1 and LUN 2, respectively. Great confusion may occur on the PRIME if the user does not take this situation into consideration when developing command files and defining the OPEN commands.

The CHAINT Organization Diagrams

The control flow for the CHAINT program is shown in figure A-1, and the calling hierarchy among the subroutines is shown in figure A-2.

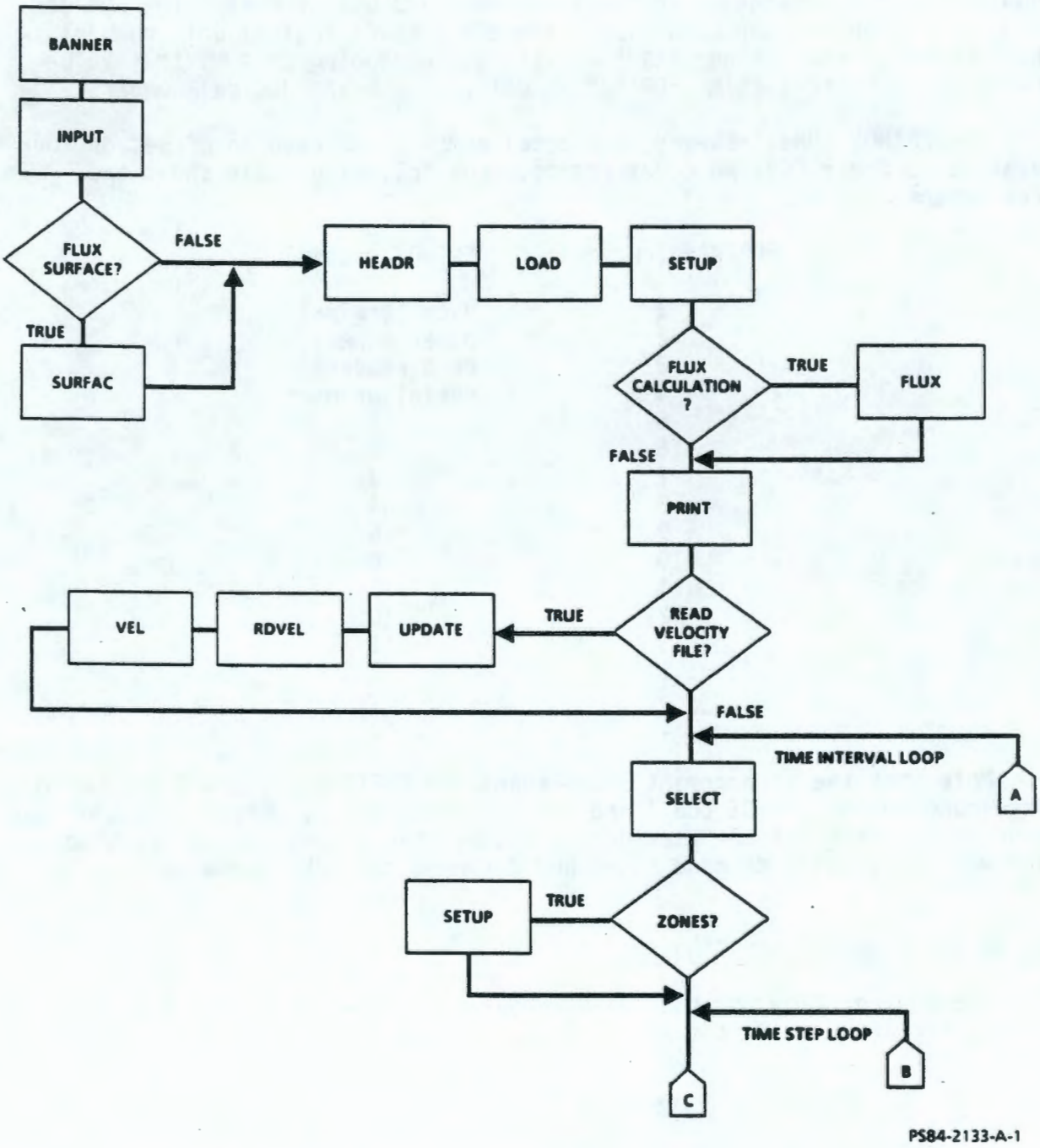


FIGURE A-1. Top-Level Control for CHAINT. (sheet 1 of 2)

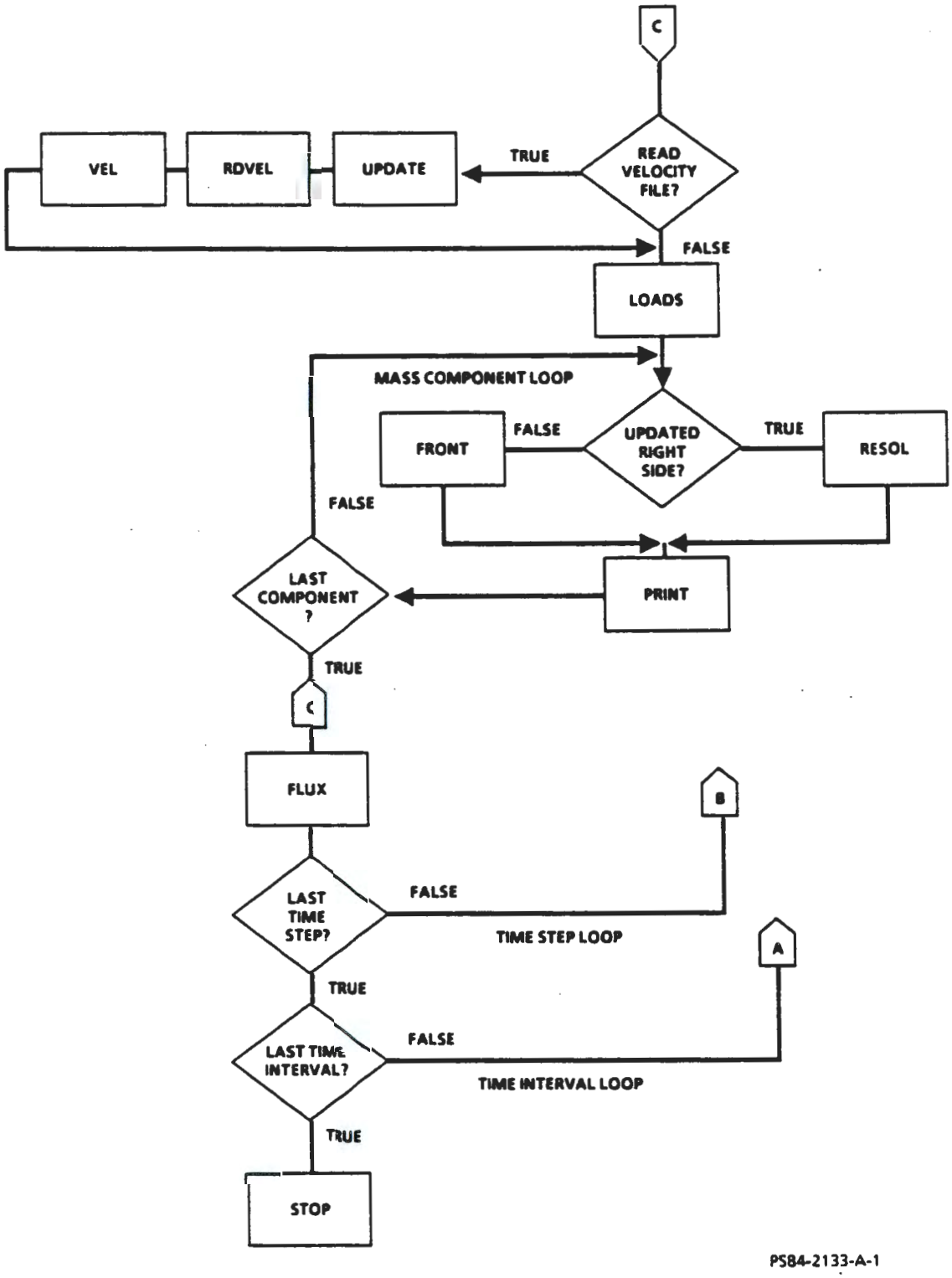
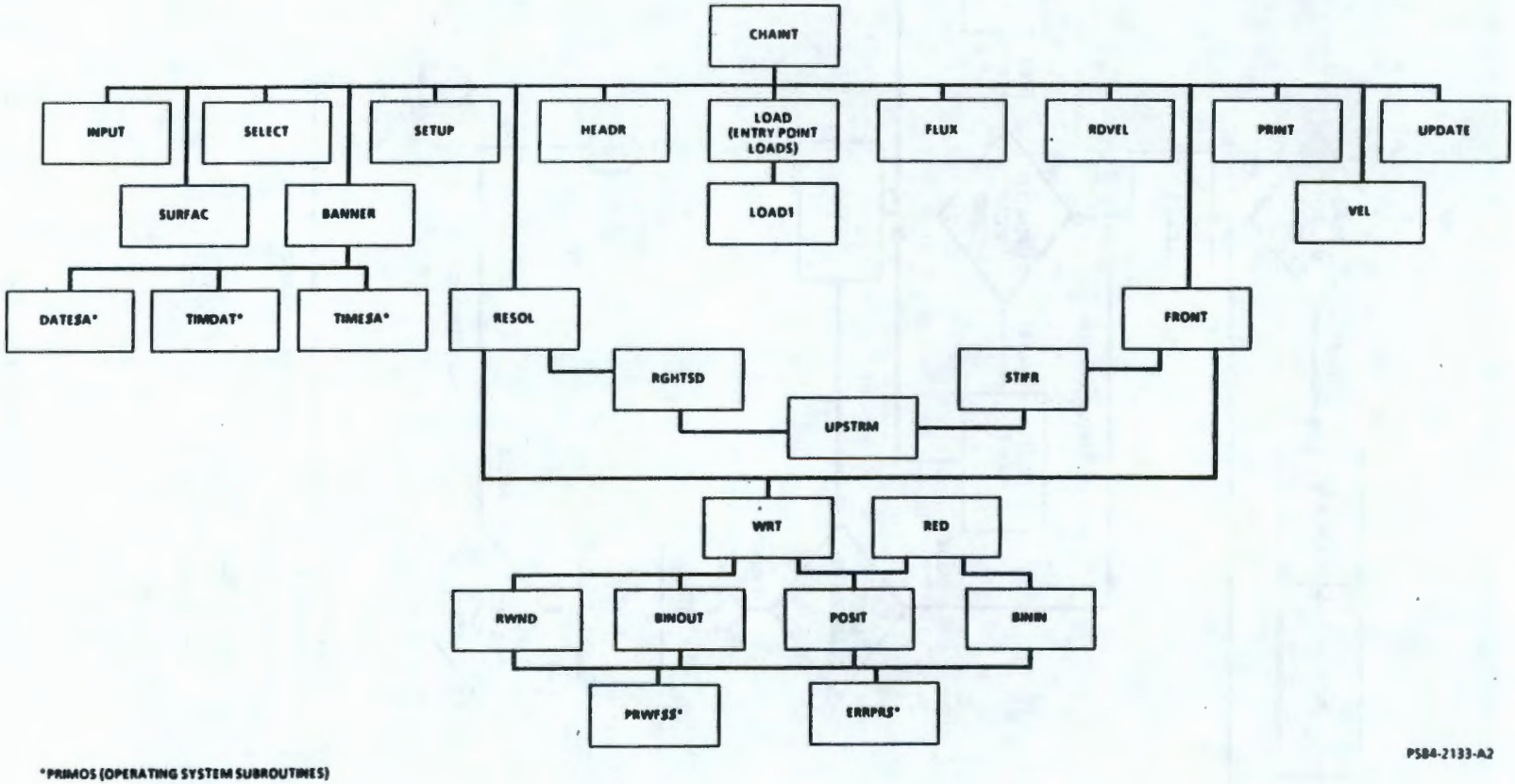


FIGURE A-1. Top-Level Control for CHAINT. (sheet 2 of 2)



*PRIMOS (OPERATING SYSTEM SUBROUTINES)

FIGURE A-2. Subroutine Hierarchy for CHAINT.

APPENDIX B

PREPROCESSORS

INTRODUCTION

A finite-element code such as CHAINT requires an extensive input data set, including geometry, initial conditions, and boundary conditions. The creation of this data set can be automated to some extent by providing "tools" to help the modeler develop and handle the requisite data. The tools used to create the data, known collectively as "preprocessors," deal mostly with the input geometry data. Geometries may be created, refined, modified, optimized, verified, and plotted. Two other preprocessors exist for creating initial and boundary condition data.

This appendix lists the CHAINT-compatible preprocessors and gives a brief description of each. It will then give a brief discussion on the steps that must be followed to use the preprocessors to generate a data set to be used for a simulation.

Note that this section is not intended to be an instruction manual for any of the preprocessors described. Detailed instructions will be found in the manual dealing with the auxiliary programs useful to the MAGNUM-2D/CHAINT user.

CHAINT PREPROCESSORS

The FEMESH code is used to generate arbitrarily shaped, finite-element geometries. The input for FEMESH is a coarse finite-element geometry of quadrilateral elements followed by some refinement specifications telling FEMESH how the coarse mesh is to be subdivided. This input must be in coded form (ASCII, etc.). The input format for the coarse geometry is exactly like that required for the MAGNUM-2D or CHAINT geometry. This allows the user to generate the coarse mesh "by hand" using a standard editor program. The user may also generate the coarse mesh using GEN and later add the refinement data by hand using an editor. The FEMESH code will generate triangular, as well as quadrilateral elements, but the input is restricted to quadrilaterals.

The GEN code is a simple processor for generating regular, rectangular finite element geometries of quadrilateral or line elements. No prior preparation of input data is required. The program prompts the user for all required input. The output geometry may be chosen as a set of quadrilaterals or a network of line elements. The lower left-hand corner of the rectangular area generated may start at whatever coordinates the user requests. All the elements will have the same material type specified. This parameter is also prompted by the program. The data generated by GEN is written to a file in coded form and may be suitably modified for use by the FEMESH code by adding the refinement data required (see FEMESH).

The MOD code allows the user to make simple modifications to a geometry including node position, geometry scaling, rotating, mirroring, or translating; to change the slope, angle, material type, or connectivity; to recalculate the midside node positions; or to create new elements.

The PLT code is used for plotting two-dimensional finite-element geometries. All three element types (quadrilaterals, triangles, and lines) are recognized. The plots produced are the mesh alone; the mesh with node, element, or material types numbered; single elements; and subregions of the entire mesh with all the above options. (Note: This program makes use of the DISSPLA* graphics system. This library of FORTRAN graphics routines is necessary to run PLT on any computer system.)

The PURGE code is used to verify a geometry. Checks are made for some of the more common errors. These include errors in element connectivity specification, midside node placement, unused nodes and elements, duplicate nodes, node rotation, free elements, ill-defined elements, aspect ratios that are potentially unacceptable, elements that overlap or are distorted, and correctness of the ordering array. Obvious errors, such as unused nodes and elements, are corrected while more devious errors are noted for the user to correct.

The REFINE code allows single elements to be divided into two smaller elements or two smaller elements to be combined into one larger element.

The TRGEN code will generate a finite element transition geometry using triangular elements to go from a region of smaller elements (a region denser in elements) to a region of larger elements (less dense).

The BCGEN code is used to generate a boundary condition data file for input to MAGNUM or CHAINT. A geometry is read from a geometry file, and a search is made for all boundary nodes. These nodes are then listed in counterclockwise order, and two user-generated subroutines, BCHEAD and BCTEMP, are called to generate the boundary conditions for head and temperature respectively. This program may require some user modification of the code.

The ICGEN code is used to generate an initial condition data file for input to MAGNUM-2D or CHAINT. A geometry is read from a geometry file, and the initial conditions are calculated based on position (or other appropriate variable) by a function or algorithm coded into the program. This program requires user modification of the code.

The ICMOD code is more of a utility than a preprocessor. It allows the user to convert an initial condition file to a file that looks like a binary results file. This file may be gridded and contoured for inspection. Alternatively, a binary results file may be converted for use as a coded initial condition file.

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*DISSPLA is a proprietary software product of Integrated Software Systems Corporation, San Diego, CA.

MODEL GENERATION WALK THROUGH

The first step in the generation of any finite element model is the determination of the exact geometric definition of the model. This should include dimensions and locations of all features associated with the region being modeled, such as voids, varying material types, heat and fluid sources, etc. Once this data is collected, the modeler must determine the optimum form of the model to ensure accurate mathematical representation of the region and, therefore, accurate results. If the area of highest gradient can be identified beforehand, often the modeling effort is simplified and the model size is limited, since this allows the high element density to be restricted to those high-gradient regions.

One successful method for the creation of the model has the modeler start with a sketch of the region to be modeled. Any identifiable subregions are then indicated (i.e., subregions composed of a single material, voids, etc.), and a plan of attack is determined, such as modeling these subregions and merging them into a whole model. This technique will be assumed in the following discussion.

A data flow diagram for the preprocessors and files discussed in this section is shown in figure B-1. It is recommended that the reader follow this diagram while reading the following paragraphs.

Often the first program to be used, and perhaps the only one needed depending on the complexity of the model, is GEN. If it is convenient to produce the entire model or complete subregions with GEN, the task is simplified; however, GEN may also be used to generate a preliminary coarse mesh to which the refinement data is added using an editor, and this file is then run through FEMESH to refine and enhance the mesh.

Note that in creating the mesh for subregions, great care should be exercised to ensure the boundary nodes are located at common geometric points so merging the meshes is possible. If the points do not coincide or at least vary with a constant x- or y-dimension offset, it will be necessary to modify a potentially large number of coordinates before merging is feasible. This can be very time consuming and difficult.

If a transition zone is necessary between regions of varying element densities (i.e., between regions of suspected high and low gradients), then TRGEN may be used to produce the zone as a separate region.

The various "pieces" of the model may be combined or merged using MERGE. This program will take any two geometry files and attempt to merge them at their common node points; thus, the user may have to use this program several times depending on the number of subregions being combined. The MERGE code (like MESHER, MOD, and REFINE) has the ability to write the new geometry back into an old file or onto a new file, thus preserving the subregion data files for future use. A good precaution to take is to maintain all the component geometries until the model generation, or some phase of it, has been verified to be correct. This allows the user to redo a portion of the geometry from the last correct phase in case a mistake is made.

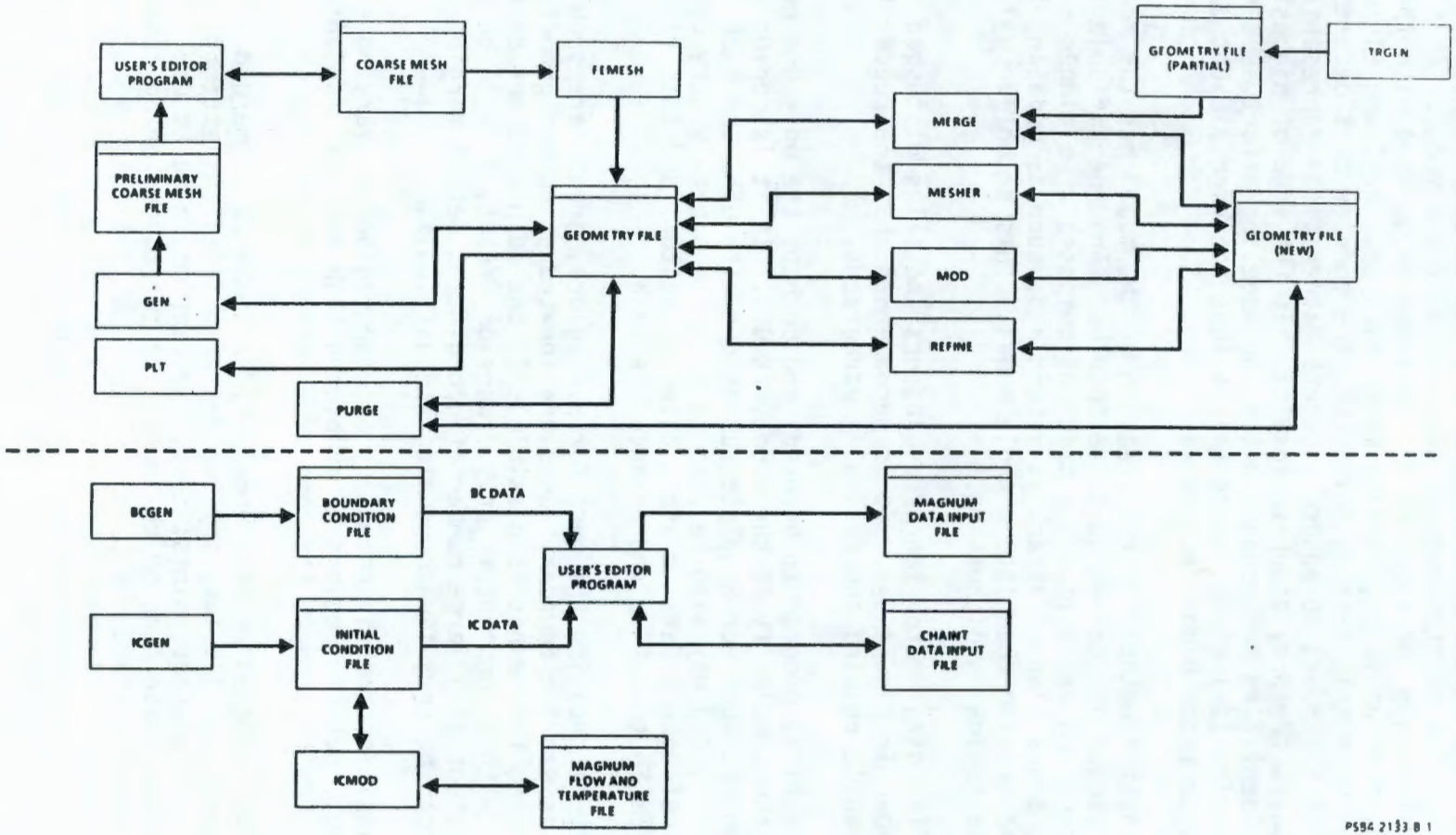

FIGURE B-1. Preprocessor Data Flow.

At any point in the model generation procedure, the program PLT may be used to view the model. It is helpful to have hard copies of the element and node number plots at hand when merging geometries.

Often the automatically generated finite element geometry is not sufficiently accurate or the region is too intricate to attempt defining adequate constraints for automatic generation. In these cases it is up to the modeler to amend and modify the geometry to produce the desired results. The MOD program will allow the user to change node locations or connectivity. This is convenient when the material boundaries require specific location of elements or midside nodes do not fall where they should when generated automatically. In addition, MOD will allow the user to mirror or translate geometries so the modeler may use any symmetry in the model. The REFINE program is useful in "fine tuning" a geometry because it allows the user to produce a fine mesh in just a few elements without defining a subregion. Both MOD and REFINE find great utilization in "refitting" a model, that is, modifying it after it is complete for sensitivity analyses or because of features revealed by the initial analysis.

After the model parts have been assembled and the actual node locations have been fine tuned, it is wise to run PURGE on the geometry. This ensures that many of the small and unobvious errors that may creep in during the creation process are removed. These errors may not be large in themselves, but they may create great variations in the final simulation results if they occur in a critical location. It is a good idea to make at least one PLT run on the final geometry file for a final visual check. A hard copy of the node number, material type, and element number plots is almost required in order to analyze the results of a simulation in detail.

After the geometry file has been created, it may be in one of two forms: binary or coded (ASCII, BCD, etc.). Either of these are readable from MAGNUM-2D or CHAINT. It may be utilized by reading the file directly from mass storage (in coded or binary form) or, in the case of a coded file, it may be edited into an input file that contains all the other data necessary for the simulation (boundary conditions, material properties, and other data as described in card types A through R).

Using an editor program, the remainder of the data required for simulation as described in the input card types is usually entered into a mass storage file, the MAGNUM-2D or CHAINT data input file. The geometry card types may be entered from the coded form of the geometry file or may be omitted and read from a binary or formatted mass storage file at execution time by specifying the logical unit number on card type C. The initial and boundary conditions, however, must be included in the data input file. If they are few enough or, in the case of initial conditions, consistent enough, they may be entered directly by using the editor. If they are numerous, the two programs ICGEN and BCGEN are used to produce files of initial and boundary conditions, respectively, which are edited into the data input file.

A data flow diagram for the MAGNUM-2D and CHAINT environment and the data files involved is shown in figure B-2. Note that for a nonrestart job, only two input files are needed: the CHAINT data input file and the geometry file.

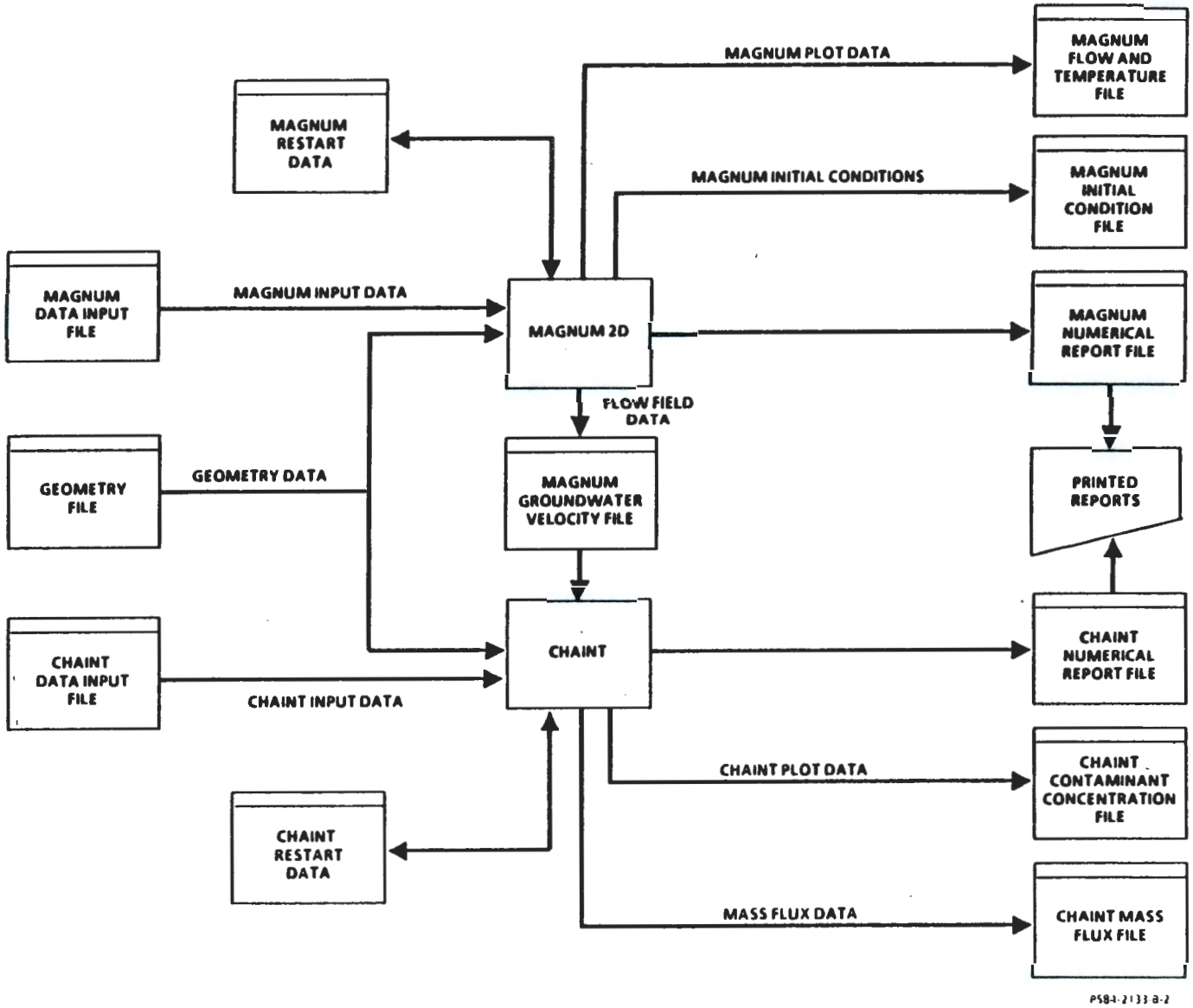

FIGURE B-2. MAGNUM-2D/CHAINT Data Flow.

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APPENDIX C

POSTPROCESSORS

INTRODUCTION

A finite element code, such as MAGNUM-2D or CHAINT, creates a large amount of output data that is often difficult to interpret in its raw form. Postprocessors provide a means of graphically displaying output data in a variety of modes. These may be two-dimensional contour plots of the results, cross-sectional plots of the data versus position, or time history plots for the data at a given location. In addition, pathlines, streamlines, velocity vectors, and mass flux data may be plotted.

This appendix will list the postprocessors available for MAGNUM-2D and CHAINT and give a brief description of each of them.

This section is not intended to be an instruction manual for any of the postprocessors described. Detailed instructions will be found in the manual dealing with the auxiliary programs useful to the MAGNUM-2D/CHAINT user.

All graphics postprocessors utilize proprietary graphics software.

CHAINT POSTPROCESSORS

A data flow diagram for the postprocessors and files discussed in this section is shown in figure C-1. Note from figure B-2 that there are three files output from CHAINT but that only two show in figure C-1. These are the only files that are used in postprocessing. They are the geometry file, the CHAINT contaminant concentration file, and the CHAINT mass flux file.

The CHTFLX program produces mass flux plots from the CHAINT mass flux file. The program computes both mass flux and total (time integrated) flux of a contaminant through a surface of finite elements. Plots are made with units of fractional release (fraction of total mass) and total release (curies). Both the raw flux data (CHAINT mass flux file) and release data are printed out to the screen or to a user defined output file. The program CHTFLX has the ability to take the required data from the CHAINT contaminant concentration file along with some material constants which the user must enter and generate the same plots. This feature allows the user to investigate flux boundaries other than those defined in the CHAINT run, but the initial conditions and possibly some resolution may be lost.

The GRIDDER postprocessor interpolates nonregularly spaced nodal data onto a regular rectangular grid to allow contouring. The sister program LEGRID will grid line elements only. They accept the MAGNUM-2D flow and temperature file as input and place the output data in an output file that may be used by CONTOUR, HISTORY, and PARAM.

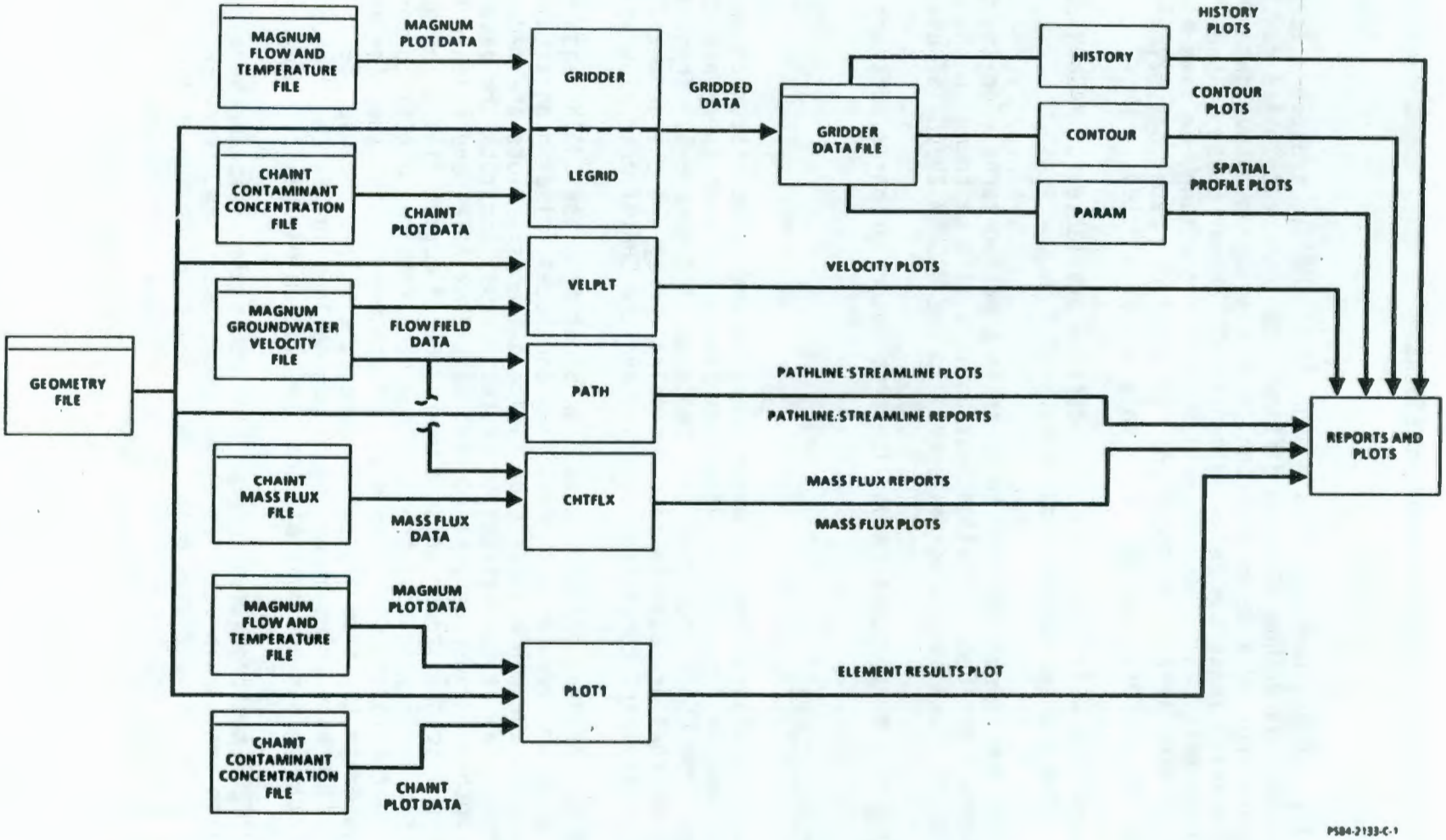

FIGURE C-1. Postprocessor Data Flow.

The CONTOUR postprocessor is used to draw contour line plots from data given as a function of two variables. The CHAINT contaminant concentration data must be interpolated onto a regular, rectangular grid using GRIDDER prior to using CONTOUR. This program is totally interactive, and the user is prompted to enter commands to set the desired plotting options, such as contour levels, background, and time plane.

The HISTORY postprocessor is used to plot results data as a function of time. The data histories corresponding to chosen locations in a finite element geometry are plotted. The histories of several points may be plotted on a single graph. The CHAINT contaminant concentration data must be interpolated onto a regular, rectangular grid using GRIDDER prior to using HISTORY.

The PARAM postprocessor is used to plot data cross sections. Data is plotted as a function of x or y, with either y, x, or time being varied as a parameter. Several curves may be plotted on a single graph. The CHAINT contaminant concentration data must be interpolated onto a regular, rectangular grid using GRIDDER prior to using PARAM.

The PLOT1 postprocessor is used to plot the contaminant concentrations on an elemental basis. A three-dimensional surface of the data is plotted along with a two-dimensional sketch of the element with written node values at each node. This program is useful as a diagnostic tool in the analysis of data anomalies. An error of insufficient geometry resolution can often be determined by examining the surface plot for data corresponding to a single element. The geometry file is also required as input for PLOT1.

9 3 1 2 4 1 7 1 7 9 4

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APPENDIX D

EXAMPLE CASES

Reproduced listings of the PRIMOS commands, input, and printed output for some example problems are contained in the Figures and Listings sections of this appendix.

The first example is a simple transport problem. The model is shown in figure D-1. A single row of elements with a constant uniform velocity field flowing from left to right is defined with the initial concentration specified in the element at the left-most end. The concentration cross sections at selected times in graphic form as produced from the postprocessor PARAM is shown in figure D-2. The geometry in this example is specified in the data input file, listing D-1. The PRIMOS commands used to run this example is shown in listing D-2. The resulting output is given in listing D-3.

The second example is a two-dimensional transport problem with a mass load (mass release rate). The model is shown in figure D-3. Note that figure D-3 is only the mesh; the node numbering option in the PLT program was not used. In addition, it is a subplot of the entire geometry. This model is typical of the type that might be used to model a repository simulation (although simplified) showing perhaps a bored repository with provisions for modeling the host rock, the grout or backfill, and the storage package. The inner semicircular area containing elements 70, 71, 72, 77, 84, 85, 89, and 90 are mass release elements. Both the initial and boundary conditions are specified as concentrations of 0.0 mg/L. There are two materials specified as the contaminant. One is assumed to be the decay daughter of the other. Thus, the mass loading is specified for only one constituent. A mass flux boundary is set using elements 47, 48, 61, 74, 87, 99, and 111. The data for mass flux across this boundary will be written to LUN 13. This simulation is set to run for 100 yr. The concentrations at time 100.0 yr for components 1 and 2 are shown in figures D-4 and D-5, respectively. The concentration profiles (as produced by the program PARAM) for components 1 and 2 are shown in figures D-6 and D-7, respectively. These profiles were taken roughly through the center of the repository. The data input file is shown in listing D-4. Note that the geometry, in this case, has been defined on an external mass storage file and has been specified as LUN 12. The PRIMOS commands used to run this example are shown in listing D-5. Note also, the specification of PRIMOS unit 10 to correspond to the file name GEOM, and PRIMOS unit 11 to correspond to the file MASFLX. The resulting output is shown in listing D-6.

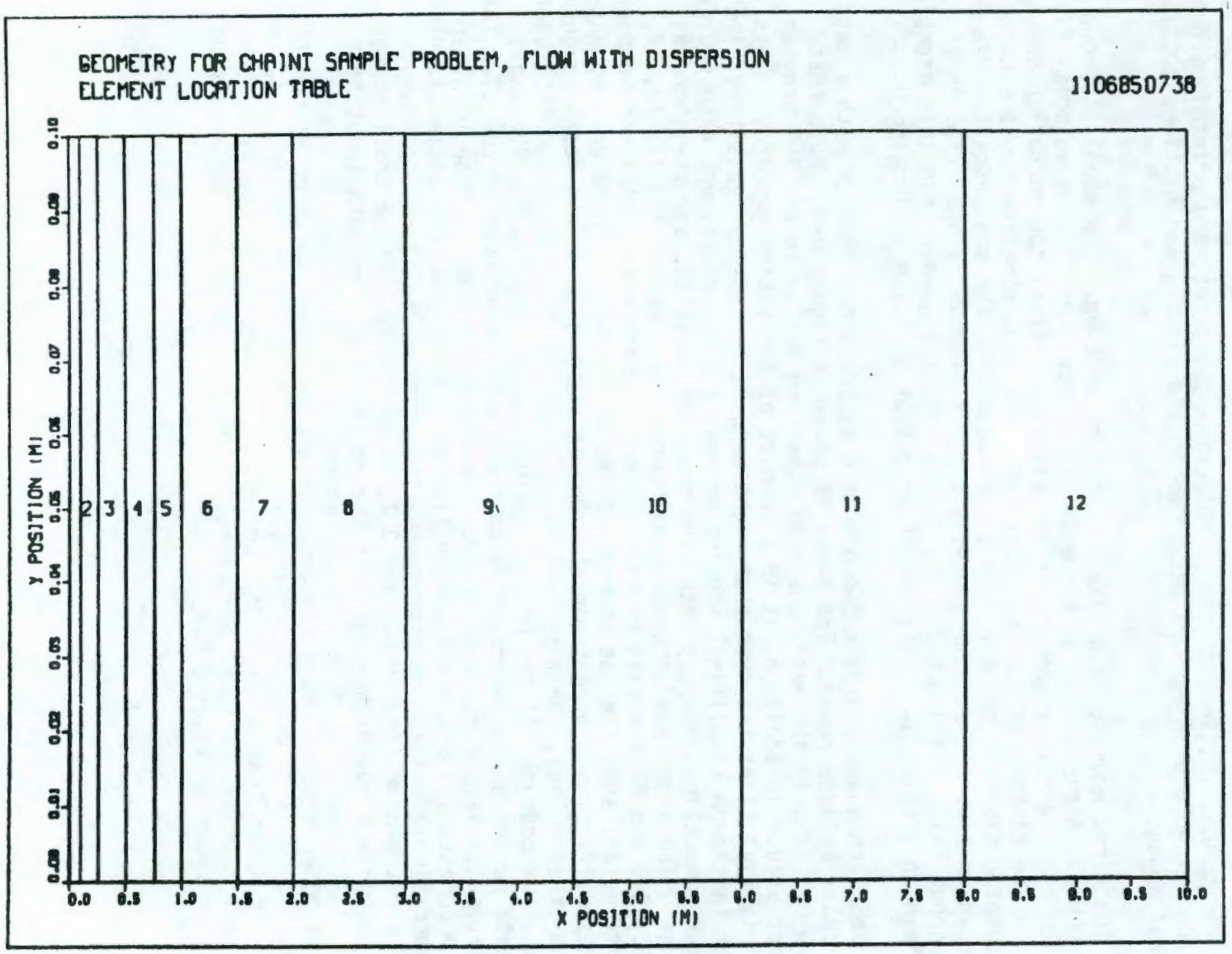

FIGURE D-1. Element Numbering for Test Case One.

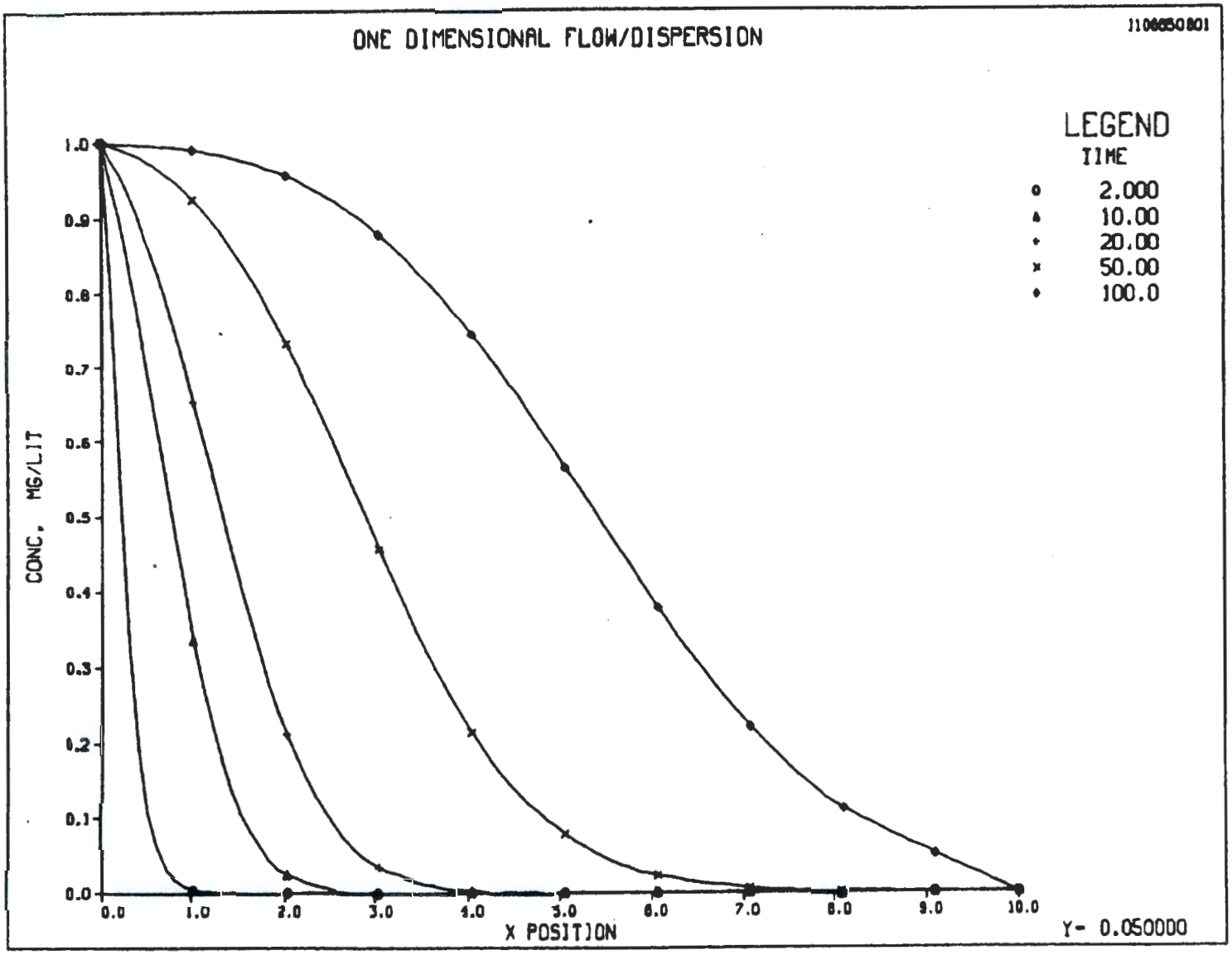

FIGURE D-2. Concentration Cross Sections at Selected Times.

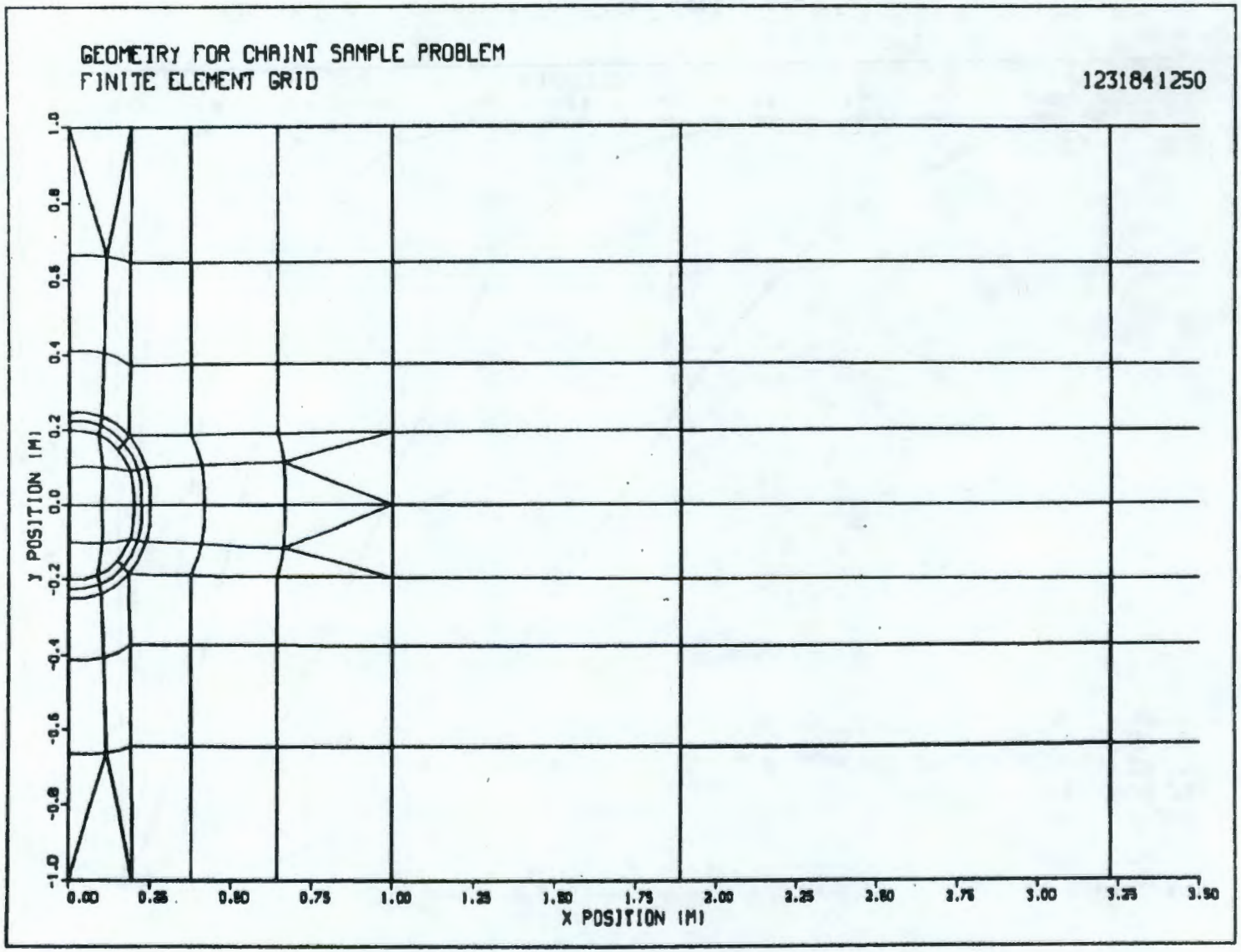

FIGURE D-3. Subplot of Finite-Element Grid for Test Case Two.

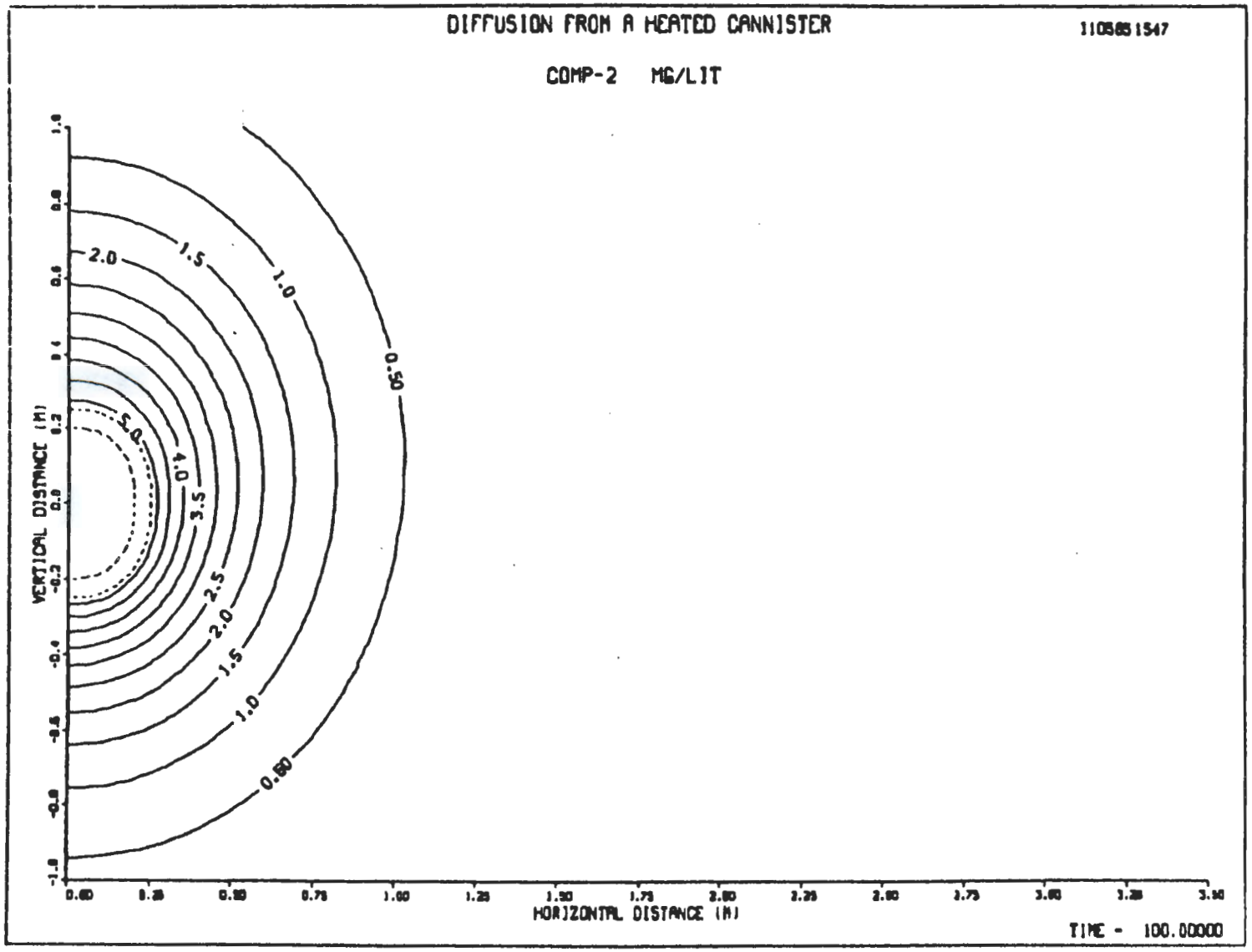

FIGURE D-4. Concentration Contours for Component One at 100 Years.

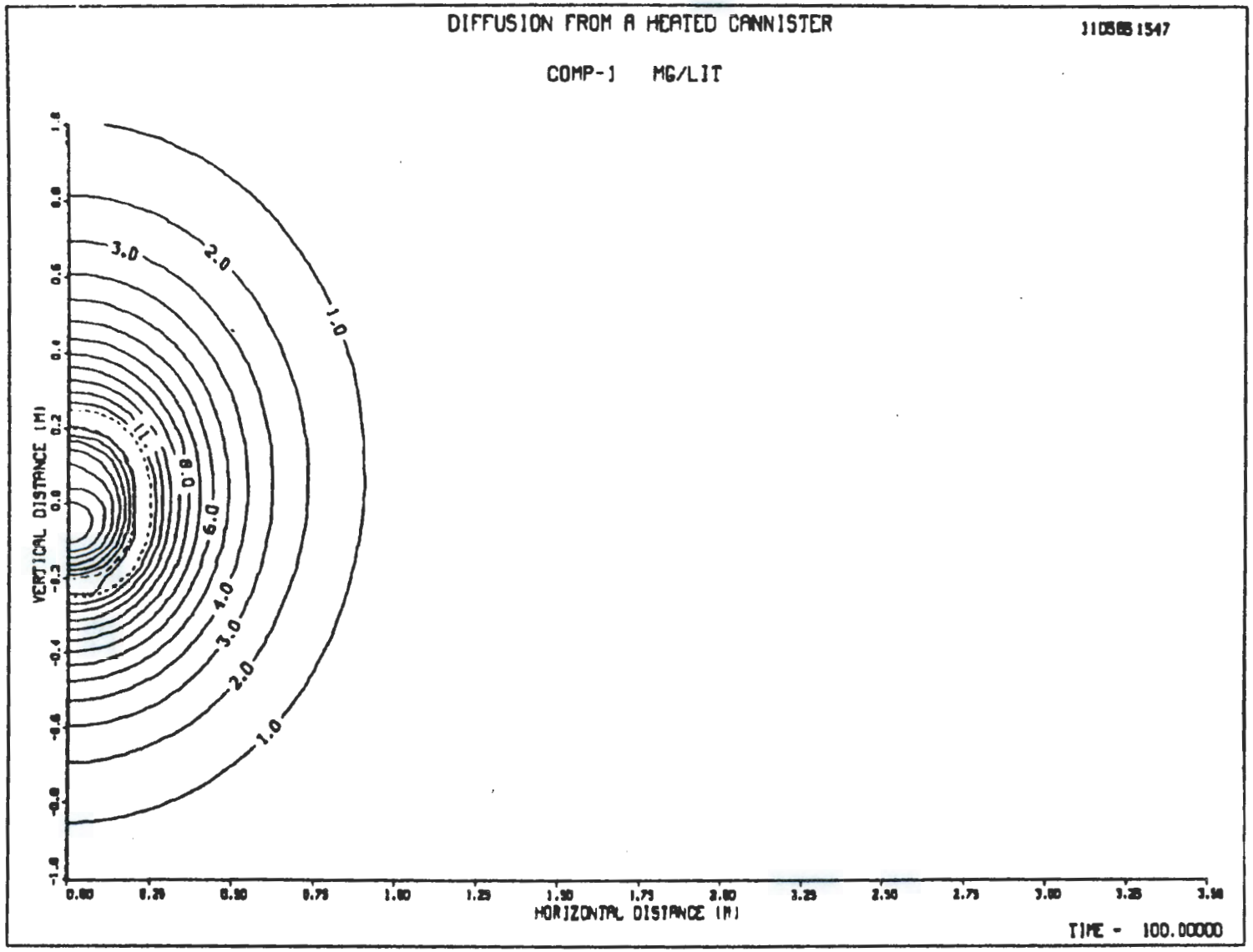

FIGURE D-5. Concentration Contours for Component Two at 100 Years.

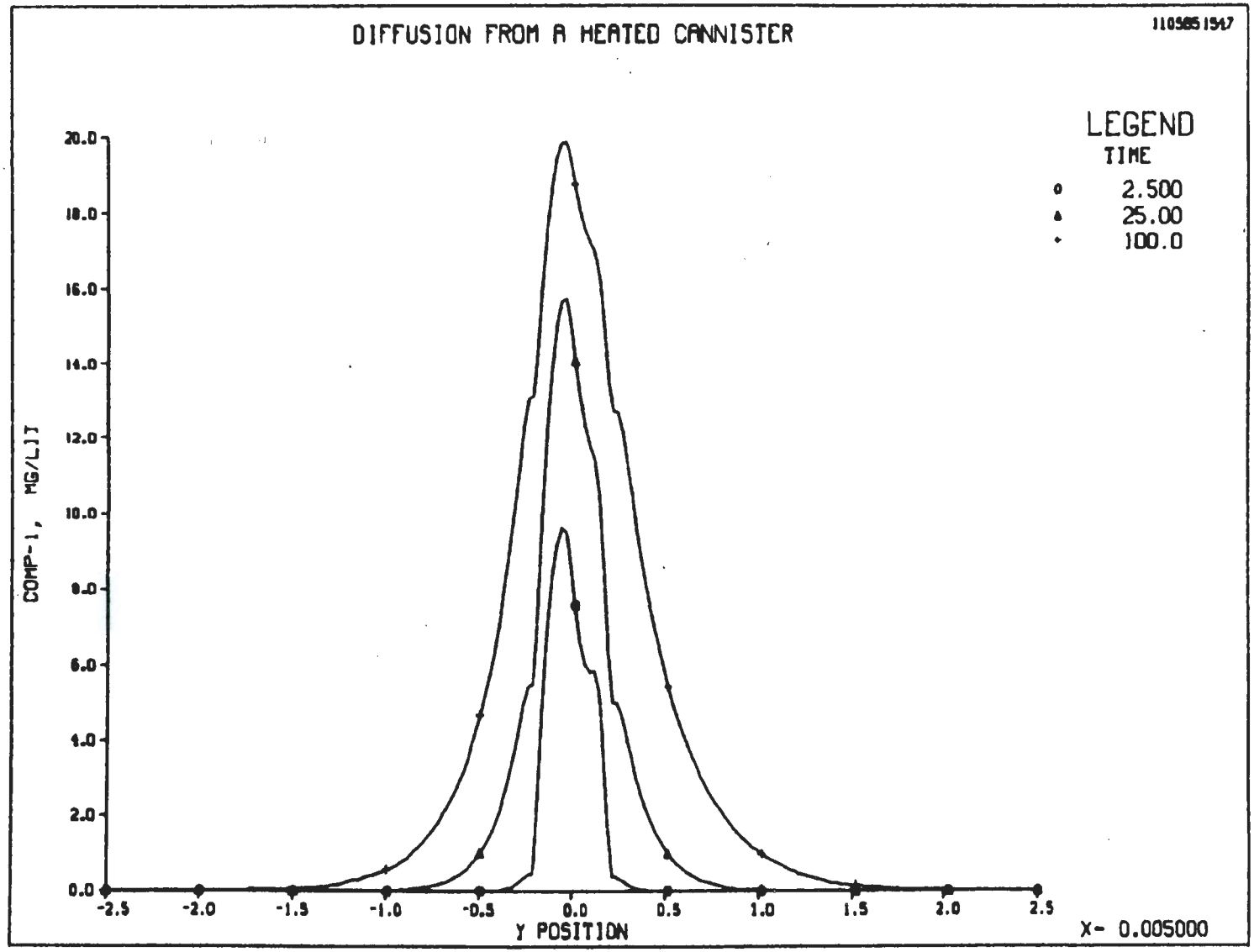

FIGURE D-6. Concentration Profiles at Selected Times for Component One.

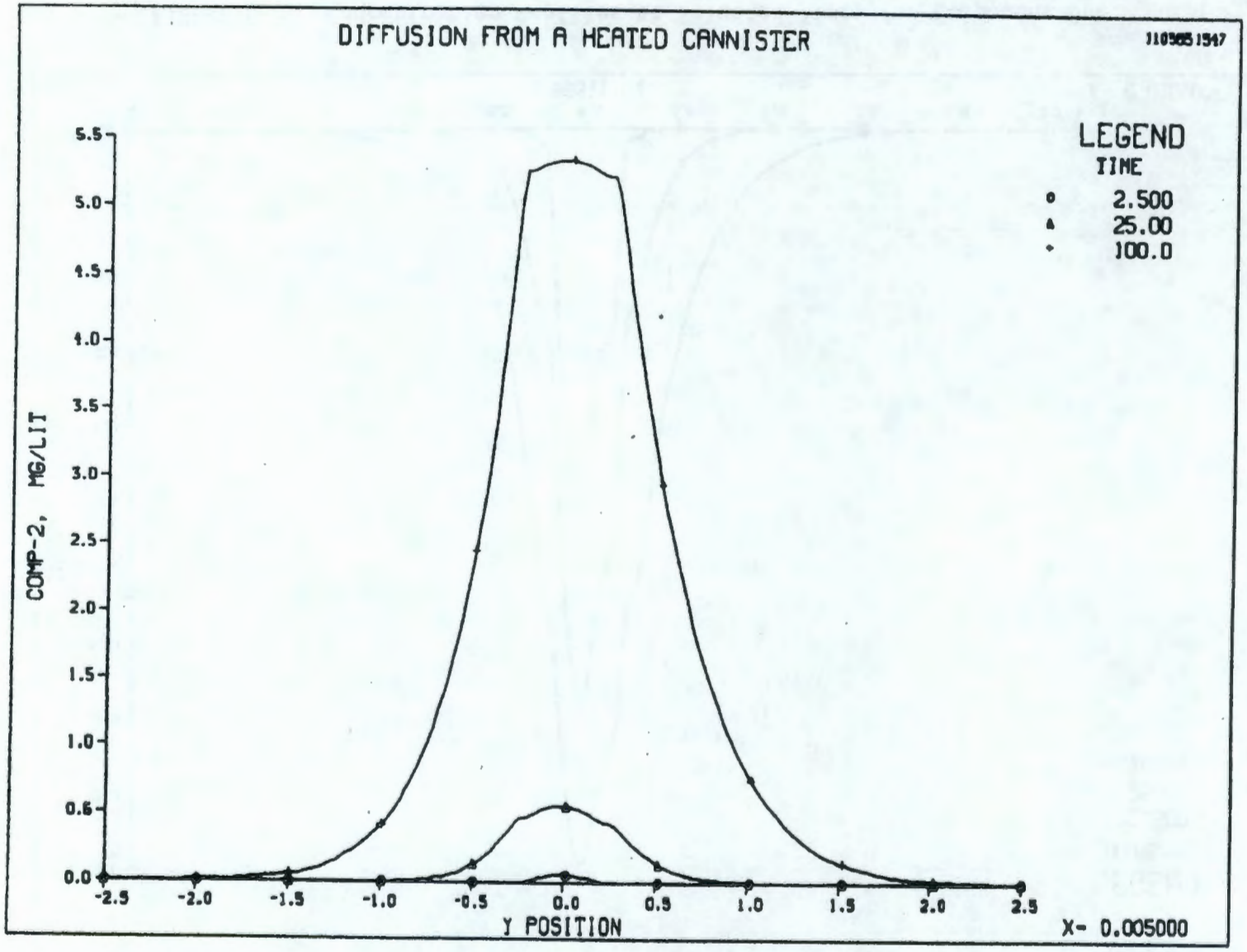

FIGURE D-7. Concentration Profiles at Selected Times for Component Two.

LISTING D-1. Input Data File for Test Case One. (Sheet 1 of 2)

```
ONE DIMENSIONAL FLOW/DISPERSION
    1   12   63    6    1    1    2    0    1    0                /*CNTRL
    0    0    0    0  -11    0   13                                /*FILE UNITS
         0.        1.8       0.0       0.0       0.0       0.0    /*STRT TME
    4    4        1.0
    3    3        2.0
    2    2        5.0
    8    8       10.0
9999
         1    1.0E-1    1.0E-1    2900.0       0.1       0.0   ROCK
1                                                                 /*CON SEL
    1  1.0   1.0E+11    0       0.0    0       0.0  CONCEN   0.0E+00
         1   2.0E-01                                            /*MOL DIFF
         1   0.31035                                             /*SORPTION
    1    1    2    3   27   41   40   39   26    1    1         /*GEOMETRY
    2    3    4    5   28   43   42   41   27    1    2
    3    5    6    7   29   45   44   43   28    1    3
    4    7    8    9   30   47   46   45   29    1    4
    5    9   10   11   31   49   48   47   30    1    5
    6   11   12   13   32   51   50   49   31    1    6
    7   13   14   15   33   53   52   51   32    1    7
    8   15   16   17   34   55   54   53   33    1    8
    9   17   18   19   35   57   56   55   34    1    9
   10   19   20   21   36   59   58   57   35    1   10
   11   21   22   23   37   61   60   59   36    1   11
   12   23   24   25   38   63   62   61   37    1   12
    1        0.000        0.000        0.00        0.00
    2        0.050        0.000        0.00        0.00
    3        0.100        0.000        0.00        0.00
    4        0.175        0.000        0.00        0.00
    5        0.250        0.000        0.00        0.00
    6        0.375        0.000        0.00        0.00
    7        0.500        0.000        0.00        0.00
    8        0.625        0.000        0.00        0.00
    9        0.750        0.000        0.00        0.00
   10        0.875        0.000        0.00        0.00
   11        1.000        0.000        0.00        0.00
   12        1.250        0.000        0.00        0.00
   13        1.500        0.000        0.00        0.00
   14        1.750        0.000        0.00        0.00
   15        2.000        0.000        0.00        0.00
   16        2.500        0.000        0.00        0.00
   17        3.000        0.000        0.00        0.00
   18        3.750        0.000        0.00        0.00
   19        4.500        0.000        0.00        0.00
   20        5.250        0.000        0.00        0.00
   21        6.000        0.000        0.00        0.00
   22        7.000        0.000        0.00        0.00
   23        8.000        0.000        0.00        0.00
   24        9.000        0.000        0.00        0.00
   25       10.000        0.000        0.00        0.00
   26        0.000        0.050        0.00        0.00
   27        0.100        0.050        0.00        0.00
```

LISTING D-1. Input Data File for Test Case One. (Sheet 2 of 2)

```
28      0.250      0.050      0.00      0.00
29      0.500      0.050      0.00      0.00
30      0.750      0.050      0.00      0.00
31      1.000      0.050      0.00      0.00
32      1.500      0.050      0.00      0.00
33      2.000      0.050      0.00      0.00
34      3.000      0.050      0.00      0.00
35      4.500      0.050      0.00      0.00
36      6.000      0.050      0.00      0.00
37      8.000      0.050      0.00      0.00
38     10.000      0.050      0.00      0.00
39      0.000      0.100      0.00      0.00
40      0.050      0.100      0.00      0.00
41      0.100      0.100      0.00      0.00
42      0.175      0.100      0.00      0.00
43      0.250      0.100      0.00      0.00
44      0.375      0.100      0.00      0.00
45      0.500      0.100      0.00      0.00
46      0.625      0.100      0.00      0.00
47      0.750      0.100      0.00      0.00
48      0.875      0.100      0.00      0.00
49      1.000      0.100      0.00      0.00
50      1.250      0.100      0.00      0.00
51      1.500      0.100      0.00      0.00
52      1.750      0.100      0.00      0.00
53      2.000      0.100      0.00      0.00
54      2.500      0.100      0.00      0.00
55      3.000      0.100      0.00      0.00
56      3.750      0.100      0.00      0.00
57      4.500      0.100      0.00      0.00
58      5.250      0.100      0.00      0.00
59      6.000      0.100      0.00      0.00
60      7.000      0.100      0.00      0.00
61      8.000      0.100      0.00      0.00
62      9.000      0.100      0.00      0.00
63     10.000      0.100      0.00      0.00
     1      0.0                                  /*INI CON
     1      1.0                                  /*BND CON
    25      0.0
    26      1.0
    38      0.0
    39      1.0
    63      0.0
     1      0.05       0.0                       /*VEL
1                                                /*MASFLX
1
3
     0                                           /*LOAD
```

LISTING D-2. The PRIMOS Command File for Test Case One.

```
EAT SEERUN
EAT PRT
EAT MASFLX
EAT RLT
COMO SEERUN
TIME
DATE
OPEN DATA 1 1
OPEN PRT 2 3
OPEN WORKSPACE 14 3
OPEN RLT 7 3
OPEN MASFLX 11 3
SEG XQT>*CHAINT DML
TIME
CLOSE WORKSPACE
EAT WORKSPACE
COMO -E
CLOSE ALL
```

9 2 1 2 4 1 Z 1 8 0 6

LISTING D-3. Output Report File for Test Case One. (Sheet 1 of 9)

```
 ****  *  *   ***   ***  ***  *  *****
** **  *  *  * *   *   *  *  *  * * *
*     *  *  ** **  *   *  **  *  *
*     *****  *  *  *   *  *  *  *
*     *  *  *******  *   *  **  *
** **  *  *  *  *    *   *  *  *  *
 ****  *  *  **   **  ***  *  ***  *

VERSION  2.1 (Revision 1.)

WED, NOV 06 1985

08:01:04

USER = LANGFORD

I.D. = 1106850801
```

LISTING D-3. Output Report File for Test Case One. (Sheet 2 of 9)

```
***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****
*** MULTICOMPONENT NUCLIDE TRANSPORT WITH DECAY CHAIN PROCESSES ***

     ONE DIMENSIONAL FLOW/DISPERSION


...PROBLEM CONTROL PARAMETERS...

NUMBER OF CONSTITUENTS.......................................... 1
NUMBER OF ELEMENTS.............................................. 12
NUMBER OF NODES................................................. 63
NUMBER OF SPECIFIED BOUNDARY NODES.............................. 6
NUMBER OF MATERIAL TYPES........................................ 1
INPUT ECHO PRINT OPTION  (0-NONE, 1-PRNT)....................... 1
OUTPUT PRINT OPTION  (1-FULL, 2-ABRV)........................... 2
VEL FIELD TYPE  (0-ONE CARD, 1-BY ROCK TYPE
                 2-VARYING ON FILE, 3-STEADY ON FILE)...........  0
NUMBER OF MASS FLUX CONSTITUENTS................................ 1
COORD SYSTEM (0-CARTESIAN, <>0-RADIAL ABOUT X=0.0)...............0
CONTAMINANT INTEGRATION OPTION (0-INHIBIT, 1-PERFORM)...........0


INITIAL CONDITION TYPE (<>0-MULT CARDS, 0-SINGLE CARD...        0
INPUT VELOCITY FILE (LU)........................................0
INPUT RESTART FILE (LU)..........................................0
OUTPUT RESTART FILE (LU)........................................0
PLOT OUTPUT FILE (LU) (0-NONE, <0-STP SAV, >0-INTV SAVE)      -11
INPUT GEOMETRY FILE (LU)........................................0
OUTPUT MASS FLUX FILE (LU)....................................13

STARTING TIME (YEARS)..........................              0.0

X SCALE FACTOR.................................            1.000
Y SCALE FACTOR.................................            1.000
U SCALE FACTOR.................................            1.000
V SCALE FACTOR.................................            1.000

WEIGHTING FACTOR...............................            1.800
```

.....TIME CONTROL AND RUN SPECIFICATIONS.....

NUMBER OF TIME STEPS	PRINT INTERVAL	TIME STEP (YRS)	TIME (YRS)	ZONEL (M)	ZONER (M)	ZONET (M)	ZONEB (M)
4	4	1.000	4.000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	3	2.000	10.00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2	5.000	20.00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8	8	10.00	100.0	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

LISTING D-3. Output Report File for Test Case One. (Sheet 3 of 9)

.....ROCK CHARACTERISTICS.....

NUMBER	X DISPERSIVITY (M)	Y DISPERSIVITY (M)	DENSITY (KG/M3)	POROSITY	FRAC WIDTH (M)	
1	1.00000E-01	1.00000E-01	2900.00	0.10000	0.00000E-01	ROCK

.....INPUT DECAY CHAIN DATA.....

CONSTITUENT	NAME	ATOMIC WEIGHT	HALF LIFE (YEARS)	DAUGHTER CONSTITUENT 1	SPLITTING FRACTION	DAUGHTER CONSTITUENT 2	SPLITTING FRACTION	CUT-OFF THRESHOLD
1	CONC	1.00	1.00000E+11	0	0.0000	0	0.0000	0.000E-01

"*" MEANS CONSTITUENT IS NON-COMPUTATIONAL

.....NUCLIDE MOLECULAR DIFFUSION COEFFICIENTS .....

CONSTITUENT		ROCK TYPES 1) ROCK
1	CONC	2.00E-01

.....NUCLIDE SORPTION (ML/GM).....

CONSTITUENT		ROCK TYPES 1) ROCK
1	CONC	3.10E-01

.....DECAY CHAIN CONNECTIVITY AND DECAY RATES.....

CONSTITUENT		DECAY RATE
1)	CONC	6.93E-12

LISTING D-3. Output Report File for Test Case One. (Sheet 4 of 9)

.....SPECIFIED BOUNDARY NODES AND VALUES.....

BOUNDARY VALUES FOR CONSTITUENTS 1 THROUGH 1

NODE	CONC
1	1.000E+00
25	0.000E-01
26	1.000E+00
38	0.000E-01
39	1.000E+00
63	0.000E-01

.....CONSTANT DARCY VELOCITY SPECIFIED.....

UL	X VELOCITY (M/YR)	5.000E-02
VL	Y VELOCITY (M/YR)	0.000E-01

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****
*** MULTICOMPONENT NUCLIDE TRANSPORT WITH DECAY CHAIN PROCESSES ***

ONE DIMENSIONAL FLOW/DISPERSION

.....NODAL CONNECTIONS AND MATERIAL NUMBERS.....

ELEMENT	NODES(COUNTERCLOCKWISE)								TYPE	ORDER.
M	N1	N2	N3	N4	N5	N6	N7	N8		
1	1	2	3	27	41	40	39	26	1	1.
2	3	4	5	28	43	42	41	27	1	2.
3	5	6	7	29	45	44	43	28	1	3.
4	7	8	9	30	47	46	45	29	1	4.
5	9	10	11	31	49	48	47	30	1	5.
6	11	12	13	32	51	50	49	31	1	6.

ELEMENT	NODES(COUNTERCLOCKWISE)								TYPE	ORDER
M	N1	N2	N3	N4	N5	N6	N7	N8		
7	13	14	15	33	53	52	51	32	1	7
8	15	16	17	34	55	54	53	33	1	8
9	17	18	19	35	57	56	55	34	1	9
10	19	20	21	36	59	58	57	35	1	10
11	21	22	23	37	61	60	59	36	1	11
12	23	24	25	38	63	62	61	37	1	12

LISTING D-3. Output Report File for Test Case One. (Sheet 5 of 9)

.....NODE POINT COORDINATES (M).....

NODE	X CORD	Y CORD,	NODE	X CORD	Y CORD,	NODE	X CORD	Y CORD,	NODE	X CORD	Y CORD
1	0.00	0.00,	17	3.00	0.00,	33	2.00	0.05,	49	1.00	0.10
2	0.05	0.00,	18	3.75	0.00,	34	3.00	0.05,	50	1.25	0.10
3	0.10	0.00,	19	4.50	0.00,	35	4.50	0.05,	51	1.50	0.10
4	0.18	0.00,	20	5.25	0.00,	36	6.00	0.05,	52	1.75	0.10
5	0.25	0.00,	21	6.00	0.00,	37	8.00	0.05,	53	2.00	0.10
6	0.37	0.00,	22	7.00	0.00,	38	10.00	0.05,	54	2.50	0.10
7	0.50	0.00,	23	8.00	0.00,	39	0.00	0.10,	55	3.00	0.10
8	0.62	0.00,	24	9.00	0.00,	40	0.05	0.10,	56	3.75	0.10
9	0.75	0.00,	25	10.00	0.00,	41	0.10	0.10,	57	4.50	0.10
10	0.87	0.00,	26	0.00	0.05,	42	0.18	0.10,	58	5.25	0.10
11	1.00	0.00,	27	0.10	0.05,	43	0.25	0.10,	59	6.00	0.10
12	1.25	0.00,	28	0.25	0.05,	44	0.37	0.10,	60	7.00	0.10
13	1.50	0.00,	29	0.50	0.05,	45	0.50	0.10,	61	8.00	0.10
14	1.75	0.00,	30	0.75	0.05,	46	0.62	0.10,	62	9.00	0.10
15	2.00	0.00,	31	1.00	0.05,	47	0.75	0.10,	63	10.00	0.10
16	2.50	0.00,	32	1.50	0.05,	48	0.87	0.10,			

.....MASS FLUX COMPUTATIONAL DATA.....

```
 DATA FOR THE FOLLOWING     1 CONSTITUENTS WILL BE INCLUDED IN THE MASS FLUX COMPUTATIONS.

      1)    CONC

MASS FLUX SURFACE NUMBER  1 IS DEFINED BY THE FOLLOWING   1 ELEMENTS.
      3


FLUX SURFACE NUMBER  1 IS OPEN,
DEFINED BY THE FOLLOWING    2 NODES
     44       6
```

```
          **** INPUT BINARY FILE TRACEBACK INFORMATION *****


     GEOMETRY FILE READ ON UNIT     5, CREATED BY   CHAINT  2.2
              THE RUN I.D. IS 1106850801,  THE USER IS LANGFORD
              THE TITLE IS:
```

LISTING D-3. Output Report File for Test Case One. (Sheet 6 of 9)

```
        THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED, SIMULATION TIME =  0.000E-01

 CONSTITUENT  USAGE     DECAY RATE(S)

   1)   CONC     1     6.931E-12

***** WARNING *****  PECLET NUMBER AT ELEMENT    8 ( ROCK    ) IS  1.0000E+00

***** WARNING *****  PECLET NUMBER AT ELEMENT    9 ( ROCK    ) IS  1.5000E+00

***** WARNING *****  PECLET NUMBER AT ELEMENT   10 ( ROCK    ) IS  1.5000E+00

***** WARNING *****  PECLET NUMBER AT ELEMENT   11 ( ROCK    ) IS  2.0000E+00

***** WARNING *****  PECLET NUMBER AT ELEMENT   12 ( ROCK    ) IS  2.0000E+00
```

```
                    ...RESULTS AFTER    4.000     YEARS OF SIMULATION...

                .....  CONCENTRATIONS FOR CONSTITUENT NUMBER  1     CONC,  MG/LIT  .....

 1 1.0000E+00    9 1.4567E-01   17 9.8792E-06   25 0.0000E-01   33 2.1179E-04   41 8.8980E-01   49 4.6744E-02   57 8.5667E-07
 2 9.5582E-01   10 8.4588E-02   18 0.0000E-01   26 1.0000E+00   34 9.8792E-06   42 7.8211E-01   50 1.3221E-02   58 0.0000E-01
 3 8.8980E-01   11 4.6744E-02   19 8.5668E-07   27 8.8980E-01   35 8.5668E-07   43 6.8039E-01   51 3.5184E-03   59 6.5824E-08
 4 7.8211E-01   12 1.3221E-02   20 0.0000E-01   28 6.8039E-01   36 6.5824E-08   44 5.1685E-01   52 8.7342E-04   60 0.0000E-01
 5 6.8039E-01   13 3.5184E-03   21 6.5824E-08   29 3.6460E-01   37 6.9903E-09   45 3.6460E-01   53 2.1179E-04   61 6.9902E-09
 6 5.1685E-01   14 8.7342E-04   22 0.0000E-01   30 1.4567E-01   38 0.0000E-01   46 2.3814E-01   54 5.7088E-06   62 0.0000E-01
 7 3.6460E-01   15 2.1179E-04   23 6.9902E-09   31 4.6744E-02   39 1.0000E+00   47 1.4567E-01   55 9.8792E-06   63 0.0000E-01
 8 2.3814E-01   16 5.7088E-06   24 0.0000E-01   32 3.5184E-03   40 9.5582E-01   48 8.4588E-02   56 0.0000E-01

   CONSTITUENT   CONC DIAGNOSTICS
         MAXIMUM VALUE IS          9.558E-01
         MAXIMUM CHANGE IS         1.204E-01 AT NODE   26, MAXIMUM FRACTIONAL CHANGE IS      3.068E+00
         MAXIMUM CORRECTION IS     1.285E-01 AT NODE   37, MAXIMUM FRACTIONAL CORRECTION IS  1.113E+01
   APPROXIMATE MAXIMUM PECLET NUMBERS ARE
     2.0000E+00 AT ELEMENT    11 FOR MATERIAL TYPE  ROCK
```

LISTING D-3. Output Report File for Test Case One. (Sheet 7 of 9)

```
        THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED, SIMULATION TIME =  4.000E+00

CONSTITUENT  USAGE     DECAY RATE(S)

  1)   CONC    1    6.931E-12
```

```
                          ...RESULTS AFTER   10.00     YEARS OF SIMULATION...

                    ..... CONCENTRATIONS FOR CONSTITUENT NUMBER  1     CONC,  MG/LIT  .....

 1 1.0000E+00    9 5.1325E-01   17 8.7025E-04   25 0.0000E-01   33 2.4692E-02   41 9.5232E-01   49 3.4188E-01   57 3.4941E-05
 2 9.7397E-01   10 4.2413E-01   18 4.9922E-05   26 1.0000E+00   34 8.7025E-04   42 9.1496E-01   50 2.0562E-01   58 2.7766E-06
 3 9.5232E-01   11 3.4188E-01   19 3.4940E-05   27 9.5232E-01   35 3.4940E-05   43 8.6975E-01   51 1.1149E-01   59 1.1457E-06
 4 9.1496E-01   12 2.0562E-01   20 2.7766E-06   28 8.6975E-01   36 1.1457E-06   44 7.8703E-01   52 5.5306E-02   60 4.7663E-08
 5 8.6975E-01   13 1.1149E-01   21 1.1457E-06   29 6.9858E-01   37 5.1882E-08   45 6.9858E-01   53 2.4692E-02   61 5.1883E-08
 6 7.8703E-01   14 5.5306E-02   22 4.7665E-08   30 5.1325E-01   38 0.0000E-01   46 6.0605E-01   54 4.4535E-03   62 4.4955E-09
 7 6.9858E-01   15 2.4692E-02   23 5.1880E-08   31 3.4188E-01   39 1.0000E+00   47 5.1325E-01   55 8.7025E-04   63 0.0000E-01
 8 6.0605E-01   16 4.4535E-03   24 4.4959E-09   32 1.1149E-01   40 9.7397E-01   48 4.2413E-01   56 4.9922E-05

  CONSTITUENT   CONC DIAGNOSTICS
        MAXIMUM VALUE IS          9.740E-01
        MAXIMUM CHANGE IS         9.918E-02 AT NODE    9, MAXIMUM FRACTIONAL CHANGE IS       3.998E+00
        MAXIMUM CORRECTION IS     3.646E-01 AT NODE   35, MAXIMUM FRACTIONAL CORRECTION IS  1.461E+01
  APPROXIMATE MAXIMUM PECLET NUMBERS ARE
    2.0000E+00 AT ELEMENT    11 FOR MATERIAL TYPE  ROCK
```

```
        THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED, SIMULATION TIME =  1.000E+01

CONSTITUENT  USAGE     DECAY RATE(S)

  1)   CONC    1    6.931E-12
```

LISTING D-3. Output Report File for Test Case One. (Sheet 8 of 9)

...RESULTS AFTER 20.00 YEARS OF SIMULATION...

..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 CONC, MG/LIT .....

1	1.0000E+00	9	7.7025E-01	17	3.4038E-02	25	0.0000E-01	33	2.1768E-01	41	9.8038E-01	49	6.5658E-01	57	1.3766E-03
2	9.8872E-01	10	7.1486E-01	18	6.7448E-03	26	1.0000E+00	34	3.4038E-02	42	9.6522E-01	50	5.3542E-01	58	2.5778E-04
3	9.8038E-01	11	6.5658E-01	19	1.3766E-03	27	9.8038E-01	35	1.3766E-03	43	9.4586E-01	51	4.1669E-01	59	5.4120E-05
4	9.6522E-01	12	5.3542E-01	20	2.5778E-04	28	9.4586E-01	36	5.4120E-05	44	9.0958E-01	52	3.0859E-01	60	5.0053E-06
5	9.4586E-01	13	4.1669E-01	21	5.4119E-05	29	8.6844E-01	37	1.9060E-06	45	8.6844E-01	53	2.1768E-01	61	1.9061E-06
6	9.0958E-01	14	3.0859E-01	22	5.0054E-06	30	7.7025E-01	38	0.0000E-01	46	8.2177E-01	54	9.5361E-02	62	2.0044E-07
7	8.6844E-01	15	2.1768E-01	23	1.9060E-06	31	6.5658E-01	39	1.0000E+00	47	7.7025E-01	55	3.4038E-02	63	0.0000E-01
8	8.2177E-01	16	9.5361E-02	24	2.0045E-07	32	4.1669E-01	40	9.8872E-01	48	7.1486E-01	56	6.7448E-03		

CONSTITUENT CONC DIAGNOSTICS
MAXIMUM VALUE IS 9.887E-01
MAXIMUM CHANGE IS 1.483E-01 AT NODE 12, MAXIMUM FRACTIONAL CHANGE IS 4.745E+00
MAXIMUM CORRECTION IS 3.261E-01 AT NODE 35, MAXIMUM FRACTIONAL CORRECTION IS 2.076E+01
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
2.0000E+00 AT ELEMENT 11 FOR MATERIAL TYPE ROCK

...RESULTS AFTER 100.0 YEARS OF SIMULATION...

..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 CONC, MG/LIT .....

1	1.0000E+00	9	9.9375E-01	17	8.7980E-01	25	0.0000E-01	33	9.5596E-01	41	9.9950E-01	49	9.8968E-01	57	6.6584E-01
2	9.9948E-01	10	9.9188E-01	18	7.8625E-01	26	1.0000E+00	34	8.7980E-01	42	9.9927E-01	50	9.8418E-01	58	5.2669E-01
3	9.9950E-01	11	9.8968E-01	19	6.6584E-01	27	9.9950E-01	35	6.6584E-01	43	9.9869E-01	51	9.7693E-01	59	3.8870E-01
4	9.9927E-01	12	9.8418E-01	20	5.2669E-01	28	9.9869E-01	36	3.8870E-01	44	9.9775E-01	52	9.6764E-01	60	2.3022E-01
5	9.9869E-01	13	9.7693E-01	21	3.8870E-01	29	9.9669E-01	37	1.1624E-01	45	9.9669E-01	53	9.5596E-01	61	1.1624E-01
6	9.9775E-01	14	9.6764E-01	22	2.3022E-01	30	9.9375E-01	38	0.0000E-01	46	9.9535E-01	54	9.2434E-01	62	5.5405E-02
7	9.9669E-01	15	9.5596E-01	23	1.1624E-01	31	9.8968E-01	39	1.0000E+00	47	9.9375E-01	55	8.7980E-01	63	0.0000E-01
8	9.9535E-01	16	9.2434E-01	24	5.5405E-02	32	9.7693E-01	40	9.9948E-01	48	9.9188E-01	56	7.8625E-01		

CONSTITUENT CONC DIAGNOSTICS
MAXIMUM VALUE IS 9.995E-01
MAXIMUM CHANGE IS 9.799E-02 AT NODE 19, MAXIMUM FRACTIONAL CHANGE IS 8.979E-01
MAXIMUM CORRECTION IS 1.482E-01 AT NODE 35, MAXIMUM FRACTIONAL CORRECTION IS 9.166E+02
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
2.0000E+00 AT ELEMENT 11 FOR MATERIAL TYPE ROCK

LISTING D-3. Output Report File for Test Case One. (Sheet 9 of 9)

```
THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED, SIMULATION TIME =  2.000E+01
CONSTITUENT  USAGE     DECAY RATE(S)

 1)   CONC     1     6.931E-12
```

LISTING D-4. Input Data File for Test Case Two. (Sheet 1 of 2)

```
SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER
    2  136  445   30    3    1    1    3    1    0    1                /*CNTRL
    0    8    0    0  -11   12   13                                    /*FILES
        0.        1.5       0.0       0.0       0.0       0.0         /*STRT TME
    2    2       1.25
    3    4       2.50
    3    3       5.00
    2    2      12.50
    2    2      25.00
9999
         1    1.0E-0    1.0E-0    2500.0      0.01       0.0  CANIST
         2    1.0E-0    1.0E-1    1800.0      0.30       0.0  PCKNG
         3    2.0E-1    2.0E-1    2780.0    2.2E-4       0.0  HOST
1 1                                                                    /*CONSTS
    1 238.  8.774E+01    2       1.00    0      0.00COMP-1       0.00E+00
    2 234.  4.468E+09    0       0.00    0      0.00COMP-2       0.00E+00
         1   6.30E-3   6.30E-3   6.30E-3                              /*DML
         2   6.30E-3   6.30E-3   6.30E-3
         1       0.0  1.666E-1   1.98E-4                              /*SORPTION
         2       0.0    2.5E-1   1.98E-4
         1     0.000                                                  /*INI CON
         2     0.000
       441     0.000     0.000                                        /*B.C.
       442     0.000     0.000
       435     0.000     0.000
       436     0.000     0.000
       429     0.000     0.000
       430     0.000     0.000
       424     0.000     0.000
       425     0.000     0.000
       426     0.000     0.000
       431     0.000     0.000
       432     0.000     0.000
       437     0.000     0.000
       438     0.000     0.000
       445     0.000     0.000
       443     0.000     0.000
         1     0.000     0.000
         2     0.000     0.000
         3     0.000     0.000
         4     0.000     0.000
         5     0.000     0.000
         6     0.000     0.000
         7     0.000     0.000
         8     0.000     0.000
         9     0.000     0.000
        10     0.000     0.000
        11     0.000     0.000
        12     0.000     0.000
        13     0.000     0.000
        14     0.000     0.000
        15     0.000     0.000
    1                                                                  /*FLX CONS
```

LISTING D-4. Input Data File for Test Case Two. (Sheet 2 of 2)

```
 8                                                                  /*FLX ELMS
47   48   50   61   74   87   99  111
      8        1.0       0.0                                        /*LOADING
     70        71        72        77        84        84        89        90
  0.0     0.10     0.0
  10.     0.10     0.0
  25.     0.09     0.0
  50.     0.08     0.0
 100.     0.06     0.0
 150.     0.02     0.0
 250.     0.01     0.0
 500.    0.005     0.0
 -1.0     0.0
```

LISTING D-5. The PRIMOS Command File for Test Case Two.

```
EAT SEERUN
EAT PRT
EAT RLT
EAT MASFLX
COMO SEERUN
DATE
TIME
OPEN DATA 1 1
OPEN PRT 2 3
OPEN WORKSPACE 14 3
OPEN RLT 7 3
OPEN *>MAGRUN>GEOM 10 1
OPEN *>MAGRUN>VEL 4 1
OPEN MASFLX 11 3
SEQ XQT>*CHAINT.DML
TIME
CLOSE WORKSPACE
EAT WORKSPACE
COMO -E
CLOSE ALL
```

LISTING D-6. Output Report File for Test Case Two. (Sheet 1 of 51)

```
 ****  *  *   ***   ***  ***  *  *****
**  **  *  *   * *   *   *  *  *  * *
*      *  *  ** **  *   *  ** *  *
*      *****  *  *  *   *  *  *  *
*      *  *  *******  *   *  ** *  *
**  **  *  *  *  *   *   *  *  *  *
 ****   *  *  **   **  ***  *  ***  *
```

VERSION 2.1 (Revision 1.)

TUE, NOV 05 1985

15:47:22

USER = LANGFORD

I.D. = 1105851547

LISTING D-6. Output Report File for Test Case Two. (Sheet 2 of 51)

```
***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****
*** MULTICOMPONENT NUCLIDE TRANSPORT WITH DECAY CHAIN PROCESSES ***

     SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER


...PROBLEM CONTROL PARAMETERS...

NUMBER OF CONSTITUENTS.....                                  2
NUMBER OF ELEMENTS.....                                    136
NUMBER OF NODES.....                                       445
NUMBER OF SPECIFIED BOUNDARY NODES.....                     30
NUMBER OF MATERIAL TYPES.....                                3
INPUT ECHO PRINT OPTION  (0-NONE, 1-PRNT).....               1
OUTPUT PRINT OPTION  (1-FULL, 2-ABRV).....                   1
VEL FIELD TYPE  (0-ONE CARD, 1-BY ROCK TYPE
                 2-VARYING ON FILE, 3-STEADY ON FILE)...     3
NUMBER OF MASS FLUX CONSTITUENTS.....                        1
COORD SYSTEM (0-CARTESIAN, <>0-RADIAL ABOUT X=0.0).....      0
CONTAMINANT INTEGRATION OPTION (0-INHIBIT, 1-PERFORM)...     1


INITIAL CONDITION TYPE (<>0-MULT CARDS, 0-SINGLE CARD...     0
INPUT VELOCITY FILE (LU).....                                8
INPUT RESTART FILE (LU).....                                 0
OUTPUT RESTART FILE (LU).....                                0
PLOT OUTPUT FILE (LU) (0-NONE, <0-STP SAV, >0-INTV SAVE)   -11
INPUT GEOMETRY FILE (LU).....                               12
OUTPUT MASS FLUX FILE (LU).....                             13

STARTING TIME (YEARS).....                                 0.0

X SCALE FACTOR.....                                      1.000
Y SCALE FACTOR.....                                      1.000
U SCALE FACTOR.....                                      1.000
V SCALE FACTOR.....                                      1.000

WEIGHTING FACTOR.....                                    1.500
```

.....TIME CONTROL AND RUN SPECIFICATIONS.....

NUMBER OF TIME STEPS	PRINT INTERVAL	TIME STEP (YRS)	TIME (YRS)	ZONEL (M)	ZONER (M)	ZONET (M)	ZONEB (M)
2	2	1.250	2.500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	4	2.500	10.00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	3	5.000	25.00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2	12.50	50.00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2	25.00	100.0	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 3 of 51)

.....ROCK CHARACTERISTICS.....

NUMBER	X DISPERSIVITY (M)	Y DISPERSIVITY (M)	DENSITY (KG/M3)	POROSITY	FRAC WIDTH (M)	
1	1.00000E+00	1.00000E+00	2500.00	0.01000	0.00000E-01	CANIST
2	1.00000E+00	1.00000E-01	1600.00	0.30000	0.00000E-01	PCKNG
3	2.00000E-01	2.00000E-01	2780.00	0.00022	0.00000E-01	HOST

LISTING D-6. Output Report File for Test Case Two. (Sheet 4 of 51)

.....INPUT DECAY CHAIN DATA.....

CONSTITUENT	NAME	ATOMIC WEIGHT	HALF LIFE (YEARS)	DAUGHTER CONSTITUENT 1	SPLITTING FRACTION	DAUGHTER CONSTITUENT 2	SPLITTING FRACTION	CUT-OFF THRESHOLD
1	COMP-1	238.00	8.77400E+01	2	1.0000	0	0.0000	0.000E-01
2	COMP-2	234.00	4.46800E+09	0	0.0000	0	0.0000	0.000E-01

"*" MEANS CONSTITUENT IS NON-COMPUTATIONAL

LISTING D-6. Output Report File for Test Case Two. (Sheet 5 of 51)

.....NUCLIDE MOLECULAR DIFFUSION COEFFICIENTS .....

CONSTITUENT		ROCK TYPES 1) CANIST	2) PCKNG	3) HOST
1	COMP-1	6.30E-03	6.30E-03	6.30E-03
2	COMP-2	6.30E-03	6.30E-03	6.30E-03

LISTING D-6. Output Report File for Test Case Two. (Sheet 6 of 51)

.....NUCLIDE SORPTION (ML/GM).....

CONSTITUENT		ROCK TYPES 1) CANIST	2) PCKNG	3) HOST
1	COMP-1	0.00E-01	1.67E-01	1.98E-04
2	COMP-2	0.00E-01	2.50E-01	1.98E-04

LISTING D-6. Output Report File for Test Case Two. (Sheet 7 of 51)

.....DECAY CHAIN CONNECTIVITY AND DECAY RATES.....

CONSTITUENT		DECAY RATE	
1)	COMP-1	7.90E-03	
2)	COMP-2	7.77E-03	1.55E-10

LISTING D-6. Output Report File for Test Case Two. (Sheet 8 of 51)

.....SPECIFIED BOUNDARY NODES AND VALUES.....

BOUNDARY VALUES FOR CONSTITUENTS 1 THROUGH 2

NODE	COMP-1	COMP-2
441	0.000E-01	0.000E-01
442	0.000E-01	0.000E-01
435	0.000E-01	0.000E-01
436	0.000E-01	0.000E-01
429	0.000E-01	0.000E-01
430	0.000E-01	0.000E-01
424	0.000E-01	0.000E-01
425	0.000E-01	0.000E-01
426	0.000E-01	0.000E-01
431	0.000E-01	0.000E-01
432	0.000E-01	0.000E-01
437	0.000E-01	0.000E-01
438	0.000E-01	0.000E-01
445	0.000E-01	0.000E-01
443	0.000E-01	0.000E-01
1	0.000E-01	0.000E-01
2	0.000E-01	0.000E-01
3	0.000E-01	0.000E-01
4	0.000E-01	0.000E-01
5	0.000E-01	0.000E-01
6	0.000E-01	0.000E-01
7	0.000E-01	0.000E-01
8	0.000E-01	0.000E-01
9	0.000E-01	0.000E-01
10	0.000E-01	0.000E-01
11	0.000E-01	0.000E-01
12	0.000E-01	0.000E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 9 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****
*** MULTICOMPONENT NUCLIDE TRANSPORT WITH DECAY CHAIN PROCESSES ***

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

.....NODAL CONNECTIONS AND MATERIAL NUMBERS.....

ELEMENT	NODES(COUNTERCLOCKWISE)								TYPE	ORDER.
M	N1	N2	N3	N4	N5	N6	N7	N8		
1	1	2	3	16	17	18	19	20	3	1.
2	17	16	3	4	5	21	22	23	3	2.
3	22	21	5	6	7	24	25	26	3	3.
4	25	24	7	8	9	27	28	29	3	4.
5	28	27	9	10	11	30	31	32	3	5.
6	31	30	11	12	13	33	34	35	3	6.
7	34	33	13	14	15	36	37	38	3	7.
8	19	18	17	39	40	41	42	43	3	8.
9	40	39	17	23	22	44	45	46	3	9.
10	45	44	22	26	25	47	48	49	3	10.
11	48	47	25	29	28	50	51	52	3	11.
12	51	50	28	32	31	53	54	55	3	12.
13	54	53	31	35	34	56	57	58	3	13.
14	57	56	34	38	37	59	60	61	3	14.
15	42	41	40	62	63	64	65	66	3	15.
16	63	62	40	46	45	67	68	69	3	16.
17	68	67	45	49	48	70	71	72	3	17.
18	71	70	48	52	51	73	74	75	3	18.
19	74	73	51	55	54	76	77	78	3	19.
20	77	76	54	58	57	79	80	81	3	20.
21	80	79	57	61	60	82	83	84	3	21.
22	65	64	63	85	86	87	0	0	3	22.
23	86	85	63	88	89	90	0	0	3	23.
24	89	88	63	69	68	91	92	93	3	24.
25	65	87	86	94	95	96	0	0	3	25.
26	92	91	68	72	71	97	98	99	3	26.
27	98	97	71	75	74	100	101	102	3	27.
28	101	100	74	78	77	103	104	105	3	28.
29	104	103	77	81	80	106	107	108	3	29.
30	107	106	80	84	83	109	110	111	3	30.
31	112	113	95	94	86	114	115	116	3	31.
32	115	114	86	90	89	117	118	119	3	32.
33	118	117	89	93	92	120	121	122	3	33.
34	121	120	92	99	98	123	124	125	3	34.
35	124	123	98	102	101	126	127	128	3	35.
36	127	126	101	105	104	129	130	131	3	36.
37	130	129	104	108	107	132	133	134	3	37.
38	133	132	107	111	110	135	136	137	3	38.
39	138	139	112	116	115	140	141	142	3	39.
40	141	140	115	119	118	143	144	145	3	40.
41	144	143	118	122	121	146	147	148	3	41.
42	147	146	121	125	124	149	150	151	3	42.
43	150	149	124	128	127	152	153	154	3	43.
44	153	152	127	131	130	155	156	157	3	44.
45	156	155	130	134	133	158	159	160	3	45.

ELEMENT	NODES(COUNTERCLOCKWISE)								TYPE	ORDER
M	N1	N2	N3	N4	N5	N6	N7	N8		
69	191	195	194	234	235	236	232	231	3	69
70	237	238	196	200	199	239	240	241	1	70
71	240	239	199	203	202	205	204	242	1	71
72	243	244	240	242	204	219	218	245	1	72
73	207	211	210	246	247	248	249	250	3	73
74	212	214	207	250	249	251	252	253	2	74
75	210	217	216	224	223	254	247	246	3	75
76	218	220	212	253	252	255	256	257	2	76
77	243	245	218	257	256	258	259	260	1	77
78	226	261	262	263	223	227	0	0	3	78
79	247	254	223	263	262	264	265	266	3	79
80	262	261	226	267	268	269	270	271	3	80
81	226	230	229	272	273	274	268	267	3	81
82	229	233	232	275	276	277	273	272	3	82
83	232	236	235	278	279	280	276	275	3	83
84	281	282	237	241	240	244	243	283	1	84
85	281	283	243	260	259	284	285	286	1	85
86	249	248	247	266	265	287	288	289	3	86
87	252	251	249	289	288	290	291	292	2	87
88	256	255	252	292	291	293	294	295	2	88
89	259	258	256	295	294	296	297	298	1	89
90	285	284	259	298	297	299	300	301	1	90
91	265	264	262	271	270	302	303	304	3	91
92	288	287	265	304	303	305	306	307	3	92
93	270	269	268	308	309	310	311	312	3	93
94	268	274	273	313	314	315	309	308	3	94
95	303	302	270	312	311	316	317	318	3	95
96	273	277	276	319	320	321	314	313	3	96
97	276	280	279	322	323	324	320	319	3	97
98	325	326	288	307	306	327	328	329	3	98
99	330	331	291	290	288	326	325	332	2	99
100	297	296	294	293	291	331	330	333	2	100
101	300	299	297	333	330	334	335	336	2	101
102	306	305	303	318	317	337	338	339	3	102
103	328	327	306	339	338	340	341	342	3	103
104	311	310	309	343	344	345	346	347	3	104
105	309	315	314	348	349	350	344	343	3	105
106	317	316	311	347	346	351	352	353	3	106
107	314	321	320	354	355	356	349	348	3	107
108	338	337	317	353	352	357	358	359	3	108
109	320	324	323	360	361	362	355	354	3	109
110	363	364	325	329	328	365	366	367	3	110
111	335	334	330	332	325	364	363	368	2	111
112	366	365	328	342	341	369	370	371	3	112
113	341	340	338	359	358	372	0	0	3	113

LISTING D-6. Output Report File for Test Case Two. (Sheet 10 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****
*** MULTICOMPONENT NUCLIDE TRANSPORT WITH DECAY CHAIN PROCESSES ***

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

.....NODAL CONNECTIONS AND MATERIAL NUMBERS.....

ELEMENT	NODES(COUNTERCLOCKWISE)								TYPE	ORDER,
M	N1	N2	N3	N4	N5	N6	N7	N8		
46	159	158	133	137	136	161	162	163	3	46,
47	164	165	138	142	141	166	167	168	2	47,
48	167	166	141	145	144	169	170	171	2	48,
49	172	173	144	148	147	174	175	176	3	49,
50	177	178	170	169	144	173	172	179	2	50,
51	175	174	147	151	150	180	181	182	3	51,
52	153	183	181	180	150	154	0	0	3	52,
53	184	185	181	183	153	186	0	0	3	53,
54	184	186	152	157	156	187	188	189	3	54,
55	188	187	156	160	159	190	191	192	3	55,
56	191	190	159	163	162	193	194	195	3	56,
57	196	197	164	168	167	198	199	200	2	57,
58	199	198	167	171	170	201	202	203	2	58,
59	204	205	202	201	170	178	177	206	2	59,
60	207	208	172	176	175	209	210	211	3	60,
61	212	213	177	179	172	208	207	214	2	61,
62	210	209	175	182	181	215	216	217	3	62,
63	218	219	204	206	177	213	212	220	2	63,
64	216	215	181	185	184	221	0	0	3	64,
65	216	221	184	222	223	224	0	0	3	65,
66	184	225	226	227	223	222	0	0	3	66,
67	184	189	188	228	229	230	226	225	3	67,
68	188	192	191	231	232	233	229	228	3	68,

ELEMENT	NODES(COUNTERCLOCKWISE)								TYPE	ORDER
M	N1	N2	N3	N4	N5	N6	N7	N8		
114	373	374	341	372	358	375	0	0	3	114
115	373	376	370	369	341	374	0	0	3	115
116	346	345	344	377	378	379	380	381	3	116
117	344	350	349	382	383	384	378	377	3	117
118	352	351	346	381	380	385	386	387	3	118
119	349	356	355	388	389	390	383	382	3	119
120	358	357	352	387	386	391	392	393	3	120
121	355	362	361	394	395	396	389	388	3	121
122	397	398	373	375	358	393	392	399	3	122
123	380	379	378	400	401	402	403	404	3	123
124	378	384	383	405	406	407	401	400	3	124
125	386	385	380	404	403	408	409	410	3	125
126	383	390	389	411	412	413	406	405	3	126
127	392	391	386	410	409	414	415	416	3	127
128	389	396	395	417	418	419	412	411	3	128
129	420	421	397	399	392	416	415	422	3	129
130	403	402	401	423	424	425	426	427	3	130
131	401	407	406	428	429	430	424	423	3	131
132	409	408	403	427	426	431	432	433	3	132
133	406	413	412	434	435	436	429	428	3	133
134	415	414	409	433	432	437	438	439	3	134
135	412	419	418	440	441	442	435	434	3	135
136	443	444	420	422	415	439	438	445	3	136

LISTING D-6. Output Report File for Test Case Two. (Sheet 11 of 51)

.....NODE POINT COORDINATES (M).....

NODE	X CORD	Y CORD.	NODE	X CORD	Y CORD.	NODE	X CORD	Y CORD.	NODE	X CORD	Y CORD
1	0.00	-2.50.	51	1.00	-1.50.	101	1.00	-0.64.	151	0.50	-0.19
2	0.12	-2.50.	52	0.81	-1.50.	102	0.81	-0.65.	152	1.00	-0.27
3	0.20	-2.50.	53	1.89	-1.75.	103	1.89	-0.81.	153	1.00	-0.19
4	0.28	-2.50.	54	1.89	-1.50.	104	1.89	-0.64.	154	0.81	-0.19
5	0.38	-2.50.	55	1.39	-1.50.	105	1.39	-0.64.	155	1.89	-0.28
6	0.50	-2.50.	56	3.22	-1.75.	106	3.22	-0.81.	156	1.89	-0.20
7	0.64	-2.50.	57	3.22	-1.50.	107	3.22	-0.64.	157	1.39	-0.20
8	0.81	-2.50.	58	2.50	-1.50.	108	2.50	-0.64.	158	3.22	-0.28
9	1.00	-2.50.	59	5.00	-1.75.	109	5.00	-0.81.	159	3.22	-0.20
10	1.39	-2.50.	60	5.00	-1.50.	110	5.00	-0.64.	160	2.50	-0.20
11	1.89	-2.50.	61	4.06	-1.50.	111	4.06	-0.64.	161	5.00	-0.28
12	2.50	-2.50.	62	0.20	-1.25.	112	0.00	-0.42.	162	5.00	-0.20
13	3.22	-2.50.	63	0.19	-1.00.	113	0.00	-0.53.	163	4.06	-0.20
14	4.06	-2.50.	64	0.12	-1.00.	114	0.11	-0.52.	164	0.00	-0.22
15	5.00	-2.50.	65	0.00	-1.00.	115	0.11	-0.41.	165	0.00	-0.24
16	0.20	-2.25.	66	0.00	-1.25.	116	0.06	-0.42.	166	0.10	-0.23
17	0.20	-2.00.	67	0.38	-1.25.	117	0.19	-0.50.	167	0.10	-0.21
18	0.12	-2.00.	68	0.38	-1.00.	118	0.19	-0.37.	168	0.05	-0.22
19	0.00	-2.00.	69	0.27	-1.00.	119	0.15	-0.39.	169	0.18	-0.18
20	0.00	-2.25.	70	0.64	-1.25.	120	0.38	-0.50.	170	0.17	-0.17
21	0.38	-2.25.	71	0.64	-1.00.	121	0.38	-0.38.	171	0.13	-0.20
22	0.38	-2.00.	72	0.50	-1.00.	122	0.27	-0.37.	172	0.24	-0.10
23	0.28	-2.00.	73	1.00	-1.25.	123	0.65	-0.50.	173	0.22	-0.14
24	0.64	-2.25.	74	1.00	-1.00.	124	0.65	-0.38.	174	0.39	-0.15
25	0.64	-2.00.	75	0.81	-1.00.	125	0.50	-0.38.	175	0.41	-0.11
26	0.50	-2.00.	76	1.89	-1.25.	126	1.00	-0.50.	176	0.31	-0.10
27	1.00	-2.25.	77	1.89	-1.00.	127	1.00	-0.38.	177	0.21	-0.10
28	1.00	-2.00.	78	1.39	-1.00.	128	0.81	-0.38.	178	0.20	-0.13
29	0.81	-2.00.	79	3.22	-1.25.	129	1.89	-0.50.	179	0.23	-0.10
30	1.89	-2.25.	80	3.22	-1.00.	130	1.89	-0.38.	180	0.66	-0.16
31	1.89	-2.00.	81	2.50	-1.00.	131	1.39	-0.38.	181	0.66	-0.11
32	1.39	-2.00.	82	5.00	-1.25.	132	3.22	-0.50.	182	0.52	-0.11
33	3.22	-2.25.	83	5.00	-1.00.	133	3.22	-0.38.	183	0.83	-0.15
34	3.22	-2.00.	84	4.06	-1.00.	134	2.50	-0.38.	184	1.00	0.00
35	2.50	-2.00.	85	0.15	-0.83.	135	5.00	-0.50.	185	0.83	-0.06
36	5.00	-2.25.	86	0.11	-0.66.	136	5.00	-0.38.	186	1.00	-0.12
37	5.00	-2.00.	87	0.06	-0.83.	137	4.06	-0.38.	187	1.89	-0.12
38	4.06	-2.00.	88	0.19	-0.81.	138	0.00	-0.25.	188	1.89	0.00
39	0.20	-1.75.	89	0.19	-0.65.	139	0.00	-0.32.	189	1.39	0.00
40	0.20	-1.50.	90	0.16	-0.66.	140	0.10	-0.31.	190	3.22	-0.12
41	0.12	-1.50.	91	0.38	-0.81.	141	0.10	-0.24.	191	3.22	0.00
42	0.00	-1.50.	92	0.38	-0.65.	142	0.05	-0.25.	192	2.50	0.00
43	0.00	-1.75.	93	0.27	-0.65.	143	0.19	-0.27.	193	5.00	-0.12
44	0.38	-1.75.	94	0.06	-0.67.	144	0.19	-0.19.	194	5.00	0.00
45	0.38	-1.50.	95	0.00	-0.67.	145	0.14	-0.22.	195	4.06	0.00
46	0.28	-1.50.	96	0.00	-0.82.	146	0.37	-0.27.	196	0.00	-0.20
47	0.64	-1.75.	97	0.65	-0.81.	147	0.37	-0.19.	197	0.00	-0.21
48	0.64	-1.50.	98	0.65	-0.65.	148	0.27	-0.19.	198	0.09	-0.20
49	0.50	-1.50.	99	0.50	-0.65.	149	0.65	-0.27.	199	0.09	-0.19
50	1.00	-1.75.	100	1.00	-0.81.	150	0.65	-0.19.	200	0.05	-0.20

LISTING D-6. Output Report File for Test Case Two. (Sheet 12 of 51)

.....NODE POINT COORDINATES (M).....

NODE	X CORD	Y CORD.	NODE	X CORD	Y CORD.	NODE	X CORD	Y CORD.	NODE	X CORD	Y CORD
201	0.16	-0.16.	251	0.23	0.10.	301	0.00	0.15.	351	0.50	1.00
202	0.15	-0.15.	252	0.21	0.10.	302	0.50	0.38.	352	0.38	1.00
203	0.12	-0.17.	253	0.22	0.05.	303	0.38	0.38.	353	0.38	0.81
204	0.19	-0.09.	254	0.52	0.11.	304	0.37	0.27.	354	3.22	0.81
205	0.17	-0.12.	255	0.20	0.09.	305	0.27	0.37.	355	3.22	1.00
206	0.20	-0.09.	256	0.19	0.09.	306	0.19	0.37.	356	2.50	1.00
207	0.25	0.00.	257	0.20	0.05.	307	0.19	0.27.	357	0.27	1.00
208	0.25	-0.05.	258	0.15	0.10.	308	1.00	0.50.	358	0.19	1.00
209	0.42	-0.06.	259	0.10	0.10.	309	1.00	0.64.	359	0.19	0.81
210	0.42	0.00.	260	0.10	0.05.	310	0.81	0.65.	360	5.00	0.81
211	0.32	0.00.	261	0.81	0.19.	311	0.65	0.65.	361	5.00	1.00
212	0.22	0.00.	262	0.65	0.19.	312	0.65	0.50.	362	4.06	1.00
213	0.22	-0.05.	263	0.66	0.16.	313	1.89	0.50.	363	0.00	0.25
214	0.24	0.00.	264	0.50	0.19.	314	1.89	0.64.	364	0.05	0.25
215	0.67	-0.06.	265	0.37	0.19.	315	1.39	0.64.	365	0.06	0.42
216	0.67	0.00.	266	0.39	0.15.	316	0.50	0.65.	366	0.00	0.42
217	0.53	0.00.	267	1.00	0.27.	317	0.38	0.65.	367	0.00	0.32
218	0.20	0.00.	268	1.00	0.38.	318	0.38	0.50.	368	0.00	0.24
219	0.20	-0.05.	269	0.81	0.38.	319	3.22	0.50.	369	0.06	0.67
220	0.21	0.00.	270	0.65	0.38.	320	3.22	0.64.	370	0.00	0.67
221	0.82	0.00.	271	0.65	0.27.	321	2.50	0.64.	371	0.00	0.53
222	0.83	0.06.	272	1.89	0.28.	322	5.00	0.50.	372	0.15	0.83
223	0.66	0.11.	273	1.89	0.38.	323	5.00	0.64.	373	0.00	1.00
224	0.67	0.06.	274	1.39	0.38.	324	4.06	0.64.	374	0.06	0.83
225	1.00	0.12.	275	3.22	0.28.	325	0.10	0.24.	375	0.12	1.00
226	1.00	0.19.	276	3.22	0.38.	326	0.14	0.22.	376	0.00	0.82
227	0.83	0.15.	277	2.50	0.38.	327	0.15	0.39.	377	1.00	1.25
228	1.89	0.12.	278	5.00	0.28.	328	0.11	0.41.	378	1.00	1.50
229	1.89	0.20.	279	5.00	0.38.	329	0.10	0.31.	379	0.81	1.50
230	1.39	0.20.	280	4.06	0.38.	330	0.10	0.21.	380	0.64	1.50
231	3.22	0.12.	281	0.00	0.00.	331	0.13	0.20.	381	0.64	1.25
232	3.22	0.20.	282	0.00	-0.05.	332	0.10	0.23.	382	1.89	1.25
233	2.50	0.20.	283	0.05	0.00.	333	0.09	0.20.	383	1.89	1.50
234	5.00	0.12.	284	0.05	0.10.	334	0.05	0.22.	384	1.39	1.50
235	5.00	0.20.	285	0.00	0.10.	335	0.00	0.22.	385	0.50	1.50
236	4.06	0.20.	286	0.00	0.05.	336	0.00	0.21.	386	0.38	1.50
237	0.00	-0.10.	287	0.27	0.19.	337	0.27	0.65.	387	0.38	1.25
238	0.00	-0.15.	288	0.19	0.19.	338	0.19	0.65.	388	3.22	1.25
239	0.10	-0.15.	289	0.22	0.14.	339	0.19	0.50.	389	3.22	1.50
240	0.10	-0.10.	290	0.18	0.18.	340	0.16	0.66.	390	2.50	1.50
241	0.05	-0.10.	291	0.17	0.17.	341	0.11	0.66.	391	0.28	1.50
242	0.15	-0.10.	292	0.20	0.13.	342	0.11	0.52.	392	0.20	1.50
243	0.10	0.00.	293	0.16	0.16.	343	1.00	0.81.	393	0.20	1.25
244	0.10	-0.05.	294	0.15	0.15.	344	1.00	1.00.	394	5.00	1.25
245	0.15	0.00.	295	0.17	0.12.	345	0.81	1.00.	395	5.00	1.50
246	0.42	0.06.	296	0.12	0.17.	346	0.64	1.00.	396	4.06	1.50
247	0.41	0.11.	297	0.09	0.19.	347	0.65	0.81.	397	0.00	1.50
248	0.31	0.10.	298	0.10	0.15.	348	1.89	0.81.	398	0.00	1.25
249	0.24	0.10.	299	0.05	0.20.	349	1.89	1.00.	399	0.12	1.50
250	0.25	0.05.	300	0.00	0.20.	350	1.39	1.00.	400	1.00	1.75

LISTING D-6. Output Report File for Test Case Two. (Sheet 13 of 51)

.....NODE POINT COORDINATES (M).....

NODE	X CORD	Y CORD,	NODE	X CORD	Y CORD,	NODE	X CORD	Y CORD,	NODE	X CORD	Y CORD
401	1.00	2.00,	413	2.50	2.00,	425	0.81	2.50,	437	0.28	2.50
402	0.81	2.00,	414	0.28	2.00,	426	0.64	2.50,	438	0.20	2.50
403	0.64	2.00,	415	0.20	2.00,	427	0.64	2.25,	439	0.20	2.25
404	0.64	1.75,	416	0.20	1.75,	428	1.89	2.25,	440	5.00	2.25
405	1.89	1.75,	417	5.00	1.75,	429	1.89	2.50,	441	5.00	2.50
406	1.89	2.00,	418	5.00	2.00,	430	1.39	2.50,	442	4.06	2.50
407	1.39	2.00,	419	4.06	2.00,	431	0.50	2.50,	443	0.00	2.50
408	0.50	2.00,	420	0.00	2.00,	432	0.38	2.50,	444	0.00	2.25
409	0.38	2.00,	421	0.00	1.75,	433	0.38	2.25,	445	0.12	2.50
410	0.38	1.75,	422	0.12	2.00,	434	3.22	2.25,			
411	3.22	1.75,	423	1.00	2.25,	435	3.22	2.50,			
412	3.22	2.00,	424	1.00	2.50,	436	2.50	2.50,			

LISTING D-6. Output Report File for Test Case Two. (Sheet 14 of 51)

```
.......MASS FLUX COMPUTATIONAL DATA.......


 DATA FOR THE FOLLOWING     1 CONSTITUENTS WILL BE INCLUDED IN THE MASS FLUX COMPUTATIONS.

      1) COMP-1

MASS FLUX SURFACE NUMBER  1 IS DEFINED BY THE FOLLOWING   8 ELEMENTS.
     47     48     50     61     74     87     99    111


FLUX SURFACE NUMBER  1 IS OPEN,
DEFINED BY THE FOLLOWING    9 NODES
    165    166    169    179    214    251    290    332    368
```

LISTING D-6. Output Report File for Test Case Two. (Sheet 15 of 51)

```
**** INPUT BINARY FILE TRACEBACK INFORMATION *****


GEOMETRY FILE READ ON UNIT     12, CREATED BY    MESHER  0.0
         THE RUN I.D. IS 1231841250,  THE USER IS LANGFORD
         THE TITLE IS:
          GEOMETRY FOR CHAINT SAMPLE PROBLEM

VELOCITY FILE READ ON UNIT      8, CREATED BY    MAGNUM  3.1
         THE RUN I.D. IS 1105851304,  THE USER IS LANGFORD
         THE TITLE IS:
          SAMPLE PROBLEM, FLOW AROUND A HEATED CANNISTER
         FILE TRACEBACK IS AS FOLLOWS:
            FILE TYPE  SOURCE CODE     RUN I.D.     USER
             GEOMETRY      MESHER    1231841250  LANGFORD
```

LISTING D-6. Output Report File for Test Case Two. (Sheet 16 of 51)

```
      ***** ELEMENT SOURCE LOADS *****

NUMBER OF ELEMENTS WITH SOURCE                          8
SCALE FACTOR FOR RELEASE RATE                     1.00E+00


LOADS ARE ON THE FOLLOWING ELEMENTS
      70      71      72      77      84      84      89      90

     TIME      ....LOADS....
    (YRS)      (GM/M**3-YR)

               COMP-1       COMP-2
 0.00E-01  1.0000E-01  0.0000E-01
 1.00E+01  1.0000E-01  0.0000E-01
 2.50E+01  9.0000E-02  0.0000E-01
 5.00E+01  8.0000E-02  0.0000E-01
 1.00E+02  6.0000E-02  0.0000E-01
 1.50E+02  2.0000E-02  0.0000E-01
 2.50E+02  1.0000E-02  0.0000E-01
 5.00E+02  5.0000E-03  0.0000E-01
```

LISTING D-6. Output Report File for Test Case Two. (Sheet 17 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

I N I T I A L C O N D I T I O N S

..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	0.000E-01	83	0.000E-01	124	0.000E-01
2	0.000E-01*	43	0.000E-01	84	0.000E-01	125	0.000E-01
3	0.000E-01*	44	0.000E-01	85	0.000E-01	126	0.000E-01
4	0.000E-01*	45	0.000E-01	86	0.000E-01	127	0.000E-01
5	0.000E-01*	46	0.000E-01	87	0.000E-01	128	0.000E-01
6	0.000E-01*	47	0.000E-01	88	0.000E-01	129	0.000E-01
7	0.000E-01*	48	0.000E-01	89	0.000E-01	130	0.000E-01
8	0.000E-01*	49	0.000E-01	90	0.000E-01	131	0.000E-01
9	0.000E-01*	50	0.000E-01	91	0.000E-01	132	0.000E-01
10	0.000E-01*	51	0.000E-01	92	0.000E-01	133	0.000E-01
11	0.000E-01*	52	0.000E-01	93	0.000E-01	134	0.000E-01
12	0.000E-01*	53	0.000E-01	94	0.000E-01	135	0.000E-01
13	0.000E-01*	54	0.000E-01	95	0.000E-01	136	0.000E-01
14	0.000E-01*	55	0.000E-01	96	0.000E-01	137	0.000E-01
15	0.000E-01*	56	0.000E-01	97	0.000E-01	138	0.000E-01
16	0.000E-01	57	0.000E-01	98	0.000E-01	139	0.000E-01
17	0.000E-01	58	0.000E-01	99	0.000E-01	140	0.000E-01
18	0.000E-01	59	0.000E-01	100	0.000E-01	141	0.000E-01
19	0.000E-01	60	0.000E-01	101	0.000E-01	142	0.000E-01
20	0.000E-01	61	0.000E-01	102	0.000E-01	143	0.000E-01
21	0.000E-01	62	0.000E-01	103	0.000E-01	144	0.000E-01
22	0.000E-01	63	0.000E-01	104	0.000E-01	145	0.000E-01
23	0.000E-01	64	0.000E-01	105	0.000E-01	146	0.000E-01
24	0.000E-01	65	0.000E-01	106	0.000E-01	147	0.000E-01
25	0.000E-01	66	0.000E-01	107	0.000E-01	148	0.000E-01
26	0.000E-01	67	0.000E-01	108	0.000E-01	149	0.000E-01
27	0.000E-01	68	0.000E-01	109	0.000E-01	150	0.000E-01
28	0.000E-01	69	0.000E-01	110	0.000E-01	151	0.000E-01
29	0.000E-01	70	0.000E-01	111	0.000E-01	152	0.000E-01
30	0.000E-01	71	0.000E-01	112	0.000E-01	153	0.000E-01
31	0.000E-01	72	0.000E-01	113	0.000E-01	154	0.000E-01
32	0.000E-01	73	0.000E-01	114	0.000E-01	155	0.000E-01
33	0.000E-01	74	0.000E-01	115	0.000E-01	156	0.000E-01
34	0.000E-01	75	0.000E-01	116	0.000E-01	157	0.000E-01
35	0.000E-01	76	0.000E-01	117	0.000E-01	158	0.000E-01
36	0.000E-01	77	0.000E-01	118	0.000E-01	159	0.000E-01
37	0.000E-01	78	0.000E-01	119	0.000E-01	160	0.000E-01
38	0.000E-01	79	0.000E-01	120	0.000E-01	161	0.000E-01
39	0.000E-01	80	0.000E-01	121	0.000E-01	162	0.000E-01
40	0.000E-01	81	0.000E-01	122	0.000E-01	163	0.000E-01
41	0.000E-01	82	0.000E-01	123	0.000E-01	164	0.000E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 18 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM. DIFFUSION FROM A HEATED CANNISTER

I N I T I A L C O N D I T I O N S

..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1. MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	0.000E-01	206	0.000E-01	247	0.000E-01	288	0.000E-01
166	0.000E-01	207	0.000E-01	248	0.000E-01	289	0.000E-01
167	0.000E-01	208	0.000E-01	249	0.000E-01	290	0.000E-01
168	0.000E-01	209	0.000E-01	250	0.000E-01	291	0.000E-01
169	0.000E-01	210	0.000E-01	251	0.000E-01	292	0.000E-01
170	0.000E-01	211	0.000E-01	252	0.000E-01	293	0.000E-01
171	0.000E-01	212	0.000E-01	253	0.000E-01	294	0.000E-01
172	0.000E-01	213	0.000E-01	254	0.000E-01	295	0.000E-01
173	0.000E-01	214	0.000E-01	255	0.000E-01	296	0.000E-01
174	0.000E-01	215	0.000E-01	256	0.000E-01	297	0.000E-01
175	0.000E-01	216	0.000E-01	257	0.000E-01	298	0.000E-01
176	0.000E-01	217	0.000E-01	258	0.000E-01	299	0.000E-01
177	0.000E-01	218	0.000E-01	259	0.000E-01	300	0.000E-01
178	0.000E-01	219	0.000E-01	260	0.000E-01	301	0.000E-01
179	0.000E-01	220	0.000E-01	261	0.000E-01	302	0.000E-01
180	0.000E-01	221	0.000E-01	262	0.000E-01	303	0.000E-01
181	0.000E-01	222	0.000E-01	263	0.000E-01	304	0.000E-01
182	0.000E-01	223	0.000E-01	264	0.000E-01	305	0.000E-01
183	0.000E-01	224	0.000E-01	265	0.000E-01	306	0.000E-01
184	0.000E-01	225	0.000E-01	266	0.000E-01	307	0.000E-01
185	0.000E-01	226	0.000E-01	267	0.000E-01	308	0.000E-01
186	0.000E-01	227	0.000E-01	268	0.000E-01	309	0.000E-01
187	0.000E-01	228	0.000E-01	269	0.000E-01	310	0.000E-01
188	0.000E-01	229	0.000E-01	270	0.000E-01	311	0.000E-01
189	0.000E-01	230	0.000E-01	271	0.000E-01	312	0.000E-01
190	0.000E-01	231	0.000E-01	272	0.000E-01	313	0.000E-01
191	0.000E-01	232	0.000E-01	273	0.000E-01	314	0.000E-01
192	0.000E-01	233	0.000E-01	274	0.000E-01	315	0.000E-01
193	0.000E-01	234	0.000E-01	275	0.000E-01	316	0.000E-01
194	0.000E-01	235	0.000E-01	276	0.000E-01	317	0.000E-01
195	0.000E-01	236	0.000E-01	277	0.000E-01	318	0.000E-01
196	0.000E-01	237	0.000E-01	278	0.000E-01	319	0.000E-01
197	0.000E-01	238	0.000E-01	279	0.000E-01	320	0.000E-01
198	0.000E-01	239	0.000E-01	280	0.000E-01	321	0.000E-01
199	0.000E-01	240	0.000E-01	281	0.000E-01	322	0.000E-01
200	0.000E-01	241	0.000E-01	282	0.000E-01	323	0.000E-01
201	0.000E-01	242	0.000E-01	283	0.000E-01	324	0.000E-01
202	0.000E-01	243	0.000E-01	284	0.000E-01	325	0.000E-01
203	0.000E-01	244	0.000E-01	285	0.000E-01	326	0.000E-01
204	0.000E-01	245	0.000E-01	286	0.000E-01	327	0.000E-01
205	0.000E-01	246	0.000E-01	287	0.000E-01	328	0.000E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 19 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

I N I T I A L C O N D I T I O N S
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 329 TO 445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	0.000E-01	359	0.000E-01	389	0.000E-01	419	0.000E-01
330	0.000E-01	360	0.000E-01	390	0.000E-01	420	0.000E-01
331	0.000E-01	361	0.000E-01	391	0.000E-01	421	0.000E-01
332	0.000E-01	362	0.000E-01	392	0.000E-01	422	0.000E-01
333	0.000E-01	363	0.000E-01	393	0.000E-01	423	0.000E-01
334	0.000E-01	364	0.000E-01	394	0.000E-01	424	0.000E-01*
335	0.000E-01	365	0.000E-01	395	0.000E-01	425	0.000E-01*
336	0.000E-01	366	0.000E-01	396	0.000E-01	426	0.000E-01*
337	0.000E-01	367	0.000E-01	397	0.000E-01	427	0.000E-01
338	0.000E-01	368	0.000E-01	398	0.000E-01	428	0.000E-01
339	0.000E-01	369	0.000E-01	399	0.000E-01	429	0.000E-01*
340	0.000E-01	370	0.000E-01	400	0.000E-01	430	0.000E-01*
341	0.000E-01	371	0.000E-01	401	0.000E-01	431	0.000E-01*
342	0.000E-01	372	0.000E-01	402	0.000E-01	432	0.000E-01*
343	0.000E-01	373	0.000E-01	403	0.000E-01	433	0.000E-01
344	0.000E-01	374	0.000E-01	404	0.000E-01	434	0.000E-01
345	0.000E-01	375	0.000E-01	405	0.000E-01	435	0.000E-01*
346	0.000E-01	376	0.000E-01	406	0.000E-01	436	0.000E-01*
347	0.000E-01	377	0.000E-01	407	0.000E-01	437	0.000E-01*
348	0.000E-01	378	0.000E-01	408	0.000E-01	438	0.000E-01*
349	0.000E-01	379	0.000E-01	409	0.000E-01	439	0.000E-01
350	0.000E-01	380	0.000E-01	410	0.000E-01	440	0.000E-01
351	0.000E-01	381	0.000E-01	411	0.000E-01	441	0.000E-01*
352	0.000E-01	382	0.000E-01	412	0.000E-01	442	0.000E-01*
353	0.000E-01	383	0.000E-01	413	0.000E-01	443	0.000E-01*
354	0.000E-01	384	0.000E-01	414	0.000E-01	444	0.000E-01
355	0.000E-01	385	0.000E-01	415	0.000E-01	445	0.000E-01*
356	0.000E-01	386	0.000E-01	416	0.000E-01		
357	0.000E-01	387	0.000E-01	417	0.000E-01		
358	0.000E-01	388	0.000E-01	418	0.000E-01		

LISTING D-6. Output Report File for Test Case Two. (Sheet 20 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

I N I T I A L C O N D I T I O N S

..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ..

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	0.000E-01	83	0.000E-01	124	0.000E-01
2	0.000E-01*	43	0.000E-01	84	0.000E-01	125	0.000E-01
3	0.000E-01*	44	0.000E-01	85	0.000E-01	126	0.000E-01
4	0.000E-01*	45	0.000E-01	86	0.000E-01	127	0.000E-01
5	0.000E-01*	46	0.000E-01	87	0.000E-01	128	0.000E-01
6	0.000E-01*	47	0.000E-01	88	0.000E-01	129	0.000E-01
7	0.000E-01*	48	0.000E-01	89	0.000E-01	130	0.000E-01
8	0.000E-01*	49	0.000E-01	90	0.000E-01	131	0.000E-01
9	0.000E-01*	50	0.000E-01	91	0.000E-01	132	0.000E-01
10	0.000E-01*	51	0.000E-01	92	0.000E-01	133	0.000E-01
11	0.000E-01*	52	0.000E-01	93	0.000E-01	134	0.000E-01
12	0.000E-01*	53	0.000E-01	94	0.000E-01	135	0.000E-01
13	0.000E-01*	54	0.000E-01	95	0.000E-01	136	0.000E-01
14	0.000E-01*	55	0.000E-01	96	0.000E-01	137	0.000E-01
15	0.000E-01*	56	0.000E-01	97	0.000E-01	138	0.000E-01
16	0.000E-01	57	0.000E-01	98	0.000E-01	139	0.000E-01
17	0.000E-01	58	0.000E-01	99	0.000E-01	140	0.000E-01
18	0.000E-01	59	0.000E-01	100	0.000E-01	141	0.000E-01
19	0.000E-01	60	0.000E-01	101	0.000E-01	142	0.000E-01
20	0.000E-01	61	0.000E-01	102	0.000E-01	143	0.000E-01
21	0.000E-01	62	0.000E-01	103	0.000E-01	144	0.000E-01
22	0.000E-01	63	0.000E-01	104	0.000E-01	145	0.000E-01
23	0.000E-01	64	0.000E-01	105	0.000E-01	146	0.000E-01
24	0.000E-01	65	0.000E-01	106	0.000E-01	147	0.000E-01
25	0.000E-01	66	0.000E-01	107	0.000E-01	148	0.000E-01
26	0.000E-01	67	0.000E-01	108	0.000E-01	149	0.000E-01
27	0.000E-01	68	0.000E-01	109	0.000E-01	150	0.000E-01
28	0.000E-01	69	0.000E-01	110	0.000E-01	151	0.000E-01
29	0.000E-01	70	0.000E-01	111	0.000E-01	152	0.000E-01
30	0.000E-01	71	0.000E-01	112	0.000E-01	153	0.000E-01
31	0.000E-01	72	0.000E-01	113	0.000E-01	154	0.000E-01
32	0.000E-01	73	0.000E-01	114	0.000E-01	155	0.000E-01
33	0.000E-01	74	0.000E-01	115	0.000E-01	156	0.000E-01
34	0.000E-01	75	0.000E-01	116	0.000E-01	157	0.000E-01
35	0.000E-01	76	0.000E-01	117	0.000E-01	158	0.000E-01
36	0.000E-01	77	0.000E-01	118	0.000E-01	159	0.000E-01
37	0.000E-01	78	0.000E-01	119	0.000E-01	160	0.000E-01
38	0.000E-01	79	0.000E-01	120	0.000E-01	161	0.000E-01
39	0.000E-01	80	0.000E-01	121	0.000E-01	162	0.000E-01
40	0.000E-01	81	0.000E-01	122	0.000E-01	163	0.000E-01
41	0.000E-01	82	0.000E-01	123	0.000E-01	164	0.000E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 21 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

I N I T I A L C O N D I T I O N S
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	0.000E-01	206	0.000E-01	247	0.000E-01	288	0.000E-01
166	0.000E-01	207	0.000E-01	248	0.000E-01	289	0.000E-01
167	0.000E-01	208	0.000E-01	249	0.000E-01	290	0.000E-01
168	0.000E-01	209	0.000E-01	250	0.000E-01	291	0.000E-01
169	0.000E-01	210	0.000E-01	251	0.000E-01	292	0.000E-01
170	0.000E-01	211	0.000E-01	252	0.000E-01	293	0.000E-01
171	0.000E-01	212	0.000E-01	253	0.000E-01	294	0.000E-01
172	0.000E-01	213	0.000E-01	254	0.000E-01	295	0.000E-01
173	0.000E-01	214	0.000E-01	255	0.000E-01	296	0.000E-01
174	0.000E-01	215	0.000E-01	256	0.000E-01	297	0.000E-01
175	0.000E-01	216	0.000E-01	257	0.000E-01	298	0.000E-01
176	0.000E-01	217	0.000E-01	258	0.000E-01	299	0.000E-01
177	0.000E-01	218	0.000E-01	259	0.000E-01	300	0.000E-01
178	0.000E-01	219	0.000E-01	260	0.000E-01	301	0.000E-01
179	0.000E-01	220	0.000E-01	261	0.000E-01	302	0.000E-01
180	0.000E-01	221	0.000E-01	262	0.000E-01	303	0.000E-01
181	0.000E-01	222	0.000E-01	263	0.000E-01	304	0.000E-01
182	0.000E-01	223	0.000E-01	264	0.000E-01	305	0.000E-01
183	0.000E-01	224	0.000E-01	265	0.000E-01	306	0.000E-01
184	0.000E-01	225	0.000E-01	266	0.000E-01	307	0.000E-01
185	0.000E-01	226	0.000E-01	267	0.000E-01	308	0.000E-01
186	0.000E-01	227	0.000E-01	268	0.000E-01	309	0.000E-01
187	0.000E-01	228	0.000E-01	269	0.000E-01	310	0.000E-01
188	0.000E-01	229	0.000E-01	270	0.000E-01	311	0.000E-01
189	0.000E-01	230	0.000E-01	271	0.000E-01	312	0.000E-01
190	0.000E-01	231	0.000E-01	272	0.000E-01	313	0.000E-01
191	0.000E-01	232	0.000E-01	273	0.000E-01	314	0.000E-01
192	0.000E-01	233	0.000E-01	274	0.000E-01	315	0.000E-01
193	0.000E-01	234	0.000E-01	275	0.000E-01	316	0.000E-01
194	0.000E-01	235	0.000E-01	276	0.000E-01	317	0.000E-01
195	0.000E-01	236	0.000E-01	277	0.000E-01	318	0.000E-01
196	0.000E-01	237	0.000E-01	278	0.000E-01	319	0.000E-01
197	0.000E-01	238	0.000E-01	279	0.000E-01	320	0.000E-01
198	0.000E-01	239	0.000E-01	280	0.000E-01	321	0.000E-01
199	0.000E-01	240	0.000E-01	281	0.000E-01	322	0.000E-01
200	0.000E-01	241	0.000E-01	282	0.000E-01	323	0.000E-01
201	0.000E-01	242	0.000E-01	283	0.000E-01	324	0.000E-01
202	0.000E-01	243	0.000E-01	284	0.000E-01	325	0.000E-01
203	0.000E-01	244	0.000E-01	285	0.000E-01	326	0.000E-01
204	0.000E-01	245	0.000E-01	286	0.000E-01	327	0.000E-01
205	0.000E-01	246	0.000E-01	287	0.000E-01	328	0.000E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 22 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

I N I T I A L C O N D I T I O N S

..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT ....

... OUTPUT FOR NODES 329 TO 445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	0.000E-01	359	0.000E-01	389	0.000E-01	419	0.000E-01
330	0.000E-01	360	0.000E-01	390	0.000E-01	420	0.000E-01
331	0.000E-01	361	0.000E-01	391	0.000E-01	421	0.000E-01
332	0.000E-01	362	0.000E-01	392	0.000E-01	422	0.000E-01
333	0.000E-01	363	0.000E-01	393	0.000E-01	423	0.000E-01
334	0.000E-01	364	0.000E-01	394	0.000E-01	424	0.000E-01*
335	0.000E-01	365	0.000E-01	395	0.000E-01	425	0.000E-01*
336	0.000E-01	366	0.000E-01	396	0.000E-01	426	0.000E-01*
337	0.000E-01	367	0.000E-01	397	0.000E-01	427	0.000E-01
338	0.000E-01	368	0.000E-01	398	0.000E-01	428	0.000E-01
339	0.000E-01	369	0.000E-01	399	0.000E-01	429	0.000E-01*
340	0.000E-01	370	0.000E-01	400	0.000E-01	430	0.000E-01*
341	0.000E-01	371	0.000E-01	401	0.000E-01	431	0.000E-01*
342	0.000E-01	372	0.000E-01	402	0.000E-01	432	0.000E-01*
343	0.000E-01	373	0.000E-01	403	0.000E-01	433	0.000E-01
344	0.000E-01	374	0.000E-01	404	0.000E-01	434	0.000E-01
345	0.000E-01	375	0.000E-01	405	0.000E-01	435	0.000E-01*
346	0.000E-01	376	0.000E-01	406	0.000E-01	436	0.000E-01*
347	0.000E-01	377	0.000E-01	407	0.000E-01	437	0.000E-01*
348	0.000E-01	378	0.000E-01	408	0.000E-01	438	0.000E-01*
349	0.000E-01	379	0.000E-01	409	0.000E-01	439	0.000E-01
350	0.000E-01	380	0.000E-01	410	0.000E-01	440	0.000E-01
351	0.000E-01	381	0.000E-01	411	0.000E-01	441	0.000E-01*
352	0.000E-01	382	0.000E-01	412	0.000E-01	442	0.000E-01*
353	0.000E-01	383	0.000E-01	413	0.000E-01	443	0.000E-01*
354	0.000E-01	384	0.000E-01	414	0.000E-01	444	0.000E-01
355	0.000E-01	385	0.000E-01	415	0.000E-01	445	0.000E-01*
356	0.000E-01	386	0.000E-01	416	0.000E-01		
357	0.000E-01	387	0.000E-01	417	0.000E-01		
358	0.000E-01	388	0.000E-01	418	0.000E-01		

LISTING D-6. Output Report File for Test Case Two. (Sheet 23 of 51)

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THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED, SIMULATION TIME =  0.000E-01
CONSTITUENT  USAGE     DECAY RATE(S)

 1) COMP-1     1     7.900E-03

 2) COMP-2     1     7.767E-03  1.551E-10
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LISTING D-6. Output Report File for Test Case Two. (Sheet 24 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 2.500 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	1.985E-06	83	3.631E-08	124	9.717E-04
2	0.000E-01*	43	0.000E-01	84	0.000E-01	125	0.000E-01
3	0.000E-01*	44	2.017E-05	85	1.389E-04	126	0.000E-01
4	0.000E-01*	45	5.101E-05	86	7.405E-04	127	0.000E-01
5	0.000E-01*	46	0.000E-01	87	2.349E-05	128	4.205E-04
6	0.000E-01*	47	0.000E-01	88	3.573E-04	129	7.853E-04
7	0.000E-01*	48	0.000E-01	89	1.382E-03	130	3.412E-05
8	0.000E-01*	49	1.135E-05	90	1.374E-03	131	0.000E-01
9	0.000E-01*	50	1.664E-07	91	3.836E-04	132	0.000E-01
10	0.000E-01*	51	4.029E-07	92	9.171E-04	133	0.000E-01
11	0.000E-01*	52	6.734E-08	93	0.000E-01	134	1.295E-05
12	0.000E-01*	53	1.172E-08	94	8.324E-04	135	8.949E-07
13	0.000E-01*	54	1.817E-08	95	4.973E-04	136	3.961E-06
14	0.000E-01*	55	1.038E-07	96	0.000E-01	137	0.000E-01
15	0.000E-01*	56	6.758E-09	97	0.000E-01	138	3.903E-01
16	0.000E-01	57	1.589E-08	98	0.000E-01	139	9.246E-02
17	0.000E-01	58	5.958E-09	99	2.425E-04	140	8.191E-02
18	0.000E-01	59	1.800E-09	100	4.767E-06	141	3.668E-01
19	5.280E-07	60	2.677E-09	101	1.059E-05	142	3.803E-01
20	0.000E-01	61	2.300E-09	102	0.000E-01	143	1.000E-01
21	0.000E-01	62	0.000E-01	103	4.987E-08	144	3.583E-01
22	0.000E-01	63	0.000E-01	104	0.000E-01	145	3.603E-01
23	1.774E-05	64	0.000E-01	105	3.247E-06	146	1.155E-02
24	3.000E-07	65	4.331E-05	106	2.165E-07	147	6.604E-03
25	6.262E-07	66	0.000E-01	107	4.607E-07	148	9.618E-02
26	0.000E-01	67	0.000E-01	108	0.000E-01	149	0.000E-01
27	1.198E-08	68	0.000E-01	109	1.519E-08	150	1.350E-03
28	1.456E-08	69	2.938E-04	110	0.000E-01	151	2.454E-04
29	2.699E-07	70	4.385E-06	111	7.780E-08	152	2.316E-04
30	4.951E-09	71	1.460E-05	112	1.662E-02	153	0.000E-01
31	1.131E-08	72	0.000E-01	113	1.611E-03	154	3.856E-04
32	1.127E-08	73	6.624E-08	114	1.184E-03	155	0.000E-01
33	9.210E-10	74	0.000E-01	115	1.617E-02	156	3.293E-05
34	1.378E-09	75	6.305E-06	116	1.542E-02	157	0.000E-01
35	5.477E-09	76	9.375E-08	117	4.457E-04	158	1.181E-05
36	5.386E-10	77	3.447E-07	118	8.427E-03	159	0.000E-01
37	1.153E-09	78	4.077E-09	119	1.102E-02	160	1.103E-05
38	4.150E-10	79	7.281E-09	120	0.000E-01	161	0.000E-01
39	1.763E-05	80	0.000E-01	121	0.000E-01	162	3.493E-06
40	5.187E-05	81	1.473E-07	122	1.190E-02	163	0.000E-01
41	1.821E-05	82	1.054E-08	123	2.415E-04	164	4.186E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 25 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 2.500 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	3.970E-01	206	4.152E-01	247	1.323E-02	288	3.198E-01
166	3.719E-01	207	3.641E-01	248	7.022E-02	289	3.215E-01
167	3.879E-01	208	3.616E-01	249	3.307E-01	290	3.263E-01
168	4.063E-01	209	1.335E-02	250	3.493E-01	291	3.440E-01
169	3.653E-01	210	1.435E-02	251	3.348E-01	292	3.394E-01
170	3.848E-01	211	7.568E-02	252	3.483E-01	293	4.003E-01
171	3.813E-01	212	3.899E-01	253	3.730E-01	294	4.786E-01
172	3.558E-01	213	3.863E-01	254	1.022E-03	295	3.831E-01
173	3.553E-01	214	3.701E-01	255	3.801E-01	296	3.768E-01
174	9.191E-03	215	7.278E-04	256	4.199E-01	297	4.091E-01
175	1.448E-02	216	3.501E-04	257	4.498E-01	298	3.204E+00
176	7.065E-02	217	1.451E-03	258	3.307E+00	299	4.236E-01
177	3.772E-01	218	4.703E-01	259	5.007E+00	300	4.291E-01
178	3.763E-01	219	4.642E-01	260	6.012E+00	301	4.753E+00
179	3.611E-01	220	4.218E-01	261	3.187E-04	302	0.000E-01
180	1.324E-03	221	0.000E-01	262	1.164E-03	303	0.000E-01
181	6.411E-04	222	2.562E-05	263	1.067E-03	304	1.005E-02
182	1.076E-03	223	5.727E-04	264	3.661E-04	305	1.063E-02
183	1.562E-04	224	7.044E-04	265	6.614E-03	306	9.341E-03
184	2.799E-05	225	4.930E-08	266	9.102E-03	307	9.403E-02
185	2.601E-05	226	0.000E-01	267	1.880E-04	308	0.000E-01
186	0.000E-01	227	1.309E-04	268	0.000E-01	309	7.008E-06
187	1.249E-05	228	1.072E-05	269	3.348E-04	310	0.000E-01
188	2.611E-06	229	2.745E-05	270	7.883E-04	311	0.000E-01
189	0.000E-01	230	0.000E-01	271	0.000E-01	312	1.948E-04
190	0.000E-01	231	0.000E-01	272	0.000E-01	313	6.109E-06
191	5.540E-07	232	0.000E-01	273	2.727E-05	314	1.932E-07
192	0.000E-01	233	9.069E-06	274	0.000E-01	315	1.948E-06
193	1.094E-06	234	9.200E-07	275	9.529E-06	316	1.807E-04
194	4.771E-08	235	2.896E-06	276	0.000E-01	317	7.064E-04
195	0.000E-01	236	0.000E-01	277	1.034E-05	318	0.000E-01
196	5.088E-01	237	8.714E+00	278	0.000E-01	319	0.000E-01
197	4.548E-01	238	5.965E+00	279	3.162E-06	320	2.848E-07
198	4.253E-01	239	3.957E+00	280	0.000E-01	321	4.361E-08
199	4.733E-01	240	6.594E+00	281	8.212E+00	322	6.922E-07
200	4.883E-01	241	8.222E+00	282	9.639E+00	323	2.979E-08
201	4.437E-01	242	3.849E+00	283	7.938E+00	324	3.629E-08
202	5.256E-01	243	7.281E+00	284	5.590E+00	325	3.188E-01
203	4.354E-01	244	7.791E+00	285	5.860E+00	326	3.161E-01
204	4.637E-01	245	5.345E+00	286	6.239E+00	327	1.120E-02
205	4.294E-01	246	1.266E-02	287	9.132E-02	328	1.492E-02

LISTING D-6. Output Report File for Test Case Two. (Sheet 26 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 2.500 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 329 TO 445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	7.923E-02	359	2.718E-04	389	7.030E-09	419	6.239E-10
330	3.367E-01	360	2.908E-08	390	1.149E-08	420	3.303E-07
331	3.341E-01	361	1.880E-08	391	0.000E-01	421	0.000E-01
332	3.232E-01	362	4.212E-09	392	3.887E-05	422	0.000E-01
333	3.690E-01	363	3.362E-01	393	0.000E-01	423	1.975E-08
334	3.515E-01	364	3.291E-01	394	4.345E-09	424	0.000E-01*
335	3.592E-01	365	1.441E-02	395	4.232E-09	425	0.000E-01*
336	3.866E-01	366	1.561E-02	396	2.259E-10	426	0.000E-01*
337	0.000E-01	367	8.826E-02	397	1.349E-06	427	1.515E-07
338	1.162E-03	368	3.414E-01	398	0.000E-01	428	6.960E-10
339	7.127E-04	369	7.232E-04	399	1.399E-05	429	0.000E-01*
340	1.112E-03	370	4.298E-04	400	8.995E-08	430	0.000E-01*
341	6.378E-04	371	1.675E-03	401	3.176E-08	431	0.000E-01*
342	1.249E-03	372	1.138E-04	402	1.368E-07	432	0.000E-01*
343	3.168E-06	373	3.559E-05	403	3.279E-07	433	0.000E-01
344	1.365E-07	374	2.557E-05	404	9.534E-08	434	1.258E-09
345	4.050E-06	375	3.008E-06	405	1.637E-08	435	0.000E-01*
346	9.781E-06	376	0.000E-01	406	2.620E-09	436	0.000E-01*
347	0.000E-01	377	1.745E-07	407	1.709E-08	437	0.000E-01*
348	1.780E-07	378	2.165E-07	408	0.000E-01	438	0.000E-01*
349	1.895E-07	379	2.872E-07	409	0.000E-01	439	0.000E-01
350	1.329E-07	380	5.072E-08	410	1.540E-05	440	5.607E-11
351	0.000E-01	381	2.715E-06	411	3.082E-09	441	0.000E-01*
352	0.000E-01	382	3.990E-08	412	2.154E-09	442	0.000E-01*
353	2.965E-04	383	3.216E-08	413	2.079E-09	443	0.000E-01*
354	1.369E-07	384	3.831E-08	414	1.311E-05	444	0.000E-01
355	1.439E-08	385	7.801E-06	415	0.000E-01	445	0.000E-01*
356	8.699E-08	386	3.870E-05	416	1.302E-05		
357	2.234E-04	387	0.000E-01	417	2.285E-09		
358	0.000E-01	388	1.229E-08	418	1.833E-10		

CONSTITUENT COMP-1 DIAGNOSTICS
MAXIMUM VALUE IS 9.639E+00
MAXIMUM CHANGE IS 4.553E+00 AT NODE 267, MAXIMUM FRACTIONAL CHANGE IS 7.994E+00
MAXIMUM CORRECTION IS 6.619E-02 AT NODE 310, MAXIMUM FRACTIONAL CORRECTION IS 4.609E+00
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
2.5472E-03 AT ELEMENT 72 FOR MATERIAL TYPE CANIST
4.0447E-05 AT ELEMENT 87 FOR MATERIAL TYPE PCKNG
2.0338E-01 AT ELEMENT 15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-1 PRESENT IN THE SIMULATION ENVIRONMENT IS 1.175E-02 GRAMS.

LISTING D-6. Output Report File for Test Case Two. (Sheet 27 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 2.500 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	3.520E-08	83	0.000E-01	124	6.829E-06
2	0.000E-01*	43	4.995E-09	84	5.130E-10	125	1.064E-05
3	0.000E-01*	44	1.254E-07	85	1.448E-06	126	3.400E-07
4	0.000E-01*	45	2.920E-07	86	9.971E-06	127	5.828E-07
5	0.000E-01*	46	2.701E-07	87	9.121E-07	128	2.734E-06
6	0.000E-01*	47	1.726E-08	88	1.704E-06	129	4.366E-08
7	0.000E-01*	48	3.852E-08	89	1.151E-05	130	2.252E-07
8	0.000E-01*	49	4.644E-08	90	1.321E-05	131	2.083E-07
9	0.000E-01*	50	0.000E-01	91	2.367E-06	132	1.705E-08
10	0.000E-01*	51	0.000E-01	92	5.824E-06	133	2.761E-08
11	0.000E-01*	52	2.568E-08	93	7.688E-06	134	8.272E-08
12	0.000E-01*	53	8.676E-10	94	1.123E-05	135	4.468E-09
13	0.000E-01*	54	1.885E-09	95	7.533E-06	136	2.564E-08
14	0.000E-01*	55	0.000E-01	96	5.212E-07	137	7.764E-09
15	0.000E-01*	56	0.000E-01	97	3.324E-07	138	4.052E-03
16	3.589E-08	57	0.000E-01	98	5.219E-07	139	1.477E-03
17	6.991E-08	58	7.596E-10	99	1.499E-06	140	1.361E-03
18	1.361E-08	59	1.140E-10	100	0.000E-01	141	3.874E-03
19	3.998E-09	60	2.416E-10	101	0.000E-01	142	3.983E-03
20	6.533E-10	61	0.000E-01	102	3.766E-07	143	1.450E-03
21	2.446E-08	62	4.216E-07	103	1.652E-08	144	3.760E-03
22	4.547E-08	63	1.249E-06	104	2.886E-08	145	3.799E-03
23	8.476E-08	64	4.197E-07	105	0.000E-01	146	1.376E-04
24	0.000E-01	65	4.026E-07	106	0.000E-01	147	1.963E-04
25	0.000E-01	66	0.000E-01	107	0.000E-01	148	1.398E-03
26	2.585E-08	67	3.168E-07	108	1.088E-08	149	7.103E-06
27	1.340E-09	68	7.591E-07	109	2.177E-09	150	1.124E-05
28	2.680E-09	69	1.572E-06	110	3.553E-09	151	3.102E-05
29	0.000E-01	70	0.000E-01	111	0.000E-01	152	1.388E-06
30	0.000E-01	71	0.000E-01	112	2.747E-04	153	9.391E-07
31	0.000E-01	72	4.019E-07	113	3.688E-05	154	1.919E-06
32	9.948E-10	73	1.535E-08	114	3.050E-05	155	1.617E-07
33	6.737E-11	74	3.928E-08	115	2.468E-04	156	1.570E-07
34	1.360E-10	75	0.000E-01	116	2.491E-04	157	3.217E-07
35	0.000E-01	76	0.000E-01	117	3.645E-05	158	6.509E-08
36	0.000E-01	77	0.000E-01	118	2.331E-04	159	4.543E-08
37	0.000E-01	78	1.478E-08	119	2.257E-04	160	4.439E-08
38	3.590E-11	79	8.007E-10	120	1.157E-05	161	1.747E-08
39	6.786E-08	80	1.968E-09	121	2.760E-05	162	1.533E-08
40	2.077E-07	81	0.000E-01	122	1.477E-04	163	1.265E-08
41	1.686E-07	82	0.000E-01	123	1.598E-06	164	4.172E-03

LISTING D-6. Output Report File for Test Case Two. (Sheet 28 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 2.500 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	4.082E-03	206	3.961E-03	247	1.951E-04	288	3.329E-03
166	3.894E-03	207	3.762E-03	248	1.195E-03	289	3.574E-03
167	3.957E-03	208	3.773E-03	249	3.479E-03	290	3.354E-03
168	4.088E-03	209	1.944E-04	250	3.631E-03	291	3.419E-03
169	3.789E-03	210	2.174E-04	251	3.492E-03	292	3.444E-03
170	3.867E-03	211	1.262E-03	252	3.545E-03	293	3.591E-03
171	3.882E-03	212	3.870E-03	253	3.721E-03	294	3.819E-03
172	3.740E-03	213	3.873E-03	254	2.523E-05	295	3.612E-03
173	3.735E-03	214	3.788E-03	255	3.658E-03	296	3.544E-03
174	1.838E-04	215	9.274E-06	256	3.794E-03	297	3.649E-03
175	2.003E-04	216	4.558E-06	257	3.981E-03	298	1.467E-02
176	1.218E-03	217	3.125E-05	258	1.510E-02	299	3.735E-03
177	3.826E-03	218	4.183E-03	259	2.600E-02	300	3.824E-03
178	3.819E-03	219	4.159E-03	260	3.506E-02	301	2.250E-02
179	3.762E-03	220	4.002E-03	261	1.282E-06	302	1.139E-05
180	1.209E-05	221	4.808E-07	262	1.008E-05	303	3.269E-05
181	7.888E-06	222	8.388E-07	263	1.051E-05	304	1.302E-04
182	2.597E-05	223	7.535E-06	264	3.109E-05	305	1.453E-04
183	1.605E-06	224	8.675E-06	265	2.021E-04	306	2.529E-04
184	2.450E-07	225	3.068E-07	266	1.877E-04	307	1.358E-03
185	8.976E-07	226	9.344E-07	267	1.023E-06	308	3.071E-07
186	2.989E-07	227	1.201E-06	268	6.113E-07	309	0.000E-01
187	1.276E-07	228	1.093E-07	269	1.917E-06	310	3.210E-07
188	4.002E-08	229	1.190E-07	270	5.179E-06	311	4.211E-07
189	0.000E-01	230	2.846E-07	271	7.624E-06	312	1.334E-06
190	1.002E-08	231	9.625E-09	272	1.720E-07	313	3.151E-08
191	5.055E-09	232	4.296E-08	273	1.599E-07	314	2.512E-08
192	8.767E-10	233	2.717E-08	274	2.247E-07	315	0.000E-01
193	1.122E-08	234	9.195E-09	275	4.556E-08	316	1.062E-06
194	1.627E-09	235	1.069E-08	276	2.953E-08	317	3.813E-06
195	0.000E-01	236	1.109E-08	277	5.840E-08	318	1.260E-05
196	4.522E-03	237	4.615E-02	278	1.851E-08	319	1.549E-08
197	4.320E-03	238	2.835E-02	279	1.814E-08	320	0.000E-01
198	4.094E-03	239	1.799E-02	280	8.333E-09	321	9.280E-09
199	4.261E-03	240	3.146E-02	281	5.363E-02	322	3.129E-09
200	4.389E-03	241	4.170E-02	282	5.500E-02	323	3.122E-09
201	4.070E-03	242	1.754E-02	283	5.094E-02	324	0.000E-01
202	4.341E-03	243	4.140E-02	284	3.334E-02	325	3.335E-03
203	4.085E-03	244	3.991E-02	285	3.674E-02	326	3.307E-03
204	4.126E-03	245	2.535E-02	286	4.691E-02	327	2.418E-04
205	4.021E-03	246	1.934E-04	287	1.327E-03	328	2.533E-04

LISTING D-6. Output Report File for Test Case Two. (Sheet 29 of 51)

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***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER   2.500     YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER  2   COMP-2,  MG/LIT  .....

... OUTPUT FOR NODES  329 TO  445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

 NODE   CONCENTRATION        NODE   CONCENTRATION        NODE   CONCENTRATION        NODE   CONCENTRATION
NUMBER                      NUMBER                      NUMBER                      NUMBER
   329 1.291E-03               359 1.041E-06               389 0.000E-01               419 2.960E-11
   330 3.404E-03               360 1.952E-09               390 6.508E-10               420 3.737E-09
   331 3.377E-03               361 0.000E-01               391 2.879E-07               421 3.077E-09
   332 3.352E-03               362 4.446E-10               392 1.176E-07               422 1.310E-08
   333 3.515E-03               363 3.455E-03               393 4.010E-07               423 1.132E-09
   334 3.492E-03               364 3.407E-03               394 0.000E-01               424 0.000E-01*
   335 3.551E-03               365 2.589E-04               395 2.065E-10               425 0.000E-01*
   336 3.666E-03               366 2.825E-04               396 0.000E-01               426 0.000E-01*
   337 8.355E-06               367 1.389E-03               397 2.781E-08               427 0.000E-01
   338 1.016E-05               368 3.479E-03               398 0.000E-01               428 0.000E-01
   339 4.053E-05               369 1.066E-05               399 1.261E-07               429 0.000E-01*
   340 1.155E-05               370 8.018E-06               400 0.000E-01               430 0.000E-01*
   341 9.565E-06               371 3.998E-05               401 2.274E-09               431 0.000E-01*
   342 3.370E-05               372 1.097E-06               402 0.000E-01               432 0.000E-01*
   343 0.000E-01               373 3.949E-07               403 0.000E-01               433 2.568E-08
   344 3.344E-08               374 8.903E-07               404 1.408E-08               434 5.551E-11
   345 0.000E-01               375 4.544E-07               405 7.390E-10               435 0.000E-01*
   346 0.000E-01               376 5.629E-07               406 0.000E-01               436 0.000E-01*
   347 2.743E-07               377 1.368E-08               407 8.251E-10               437 0.000E-01*
   348 1.482E-08               378 0.000E-01               408 2.193E-08               438 0.000E-01*
   349 0.000E-01               379 2.249E-08               409 4.766E-08               439 3.368E-08
   350 1.285E-08               380 3.089E-08               410 7.802E-08               440 0.000E-01
   351 3.530E-07               381 0.000E-01               411 0.000E-01               441 0.000E-01*
   352 7.973E-07               382 0.000E-01               412 1.128E-10               442 0.000E-01*
   353 1.493E-06               383 1.618E-09               413 0.000E-01               443 0.000E-01*
   354 0.000E-01               384 0.000E-01               414 4.644E-08               444 1.048E-09
   355 1.694E-09               385 2.171E-08               415 6.641E-08               445 0.000E-01*
   356 0.000E-01               386 1.726E-07               416 3.334E-08
   357 9.792E-07               387 3.284E-07               417 9.687E-11
   358 1.251E-06               388 7.032E-10               418 0.000E-01

CONSTITUENT COMP-2 DIAGNOSTICS
      MAXIMUM VALUE IS          5.500E-02
      MAXIMUM CHANGE IS         3.534E-02 AT NODE  267, MAXIMUM FRACTIONAL CHANGE IS      8.401E+00
      MAXIMUM CORRECTION IS     8.226E-03 AT NODE  271, MAXIMUM FRACTIONAL CORRECTION IS  8.214E-01
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
  2.5472E-03 AT ELEMENT    72 FOR MATERIAL TYPE CANIST
  4.0447E-05 AT ELEMENT    87 FOR MATERIAL TYPE PCKNG
  2.0338E-01 AT ELEMENT    15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-2 PRESENT IN THE SIMULATION ENVIRONMENT IS  1.219E-04 GRAMS.
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LISTING D-6. Output Report File for Test Case Two. (Sheet 30 of 51)

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        THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED, SIMULATION TIME =  2.500E+00
CONSTITUENT  USAGE     DECAY RATE(S)

  1) COMP-1     1     7.900E-03

  2) COMP-2     1     7.767E-03  1.551E-10
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LISTING D-6. Output Report File for Test Case Two. (Sheet 31 of 51)

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THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED. SIMULATION TIME =  1.000E+01
CONSTITUENT  USAGE     DECAY RATE(S)

 1) COMP-1     1     7.900E-03

 2) COMP-2     1     7.767E-03  1.551E-10
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LISTING D-6. Output Report File for Test Case Two. (Sheet 32 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 25.00 YEARS - DYNAMIC SIMULATION..
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	4.923E-04	83	0.000E-01	124	1.230E-01
2	0.000E-01*	43	4.603E-05	84	3.805E-07	125	3.431E-01
3	0.000E-01*	44	6.006E-05	85	5.243E-02	126	4.345E-03
4	0.000E-01*	45	3.415E-04	86	2.333E-01	127	7.039E-03
5	0.000E-01*	46	4.083E-04	87	5.998E-02	128	3.395E-02
6	0.000E-01*	47	2.160E-05	88	5.717E-02	129	3.491E-04
7	0.000E-01*	48	8.420E-05	89	2.361E-01	130	5.425E-04
8	0.000E-01*	49	2.239E-04	90	2.354E-01	131	2.574E-05
9	0.000E-01*	50	2.670E-06	91	3.395E-02	132	2.667E-05
10	0.000E-01*	51	7.954E-06	92	1.245E-01	133	4.938E-05
11	0.000E-01*	52	3.860E-05	93	1.813E-01	134	0.000E-01
12	0.000E-01*	53	9.252E-07	94	2.450E-01	135	1.379E-05
13	0.000E-01*	54	1.599E-06	95	2.509E-01	136	1.895E-05
14	0.000E-01*	55	1.949E-06	96	6.423E-02	137	0.000E-01
15	0.000E-01*	56	1.385E-07	97	9.103E-03	138	5.431E+00
16	6.361E-06	57	3.676E-07	98	2.518E-02	139	3.358E+00
17	4.333E-05	58	4.115E-08	99	7.239E-02	140	3.239E+00
18	1.783E-05	59	4.185E-08	100	9.001E-04	141	5.382E+00
19	4.507E-05	60	4.553E-08	101	1.873E-03	142	5.413E+00
20	1.506E-05	61	6.410E-08	102	9.060E-03	143	3.324E+00
21	2.047E-06	62	9.747E-04	103	6.776E-05	144	5.323E+00
22	9.170E-06	63	1.357E-02	104	1.223E-04	145	5.352E+00
23	5.108E-05	64	1.353E-02	105	5.362E-05	146	1.232E+00
24	1.354E-06	65	1.426E-02	106	5.240E-06	147	1.636E+00
25	8.305E-06	66	1.370E-03	107	1.366E-05	148	3.277E+00
26	7.493E-06	67	7.041E-04	108	4.437E-08	149	1.768E-01
27	6.561E-07	68	7.290E-03	109	2.645E-06	150	2.307E-01
28	9.643E-07	69	1.096E-02	110	3.998E-06	151	6.844E-01
29	4.295E-06	70	2.491E-04	111	2.490E-07	152	1.053E-02
30	7.001E-08	71	1.892E-03	112	1.733E+00	153	1.291E-02
31	1.568E-07	72	4.479E-03	113	7.351E-01	154	5.724E-02
32	5.054E-07	73	2.845E-05	114	6.991E-01	155	6.561E-04
33	0.000E-01	74	8.065E-05	115	1.660E+00	156	9.761E-04
34	0.000E-01	75	9.242E-04	116	1.685E+00	157	0.000E-01
35	1.276E-07	76	2.200E-06	117	7.088E-01	158	1.084E-04
36	1.139E-08	77	8.027E-07	118	1.688E+00	159	1.153E-04
37	2.552E-08	78	2.231E-05	119	1.644E+00	160	0.000E-01
38	7.949E-09	79	4.943E-07	120	3.482E-01	161	1.248E-05
39	4.976E-05	80	1.619E-06	121	7.183E-01	162	2.944E-05
40	6.767E-04	81	0.000E-01	122	1.253E+00	163	0.000E-01
41	6.975E-04	82	1.488E-07	123	7.180E-02	164	5.460E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 33 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 25.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	5.438E+00	206	5.329E+00	247	1.631E+00	288	4.996E+00
166	5.387E+00	207	5.205E+00	248	3.127E+00	289	5.032E+00
167	5.402E+00	208	5.242E+00	249	5.082E+00	290	5.003E+00
168	5.439E+00	209	1.610E+00	250	5.144E+00	291	5.021E+00
169	5.331E+00	210	1.663E+00	251	5.085E+00	292	5.049E+00
170	5.350E+00	211	3.191E+00	252	5.097E+00	293	5.077E+00
171	5.372E+00	212	5.232E+00	253	5.167E+00	294	5.155E+00
172	5.266E+00	213	5.269E+00	254	7.055E-01	295	5.092E+00
173	5.293E+00	214	5.212E+00	255	5.128E+00	296	5.037E+00
174	1.582E+00	215	2.418E-01	256	5.167E+00	297	5.056E+00
175	1.590E+00	216	2.499E-01	257	5.243E+00	298	8.026E+00
176	3.119E+00	217	7.180E-01	258	8.175E+00	299	5.064E+00
177	5.290E+00	218	5.315E+00	259	1.019E+01	300	5.071E+00
178	5.316E+00	219	5.349E+00	260	1.159E+01	301	9.765E+00
179	5.273E+00	220	5.266E+00	261	6.375E-02	302	4.103E-01
180	2.302E-01	221	6.644E-02	262	2.519E-01	303	8.373E-01
181	2.284E-01	222	6.323E-02	263	2.467E-01	304	1.332E+00
182	6.744E-01	223	2.409E-01	264	7.391E-01	305	1.394E+00
183	5.283E-02	224	2.487E-01	265	1.716E+00	306	1.848E+00
184	1.434E-02	225	1.411E-02	266	1.646E+00	307	3.312E+00
185	6.122E-02	226	1.420E-02	267	1.185E-02	308	5.780E-03
186	1.326E-02	227	5.763E-02	268	8.983E-03	309	2.821E-03
187	1.052E-03	228	1.055E-03	269	4.142E-02	310	1.341E-02
188	9.618E-04	229	1.063E-03	270	1.494E-01	311	3.822E-02
189	1.137E-04	230	0.000E-01	271	2.039E-01	312	9.287E-02
190	9.828E-05	231	1.129E-04	272	8.128E-04	313	4.302E-04
191	1.210E-04	232	1.238E-04	273	6.392E-04	314	1.804E-04
192	0.000E-01	233	0.000E-01	274	5.032E-05	315	6.061E-05
193	3.631E-05	234	3.261E-05	275	1.071E-04	316	1.012E-01
194	2.416E-05	235	3.165E-05	276	6.902E-05	317	1.741E-01
195	0.000E-01	236	0.000E-01	277	0.000E-01	318	4.390E-01
196	5.552E+00	237	1.442E+01	278	2.075E-05	319	3.870E-05
197	5.497E+00	238	1.121E+01	279	1.887E-05	320	1.950E-05
198	5.439E+00	239	9.018E+00	280	0.000E-01	321	0.000E-01
199	5.486E+00	240	1.184E+01	281	1.464E+01	322	1.460E-05
200	5.521E+00	241	1.375E+01	282	1.578E+01	323	5.240E-06
201	5.408E+00	242	8.866E+00	283	1.421E+01	324	0.000E-01
202	5.489E+00	243	1.301E+01	284	1.115E+01	325	4.961E+00
203	5.425E+00	244	1.330E+01	285	1.162E+01	326	4.970E+00
204	5.379E+00	245	1.047E+01	286	1.264E+01	327	1.810E+00
205	5.372E+00	246	1.633E+00	287	3.269E+00	328	1.825E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 34 of 51)

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***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER   25.00     YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER  1   COMP-1,  MG/LIT .....

... OUTPUT FOR NODES  329 TO  445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...
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NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	3.246E+00	359	8.942E-02	389	6.928E-07	419	0.000E-01
330	4.981E+00	360	2.620E-06	390	0.000E-01	420	5.104E-05
331	4.990E+00	361	5.047E-08	391	6.784E-04	421	8.757E-05
332	4.966E+00	362	3.026E-07	392	9.221E-04	422	2.778E-05
333	5.014E+00	363	4.973E+00	393	2.085E-03	423	6.431E-07
334	4.990E+00	364	4.966E+00	394	4.422E-07	424	0.000E-01*
335	4.997E+00	365	1.855E+00	395	0.000E-01	425	0.000E-01*
336	5.026E+00	366	1.900E+00	396	1.488E-07	426	0.000E-01*
337	2.518E-01	367	3.344E+00	397	7.897E-04	427	3.291E-07
338	3.198E-01	368	4.978E+00	398	2.649E-03	428	2.439E-07
339	8.598E-01	369	3.332E-01	399	9.576E-04	429	0.000E-01*
340	3.183E-01	370	3.423E-01	400	3.206E-06	430	0.000E-01*
341	3.189E-01	371	8.979E-01	401	1.397E-06	431	0.000E-01*
342	8.562E-01	372	8.328E-02	402	4.666E-06	432	0.000E-01*
343	1.471E-03	373	2.344E-02	403	5.921E-06	433	3.989E-06
344	1.948E-04	374	9.421E-02	404	3.127E-05	434	0.000E-01
345	1.627E-03	375	2.224E-02	405	1.415E-07	435	0.000E-01*
346	3.319E-03	376	1.009E-01	406	4.592E-07	436	0.000E-01*
347	1.506E-02	377	6.650E-05	407	0.000E-01	437	0.000E-01*
348	9.223E-05	378	9.172E-06	408	1.659E-05	438	0.000E-01*
349	7.772E-06	379	6.410E-05	409	1.576E-05	439	6.960E-06
350	2.670E-05	380	1.441E-04	410	7.495E-05	440	2.335E-08
351	7.882E-03	381	5.035E-04	411	2.659E-07	441	0.000E-01*
352	1.239E-02	382	7.222E-06	412	0.000E-01	442	0.000E-01*
353	5.373E-02	383	0.000E-01	413	1.780E-07	443	0.000E-01*
354	1.011E-05	384	5.097E-06	414	4.071E-05	444	1.552E-05
355	1.855E-06	385	2.879E-04	415	5.064E-05	445	0.000E-01*
356	2.612E-07	386	4.828E-04	416	8.494E-05		
357	1.732E-02	387	1.476E-03	417	0.000E-01		
358	2.164E-02	388	9.288E-08	418	4.179E-08		

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CONSTITUENT COMP-1 DIAGNOSTICS
      MAXIMUM VALUE IS          1.578E+01
      MAXIMUM CHANGE IS         9.591E-01 AT NODE  127, MAXIMUM FRACTIONAL CHANGE IS      5.964E+00
      MAXIMUM CORRECTION IS     3.074E-02 AT NODE  356, MAXIMUM FRACTIONAL CORRECTION IS  2.952E+00
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
  2.5472E-03 AT ELEMENT    72 FOR MATERIAL TYPE CANIST
  4.0447E-05 AT ELEMENT    87 FOR MATERIAL TYPE PCKNG
  2.0338E-01 AT ELEMENT    15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-1 PRESENT IN THE SIMULATION ENVIRONMENT IS  1.223E-01 GRAMS.
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LISTING D-6. Output Report File for Test Case Two. (Sheet 35 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 25.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	1.020E-04	83	0.000E-01	124	2.132E-02
2	0.000E-01*	43	1.259E-05	84	7.575E-08	125	5.293E-02
3	0.000E-01*	44	1.007E-05	85	9.757E-03	126	9.877E-04
4	0.000E-01*	45	6.391E-05	86	3.699E-02	127	1.530E-03
5	0.000E-01*	46	9.270E-05	87	1.096E-02	128	6.602E-03
6	0.000E-01*	47	5.218E-06	88	1.052E-02	129	6.409E-05
7	0.000E-01*	48	2.240E-05	89	3.732E-02	130	1.020E-04
8	0.000E-01*	49	3.932E-05	90	3.700E-02	131	2.314E-05
9	0.000E-01*	50	6.949E-07	91	6.538E-03	132	6.606E-06
10	0.000E-01*	51	2.028E-06	92	2.141E-02	133	1.051E-05
11	0.000E-01*	52	8.969E-06	93	3.007E-02	134	0.000E-01
12	0.000E-01*	53	2.859E-08	94	3.851E-02	135	1.842E-06
13	0.000E-01*	54	0.000E-01	95	3.953E-02	136	2.898E-06
14	0.000E-01*	55	9.241E-07	96	1.175E-02	137	0.000E-01
15	0.000E-01*	56	4.543E-08	97	2.012E-03	138	4.701E-01
16	1.211E-06	57	1.225E-07	98	5.354E-03	139	3.373E-01
17	7.446E-06	58	0.000E-01	99	1.287E-02	140	3.285E-01
18	4.727E-06	59	0.000E-01	100	2.239E-04	141	4.684E-01
19	6.903E-06	60	0.000E-01	101	4.435E-04	142	4.695E-01
20	2.061E-06	61	2.810E-08	102	2.017E-03	143	3.338E-01
21	9.611E-07	62	2.418E-04	103	1.502E-05	144	4.648E-01
22	3.388E-06	63	2.578E-03	104	2.812E-05	145	4.668E-01
23	5.027E-06	64	2.640E-03	105	1.360E-05	146	1.546E-01
24	6.199E-08	65	2.764E-03	106	1.131E-06	147	1.973E-01
25	9.110E-07	66	3.024E-04	107	2.560E-06	148	3.309E-01
26	3.086E-06	67	1.771E-04	108	3.479E-07	149	2.985E-02
27	6.342E-08	68	1.546E-03	109	5.109E-07	150	3.719E-02
28	1.503E-07	69	2.075E-03	110	8.683E-07	151	9.633E-02
29	9.680E-07	70	6.232E-05	111	0.000E-01	152	2.066E-03
30	4.216E-08	71	4.430E-04	112	2.036E-01	153	2.556E-03
31	7.884E-08	72	1.004E-03	113	1.008E-01	154	1.074E-02
32	0.000E-01	73	8.822E-06	114	9.670E-02	155	1.365E-04
33	0.000E-01	74	2.984E-05	115	1.965E-01	156	1.761E-04
34	0.000E-01	75	2.278E-04	116	1.991E-01	157	1.837E-05
35	3.443E-08	76	1.086E-06	117	9.787E-02	158	1.604E-05
36	4.340E-09	77	5.930E-07	118	2.004E-01	159	1.988E-05
37	8.140E-09	78	5.406E-06	119	1.957E-01	160	0.000E-01
38	0.000E-01	79	7.967E-10	120	5.330E-02	161	3.380E-06
39	1.156E-05	80	3.802E-07	121	1.003E-01	162	4.903E-06
40	1.159E-04	81	0.000E-01	122	1.560E-01	163	0.000E-01
41	1.196E-04	82	7.434E-08	123	1.284E-02	164	4.703E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 36 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM. DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 25.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	4.701E-01	206	4.609E-01	247	1.982E-01	288	4.424E-01
166	4.684E-01	207	4.545E-01	248	3.237E-01	289	4.449E-01
167	4.684E-01	208	4.576E-01	249	4.478E-01	290	4.425E-01
168	4.697E-01	209	1.952E-01	250	4.510E-01	291	4.427E-01
169	4.649E-01	210	2.007E-01	251	4.478E-01	292	4.449E-01
170	4.650E-01	211	3.282E-01	252	4.478E-01	293	4.430E-01
171	4.668E-01	212	4.547E-01	253	4.511E-01	294	4.435E-01
172	4.601E-01	213	4.579E-01	254	1.000E-01	295	4.451E-01
173	4.625E-01	214	4.546E-01	255	4.479E-01	296	4.414E-01
174	1.920E-01	215	3.899E-02	256	4.481E-01	297	4.403E-01
175	1.924E-01	216	4.051E-02	257	4.515E-01	298	4.661E-01
176	3.215E-01	217	1.010E-01	258	4.704E-01	299	4.396E-01
177	4.605E-01	218	4.554E-01	259	4.933E-01	300	4.395E-01
178	4.628E-01	219	4.586E-01	260	5.160E-01	301	4.825E-01
179	4.603E-01	220	4.550E-01	261	1.200E-02	302	6.333E-02
180	3.698E-02	221	1.245E-02	262	4.083E-02	303	1.169E-01
181	3.714E-02	222	1.184E-02	263	3.988E-02	304	1.687E-01
182	9.547E-02	223	3.930E-02	264	1.043E-01	305	1.755E-01
183	1.003E-02	224	4.019E-02	265	2.077E-01	306	2.209E-01
184	2.899E-03	225	2.866E-03	266	2.004E-01	307	3.369E-01
185	1.146E-02	226	2.828E-03	267	2.382E-03	308	1.314E-03
186	2.636E-03	227	1.097E-02	268	1.933E-03	309	6.799E-04
187	1.909E-04	228	1.915E-04	269	8.155E-03	310	2.968E-03
188	1.868E-04	229	1.941E-04	270	2.608E-02	311	7.974E-03
189	3.908E-05	230	2.015E-05	271	3.444E-02	312	1.678E-02
190	1.827E-05	231	2.122E-05	272	1.626E-04	313	8.255E-05
191	2.108E-05	232	2.150E-05	273	1.265E-04	314	4.214E-05
192	0.000E-01	233	0.000E-01	274	2.712E-05	315	1.819E-05
193	5.877E-06	234	5.142E-06	275	1.720E-05	316	1.823E-02
194	4.709E-06	235	5.417E-06	276	1.346E-05	317	3.016E-02
195	0.000E-01	236	0.000E-01	277	0.000E-01	318	6.732E-02
196	4.709E-01	237	5.439E-01	278	4.617E-06	319	9.016E-06
197	4.705E-01	238	5.119E-01	279	3.406E-06	320	3.873E-06
198	4.686E-01	239	4.917E-01	280	0.000E-01	321	2.276E-07
199	4.689E-01	240	5.143E-01	281	5.603E-01	322	2.126E-06
200	4.702E-01	241	5.348E-01	282	5.616E-01	323	1.193E-06
201	4.654E-01	242	4.875E-01	283	5.536E-01	324	0.000E-01
202	4.658E-01	243	5.312E-01	284	5.102E-01	325	4.394E-01
203	4.671E-01	244	5.290E-01	285	5.187E-01	326	4.406E-01
204	4.613E-01	245	4.971E-01	286	5.456E-01	327	2.173E-01
205	4.634E-01	246	1.983E-01	287	3.333E-01	328	2.183E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 37 of 51)

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***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER   25.00     YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER  2   COMP-2,  MG/LIT  .....

... OUTPUT FOR NODES  329 TO  445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...
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NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	3.333E-01	359	1.661E-02	389	2.071E-07	419	0.000E-01
330	4.396E-01	360	5.823E-07	390	0.000E-01	420	8.155E-06
331	4.408E-01	361	0.000E-01	391	1.436E-04	421	2.434E-05
332	4.395E-01	362	8.704E-08	392	1.749E-04	422	7.088E-06
333	4.399E-01	363	4.386E-01	393	5.193E-04	423	1.742E-07
334	4.390E-01	364	4.388E-01	394	1.537E-07	424	0.000E-01*
335	4.388E-01	365	2.215E-01	395	0.000E-01	425	0.000E-01*
336	4.391E-01	366	2.257E-01	396	4.878E-08	426	0.000E-01*
337	4.186E-02	367	3.405E-01	397	1.721E-04	427	1.935E-07
338	5.119E-02	368	4.387E-01	398	6.188E-04	428	8.306E-08
339	1.194E-01	369	5.311E-02	399	1.800E-04	429	0.000E-01*
340	5.086E-02	370	5.451E-02	400	6.524E-07	430	0.000E-01*
341	5.121E-02	371	1.239E-01	401	4.582E-07	431	0.000E-01*
342	1.191E-01	372	1.560E-02	402	9.588E-07	432	0.000E-01*
343	3.663E-04	373	4.757E-03	403	1.231E-06	433	1.023E-06
344	6.824E-05	374	1.737E-02	404	7.356E-06	434	0.000E-01
345	4.087E-04	375	4.528E-03	405	0.000E-01	435	0.000E-01*
346	8.187E-04	376	1.857E-02	406	1.493E-07	436	0.000E-01*
347	3.296E-03	377	2.203E-05	407	0.000E-01	437	0.000E-01*
348	2.171E-05	378	2.096E-06	408	4.297E-06	438	0.000E-01*
349	2.265E-06	379	1.696E-05	409	4.311E-06	439	1.193E-06
350	8.043E-06	380	3.598E-05	410	1.631E-05	440	7.041E-09
351	1.776E-03	381	1.385E-04	411	7.816E-08	441	0.000E-01*
352	2.690E-03	382	2.479E-06	412	0.000E-01	442	0.000E-01*
353	1.045E-02	383	0.000E-01	413	4.420E-08	443	0.000E-01*
354	2.103E-06	384	1.790E-06	414	5.929E-06	444	1.940E-06
355	5.505E-07	385	6.236E-05	415	8.679E-06	445	0.000E-01*
356	0.000E-01	386	1.032E-04	416	2.161E-05		
357	3.524E-03	387	3.708E-04	417	0.000E-01		
358	4.312E-03	388	0.000E-01	418	1.129E-08		

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CONSTITUENT COMP-2 DIAGNOSTICS
      MAXIMUM VALUE IS          5.616E-01
      MAXIMUM CHANGE IS         1.609E-01 AT NODE  150, MAXIMUM FRACTIONAL CHANGE IS      5.268E+00
      MAXIMUM CORRECTION IS     2.504E-02 AT NODE  353, MAXIMUM FRACTIONAL CORRECTION IS  8.753E-01
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
  2.5472E-03 AT ELEMENT    72 FOR MATERIAL TYPE CANIST
  4.0447E-05 AT ELEMENT    87 FOR MATERIAL TYPE PCKNG
  2.0338E-01 AT ELEMENT    15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-2 PRESENT IN THE SIMULATION ENVIRONMENT IS  1.291E-02 GRAMS.
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LISTING D-6. Output Report File for Test Case Two. (Sheet 38 of 51)

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        THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED. SIMULATION TIME =  2.500E+01
CONSTITUENT  USAGE     DECAY RATE(S)

  1) COMP-1     1     7.900E-03

  2) COMP-2     1     7.767E-03  1.551E-10
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LISTING D-6. Output Report File for Test Case Two. (Sheet 39 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 50.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	6.249E-03	83	0.000E-01	124	6.110E-01
2	0.000E-01*	43	1.160E-03	84	1.078E-05	125	1.217E+00
3	0.000E-01*	44	8.525E-04	85	3.285E-01	126	6.398E-02
4	0.000E-01*	45	4.425E-03	86	9.069E-01	127	8.939E-02
5	0.000E-01*	46	5.067E-03	87	3.561E-01	128	2.582E-01
6	0.000E-01*	47	4.326E-04	88	3.479E-01	129	2.592E-03
7	0.000E-01*	48	2.082E-03	89	9.129E-01	130	3.877E-03
8	0.000E-01*	49	3.234E-03	90	9.070E-01	131	6.944E-03
9	0.000E-01*	50	8.712E-05	91	2.447E-01	132	1.789E-04
10	0.000E-01*	51	3.593E-04	92	5.968E-01	133	2.571E-04
11	0.000E-01*	52	1.283E-03	93	7.716E-01	134	6.001E-05
12	0.000E-01*	53	0.000E-01	94	9.343E-01	135	3.972E-05
13	0.000E-01*	54	0.000E-01	95	9.522E-01	136	6.927E-05
14	0.000E-01*	55	2.184E-04	96	3.764E-01	137	0.000E-01
15	0.000E-01*	56	5.159E-06	97	1.035E-01	138	9.185E+00
16	4.495E-05	57	1.869E-05	98	2.199E-01	139	6.299E+00
17	3.063E-04	58	0.000E-01	99	4.047E-01	140	6.129E+00
18	3.021E-04	59	0.000E-01	100	2.116E-02	141	9.138E+00
19	3.100E-04	60	0.000E-01	101	3.840E-02	142	9.168E+00
20	5.488E-05	61	4.454E-06	102	1.057E-01	143	6.263E+00
21	3.054E-05	62	2.146E-02	103	9.066E-04	144	9.078E+00
22	1.998E-04	63	1.157E-01	104	1.322E-03	145	9.108E+00
23	3.109E-04	64	1.213E-01	105	3.937E-03	146	2.997E+00
24	2.264E-05	65	1.264E-01	106	1.246E-05	147	3.725E+00
25	1.231E-04	66	2.406E-02	107	1.011E-04	148	6.222E+00
26	1.717E-04	67	1.655E-02	108	2.425E-05	149	7.949E-01
27	1.784E-05	68	8.256E-02	109	2.531E-05	150	9.483E-01
28	5.247E-05	69	1.012E-01	110	1.007E-05	151	2.004E+00
29	6.060E-05	70	8.530E-03	111	4.964E-06	152	1.111E-01
30	5.258E-06	71	3.673E-02	112	3.810E+00	153	1.285E-01
31	8.562E-06	72	6.004E-02	113	2.036E+00	154	3.765E-01
32	1.328E-07	73	2.454E-03	114	1.967E+00	155	4.510E-03
33	0.000E-01	74	7.399E-03	115	3.691E+00	156	5.785E-03
34	2.943E-07	75	2.049E-02	116	3.733E+00	157	9.115E-03
35	6.838E-07	76	1.622E-04	117	1.989E+00	158	4.380E-04
36	2.031E-07	77	1.632E-05	118	3.751E+00	159	4.525E-04
37	1.642E-07	78	1.381E-03	119	3.672E+00	160	8.738E-06
38	0.000E-01	79	0.000E-01	120	1.211E+00	161	4.835E-05
39	1.040E-03	80	4.852E-05	121	2.036E+00	162	1.025E-04
40	6.063E-03	81	0.000E-01	122	3.005E+00	163	0.000E-01
41	6.215E-03	82	1.027E-05	123	4.102E-01	164	9.211E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 40 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...REBULTS AFTER 50.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1. MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	9.191E+00	206	9.073E+00	247	3.805E+00	288	8.736E+00
166	9.143E+00	207	8.948E+00	248	6.115E+00	289	8.773E+00
167	9.156E+00	208	8.988E+00	249	8.824E+00	290	8.742E+00
168	9.192E+00	209	3.723E+00	250	8.886E+00	291	8.759E+00
169	9.085E+00	210	3.928E+00	251	8.826E+00	292	8.789E+00
170	9.103E+00	211	6.176E+00	252	8.837E+00	293	8.809E+00
171	9.126E+00	212	8.972E+00	253	8.906E+00	294	8.878E+00
172	9.016E+00	213	9.012E+00	254	2.113E+00	295	8.826E+00
173	9.046E+00	214	8.954E+00	255	8.865E+00	296	8.769E+00
174	3.645E+00	215	9.954E-01	256	8.899E+00	297	8.782E+00
175	3.669E+00	216	1.029E+00	257	8.973E+00	298	1.143E+01
176	6.029E+00	217	2.115E+00	258	1.157E+01	299	8.787E+00
177	9.038E+00	218	9.046E+00	259	1.335E+01	300	8.792E+00
178	9.067E+00	219	9.084E+00	260	1.460E+01	301	1.297E+01
179	9.022E+00	220	9.002E+00	261	4.244E-01	302	1.487E+00
180	9.481E-01	221	4.276E-01	262	1.053E+00	303	2.431E+00
181	9.559E-01	222	4.130E-01	263	1.032E+00	304	3.324E+00
182	2.002E+00	223	1.018E+00	264	2.196E+00	305	3.459E+00
183	3.598E-01	224	1.030E+00	265	3.974E+00	306	4.240E+00
184	1.489E-01	225	1.486E-01	266	3.845E+00	307	6.432E+00
185	3.984E-01	226	1.451E-01	267	1.318E-01	308	8.826E-02
186	1.380E-01	227	3.961E-01	268	1.147E-01	309	5.961E-02
187	6.315E-03	228	6.283E-03	269	3.255E-01	310	1.599E-01
188	6.542E-03	229	6.484E-03	270	7.607E-01	311	3.316E-01
189	1.080E-02	230	1.048E-02	271	9.302E-01	312	5.512E-01
190	4.343E-04	231	5.600E-04	272	5.450E-03	313	3.409E-03
191	4.878E-04	232	5.085E-04	273	4.942E-03	314	2.154E-03
192	5.041E-05	233	4.529E-06	274	9.007E-03	315	5.961E-03
193	1.237E-04	234	8.433E-05	275	4.934E-04	316	5.923E-01
194	1.108E-04	235	1.143E-04	276	3.368E-04	317	8.645E-01
195	0.000E-01	236	0.000E-01	277	6.508E-05	318	1.573E+00
196	9.292E+00	237	1.714E+01	278	6.867E-05	319	2.741E-04
197	9.244E+00	238	1.430E+01	279	8.620E-05	320	1.420E-04
198	9.189E+00	239	1.236E+01	280	0.000E-01	321	5.087E-05
199	9.230E+00	240	1.486E+01	281	1.732E+01	322	3.921E-05
200	9.264E+00	241	1.655E+01	282	1.834E+01	323	2.369E-05
201	9.154E+00	242	1.221E+01	283	1.693E+01	324	3.362E-06
202	9.226E+00	243	1.587E+01	284	1.420E+01	325	8.697E+00
203	9.173E+00	244	1.614E+01	285	1.462E+01	326	8.709E+00
204	9.117E+00	245	1.362E+01	286	1.553E+01	327	4.183E+00
205	9.117E+00	246	3.796E+00	287	6.344E+00	328	4.209E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 41 of 51)

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***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER   50.00     YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER  1   COMP-1,  MG/LIT .....

... OUTPUT FOR NODES  329 TO  445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

  NODE   CONCENTRATION        NODE   CONCENTRATION        NODE   CONCENTRATION        NODE   CONCENTRATION
 NUMBER                      NUMBER                      NUMBER                      NUMBER
    329 6.353E+00               359 5.662E-01               389 3.176E-05               419 3.293E-07
    330 8.715E+00               360 2.669E-05               390 0.000E-01               420 7.597E-04
    331 8.727E+00               361 0.000E-01               391 1.154E-02               421 3.094E-03
    332 8.701E+00               362 1.466E-05               392 1.323E-02               422 7.741E-04
    333 8.745E+00               363 8.704E+00               393 5.013E-02               423 4.178E-05
    334 8.721E+00               364 8.699E+00               394 2.032E-05               424 0.000E-01*
    335 8.726E+00               365 4.263E+00               395 0.000E-01               425 0.000E-01*
    336 8.752E+00               366 4.337E+00               396 8.367E-06               426 0.000E-01*
    337 1.107E+00               367 6.499E+00               397 1.414E-02               427 7.276E-05
    338 1.292E+00               368 8.710E+00               398 5.556E-02               428 8.022E-06
    339 2.498E+00               369 1.331E+00               399 1.364E-02               429 0.000E-01*
    340 1.287E+00               370 1.356E+00               400 3.187E-04               430 0.000E-01*
    341 1.296E+00               371 2.583E+00               401 1.301E-04               431 0.000E-01*
    342 2.498E+00               372 5.414E-01               402 1.757E-04               432 0.000E-01*
    343 3.599E-02               373 2.343E-01               403 3.386E-04               433 1.057E-04
    344 1.528E-02               374 5.834E-01               404 1.223E-03               434 7.023E-07
    345 3.956E-02               375 2.248E-01               405 0.000E-01               435 0.000E-01*
    346 7.114E-02               376 6.141E-01               406 1.107E-05               436 0.000E-01*
    347 1.743E-01               377 5.838E-03               407 1.869E-05               437 0.000E-01*
    348 1.371E-03               378 1.081E-03               408 4.669E-04               438 0.000E-01*
    349 1.851E-04               379 3.239E-03               409 5.512E-04               439 1.360E-04
    350 2.541E-03               380 5.113E-03               410 2.256E-03               440 9.943E-08
    351 1.143E-01               381 2.016E-02               411 7.163E-06               441 0.000E-01*
    352 1.552E-01               382 3.488E-04               412 2.638E-06               442 0.000E-01*
    353 4.030E-01               383 0.000E-01               413 0.000E-01               443 0.000E-01*
    354 4.992E-05               384 4.868E-04               414 7.125E-04               444 1.441E-04
    355 6.705E-05               385 7.596E-03               415 7.334E-04               445 0.000E-01*
    356 0.000E-01               386 1.013E-02               416 2.789E-03
    357 1.876E-01               387 3.870E-02               417 0.000E-01
    358 2.128E-01               388 0.000E-01               418 0.000E-01

CONSTITUENT COMP-1 DIAGNOSTICS
      MAXIMUM VALUE IS          1.834E+01
      MAXIMUM CHANGE IS         1.706E+00 AT NODE  311, MAXIMUM FRACTIONAL CHANGE IS      7.017E+00
      MAXIMUM CORRECTION IS     4.232E-02 AT NODE  361, MAXIMUM FRACTIONAL CORRECTION IS  1.475E+00
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
  2.5472E-03 AT ELEMENT     72 FOR MATERIAL TYPE CANIST
  4.0447E-05 AT ELEMENT     87 FOR MATERIAL TYPE PCKNG
  2.0338E-01 AT ELEMENT     15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-1 PRESENT IN THE SIMULATION ENVIRONMENT IS  2.078E-01 GRAMS.
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LISTING D-6. Output Report File for Test Case Two. (Sheet 42 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 50.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	2.856E-03	83	0.000E-01	124	1.995E-01
2	0.000E-01*	43	5.990E-04	84	4.752E-06	125	3.560E-01
3	0.000E-01*	44	4.439E-04	85	1.144E-01	126	2.733E-02
4	0.000E-01*	45	2.093E-03	86	2.742E-01	127	3.706E-02
5	0.000E-01*	46	2.364E-03	87	1.224E-01	128	9.449E-02
6	0.000E-01*	47	2.496E-04	88	1.202E-01	129	9.289E-04
7	0.000E-01*	48	1.108E-03	89	2.755E-01	130	1.367E-03
8	0.000E-01*	49	1.590E-03	90	2.734E-01	131	3.902E-03
9	0.000E-01*	50	6.654E-05	91	8.839E-02	132	5.866E-05
10	0.000E-01*	51	2.472E-04	92	1.928E-01	133	7.690E-05
11	0.000E-01*	52	7.036E-04	93	2.402E-01	134	4.516E-05
12	0.000E-01*	53	0.000E-01	94	2.806E-01	135	9.199E-06
13	0.000E-01*	54	0.000E-01	95	2.854E-01	136	1.905E-05
14	0.000E-01*	55	1.296E-04	96	1.288E-01	137	2.539E-07
15	0.000E-01*	56	2.533E-06	97	4.135E-02	138	1.666E+00
16	2.565E-05	57	9.698E-06	98	8.199E-02	139	1.279E+00
17	1.489E-04	58	0.000E-01	99	1.372E-01	140	1.255E+00
18	1.567E-04	59	0.000E-01	100	9.903E-03	141	1.663E+00
19	1.520E-04	60	0.000E-01	101	1.732E-02	142	1.665E+00
20	2.683E-05	61	2.318E-06	102	4.244E-02	143	1.275E+00
21	2.010E-05	62	9.958E-03	103	3.687E-04	144	1.658E+00
22	1.130E-04	63	4.460E-02	104	5.225E-04	145	1.661E+00
23	1.446E-04	64	4.689E-02	105	2.210E-03	146	7.358E-01
24	1.390E-05	65	4.867E-02	106	1.687E-06	147	8.782E-01
25	6.995E-05	66	1.095E-02	107	3.320E-05	148	1.274E+00
26	9.761E-05	67	7.845E-03	108	2.209E-05	149	2.516E-01
27	9.371E-06	68	3.345E-02	109	9.717E-06	150	2.919E-01
28	3.002E-05	69	3.972E-02	110	2.634E-06	151	5.412E-01
29	3.873E-05	70	4.294E-03	111	2.570E-06	152	4.480E-02
30	2.513E-06	71	1.637E-02	112	8.797E-01	153	5.113E-02
31	3.930E-06	72	2.519E-02	113	5.367E-01	154	1.327E-01
32	2.815E-06	73	1.378E-03	114	5.223E-01	155	1.559E-03
33	7.077E-08	74	3.950E-03	115	8.583E-01	156	1.938E-03
34	3.798E-07	75	9.515E-03	116	8.662E-01	157	5.088E-03
35	0.000E-01	76	8.418E-05	117	5.275E-01	158	1.259E-04
36	5.701E-08	77	1.870E-05	118	8.722E-01	159	1.258E-04
37	0.000E-01	78	7.906E-04	119	8.566E-01	160	4.038E-05
38	4.467E-08	79	0.000E-01	120	3.520E-01	161	1.182E-05
39	5.412E-04	80	2.135E-05	121	5.426E-01	162	2.671E-05
40	2.687E-03	81	0.000E-01	122	7.323E-01	163	5.087E-07
41	2.760E-03	82	5.389E-06	123	1.399E-01	164	1.666E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 43 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 50.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	1.666E+00	206	1.651E+00	247	9.076E-01	288	1.622E+00
166	1.663E+00	207	1.641E+00	248	1.279E+00	289	1.626E+00
167	1.663E+00	208	1.646E+00	249	1.631E+00	290	1.622E+00
168	1.665E+00	209	8.848E-01	250	1.635E+00	291	1.622E+00
169	1.658E+00	210	9.067E-01	251	1.631E+00	292	1.626E+00
170	1.658E+00	211	1.283E+00	252	1.630E+00	293	1.623E+00
171	1.661E+00	212	1.641E+00	253	1.636E+00	294	1.623E+00
172	1.650E+00	213	1.646E+00	254	5.751E-01	295	1.626E+00
173	1.654E+00	214	1.641E+00	255	1.631E+00	296	1.620E+00
174	8.656E-01	215	3.063E-01	256	1.631E+00	297	1.618E+00
175	8.713E-01	216	3.165E-01	257	1.636E+00	298	1.646E+00
176	1.254E+00	217	5.718E-01	258	1.653E+00	299	1.617E+00
177	1.651E+00	218	1.642E+00	259	1.676E+00	300	1.617E+00
178	1.654E+00	219	1.647E+00	260	1.700E+00	301	1.662E+00
179	1.650E+00	220	1.641E+00	261	1.499E-01	302	4.372E-01
180	2.920E-01	221	1.497E-01	262	3.253E-01	303	6.516E-01
181	2.958E-01	222	1.453E-01	263	3.191E-01	304	8.242E-01
182	5.438E-01	223	3.157E-01	264	5.953E-01	305	8.536E-01
183	1.279E-01	224	3.173E-01	265	9.429E-01	306	9.977E-01
184	5.921E-02	225	5.929E-02	266	9.178E-01	307	1.331E+00
185	1.401E-01	226	5.792E-02	267	5.350E-02	308	3.788E-02
186	5.498E-02	227	1.410E-01	268	4.759E-02	309	2.693E-02
187	2.117E-03	228	2.097E-03	269	1.197E-01	310	6.449E-02
188	2.230E-03	229	2.179E-03	270	2.495E-01	311	1.237E-01
189	5.895E-03	230	5.848E-03	271	2.952E-01	312	1.893E-01
190	1.220E-04	231	1.672E-04	272	1.873E-03	313	1.227E-03
191	1.341E-04	232	1.438E-04	273	1.754E-03	314	8.543E-04
192	6.106E-05	233	4.046E-05	274	5.051E-03	315	3.385E-03
193	3.255E-05	234	1.705E-05	275	1.462E-04	316	2.025E-01
194	3.079E-05	235	2.930E-05	276	9.889E-05	317	2.814E-01
195	6.658E-07	236	1.434E-06	277	5.584E-05	318	4.604E-01
196	1.666E+00	237	1.734E+00	278	1.565E-05	319	9.183E-05
197	1.666E+00	238	1.705E+00	279	2.440E-05	320	4.551E-05
198	1.663E+00	239	1.685E+00	280	4.406E-07	321	4.041E-05
199	1.664E+00	240	1.705E+00	281	1.746E+00	322	6.944E-06
200	1.666E+00	241	1.725E+00	282	1.749E+00	323	7.312E-06
201	1.658E+00	242	1.678E+00	283	1.739E+00	324	2.335E-06
202	1.659E+00	243	1.717E+00	284	1.692E+00	325	1.617E+00
203	1.661E+00	244	1.717E+00	285	1.701E+00	326	1.619E+00
204	1.652E+00	245	1.684E+00	286	1.729E+00	327	9.886E-01
205	1.655E+00	246	9.042E-01	287	1.314E+00	328	9.932E-01

LISTING D-6. Output Report File for Test Case Two. (Sheet 44 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 50.00 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 329 TO 445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	1.323E+00	359	1.971E-01	389	1.605E-05	419	2.842E-07
330	1.617E+00	360	9.339E-06	390	0.000E-01	420	4.361E-04
331	1.620E+00	361	0.000E-01	391	5.794E-03	421	1.712E-03
332	1.617E+00	362	6.594E-06	392	6.454E-03	422	4.441E-04
333	1.618E+00	363	1.616E+00	393	2.336E-02	423	2.524E-05
334	1.616E+00	364	1.616E+00	394	1.010E-05	424	0.000E-01*
335	1.616E+00	365	1.004E+00	395	0.000E-01	425	0.000E-01*
336	1.616E+00	366	1.017E+00	396	4.226E-06	426	0.000E-01*
337	3.471E-01	367	1.345E+00	397	6.953E-03	427	4.947E-05
338	3.939E-01	368	1.616E+00	398	2.554E-02	428	3.570E-06
339	6.693E-01	369	4.046E-01	399	6.667E-03	429	0.000E-01*
340	3.929E-01	370	4.110E-01	400	2.443E-04	430	0.000E-01*
341	3.961E-01	371	6.885E-01	401	8.259E-05	431	0.000E-01*
342	6.705E-01	372	1.897E-01	402	1.261E-04	432	0.000E-01*
343	1.695E-02	373	9.164E-02	403	2.144E-04	433	7.276E-05
344	8.094E-03	374	2.021E-01	404	7.564E-04	434	6.179E-07
345	1.855E-02	375	8.824E-02	405	0.000E-01	435	0.000E-01*
346	3.191E-02	376	2.115E-01	406	4.035E-06	436	0.000E-01*
347	6.990E-02	377	3.276E-03	407	2.027E-05	437	0.000E-01*
348	5.590E-04	378	7.571E-04	408	2.858E-04	438	0.000E-01*
349	1.035E-04	379	1.856E-03	409	3.374E-04	439	8.883E-05
350	1.492E-03	380	2.864E-03	410	1.287E-03	440	0.000E-01
351	4.837E-02	381	1.020E-02	411	3.197E-06	441	0.000E-01*
352	6.362E-02	382	1.750E-04	412	1.953E-06	442	0.000E-01*
353	1.465E-01	383	0.000E-01	413	0.000E-01	443	0.000E-01*
354	1.593E-05	384	2.987E-04	414	4.016E-04	444	9.141E-05
355	2.907E-05	385	4.027E-03	415	4.169E-04	445	0.000E-01*
356	0.000E-01	386	5.173E-03	416	1.564E-03		
357	7.505E-02	387	1.845E-02	417	0.000E-01		
358	8.359E-02	388	0.000E-01	418	0.000E-01		

CONSTITUENT COMP-2 DIAGNOSTICS
MAXIMUM VALUE IS 1.749E+00
MAXIMUM CHANGE IS 6.663E-01 AT NODE 182, MAXIMUM FRACTIONAL CHANGE IS 1.200E+01
MAXIMUM CORRECTION IS 8.919E-02 AT NODE 353, MAXIMUM FRACTIONAL CORRECTION IS 1.969E+00
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
2.5472E-03 AT ELEMENT 72 FOR MATERIAL TYPE CANIST
4.0447E-05 AT ELEMENT 87 FOR MATERIAL TYPE PCKNG
2.0338E-01 AT ELEMENT 15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-2 PRESENT IN THE SIMULATION ENVIRONMENT IS 4.672E-02 GRAMS.

LISTING D-6. Output Report File for Test Case Two. (Sheet 45 of 51)

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        THE FOLLOWING DECAY CHAIN HAS BEEN SELECTED, SIMULATION TIME =  5.000E+01
CONSTITUENT  USAGE     DECAY RATE(S)

  1) COMP-1     1     7.900E-03

  2) COMP-2     1     7.767E-03  1.551E-10
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LISTING D-6. Output Report File for Test Case Two. (Sheet 46 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 100.0 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	5.436E-02	83	0.000E-01	124	1.692E+00
2	0.000E-01*	43	1.577E-02	84	4.387E-05	125	2.758E+00
3	0.000E-01*	44	1.284E-02	85	1.042E+00	126	3.584E-01
4	0.000E-01*	45	4.359E-02	86	2.169E+00	127	4.572E-01
5	0.000E-01*	46	4.756E-02	87	1.099E+00	128	9.324E-01
6	0.000E-01*	47	8.748E-03	88	1.086E+00	129	1.161E-02
7	0.000E-01*	48	2.840E-02	89	2.179E+00	130	1.560E-02
8	0.000E-01*	49	3.625E-02	90	2.166E+00	131	8.984E-02
9	0.000E-01*	50	4.012E-03	91	8.505E-01	132	5.599E-04
10	0.000E-01*	51	1.122E-02	92	1.612E+00	133	6.376E-04
11	0.000E-01*	52	1.997E-02	93	1.937E+00	134	1.066E-03
12	0.000E-01*	53	1.566E-04	94	2.212E+00	135	6.156E-05
13	0.000E-01*	54	4.496E-05	95	2.243E+00	136	1.403E-04
14	0.000E-01*	55	4.672E-03	96	1.147E+00	137	0.000E-01
15	0.000E-01*	56	4.084E-05	97	4.712E-01	138	1.303E+01
16	1.118E-03	57	1.453E-04	98	8.128E-01	139	9.585E+00
17	4.568E-03	58	0.000E-01	99	1.222E+00	140	9.383E+00
18	4.720E-03	59	0.000E-01	100	1.612E-01	141	1.299E+01
19	4.762E-03	60	0.000E-01	101	2.529E-01	142	1.302E+01
20	1.169E-03	61	3.197E-05	102	4.889E-01	143	9.563E+00
21	9.716E-04	62	1.564E-01	103	5.877E-03	144	1.295E+01
22	3.924E-03	63	4.917E-01	104	8.096E-03	145	1.297E+01
23	4.401E-03	64	5.123E-01	105	5.577E-02	146	5.405E+00
24	7.103E-04	65	5.279E-01	106	9.983E-05	147	6.429E+00
25	2.791E-03	66	1.677E-01	107	3.546E-04	148	9.555E+00
26	3.443E-03	67	1.308E-01	108	6.606E-04	149	2.066E+00
27	3.926E-04	68	3.952E-01	109	9.603E-05	150	2.356E+00
28	1.335E-03	69	4.514E-01	110	4.054E-05	151	4.045E+00
29	1.981E-03	70	8.351E-02	111	1.371E-05	152	5.341E-01
30	4.528E-05	71	2.324E-01	112	6.428E+00	153	5.937E-01
31	7.211E-05	72	3.187E-01	113	3.964E+00	154	1.239E+00
32	5.145E-04	73	3.561E-02	114	3.865E+00	155	1.701E-02
33	7.512E-06	74	8.373E-02	115	6.275E+00	156	2.023E-02
34	2.084E-05	75	1.530E-01	116	6.328E+00	157	1.119E-01
35	0.000E-01	76	2.051E-03	117	3.905E+00	158	1.031E-03
36	0.000E-01	77	2.035E-03	118	6.371E+00	159	9.536E-04
37	0.000E-01	78	2.324E-02	119	6.257E+00	160	1.162E-03
38	3.737E-06	79	0.000E-01	120	2.713E+00	161	4.661E-05
39	1.481E-02	80	2.688E-04	121	4.022E+00	162	1.698E-04
40	5.153E-02	81	1.149E-04	122	5.368E+00	163	0.000E-01
41	5.299E-02	82	8.088E-05	123	1.256E+00	164	1.305E+01

LISTING D-6. Output Report File for Test Case Two. (Sheet 47 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 100.0 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 1 COMP-1, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	1.303E+01	206	1.294E+01	247	6.683E+00	288	1.268E+01
166	1.300E+01	207	1.284E+01	248	9.581E+00	289	1.271E+01
167	1.301E+01	208	1.288E+01	249	1.275E+01	290	1.268E+01
168	1.303E+01	209	6.494E+00	250	1.280E+01	291	1.270E+01
169	1.295E+01	210	6.662E+00	251	1.275E+01	292	1.272E+01
170	1.296E+01	211	9.606E+00	252	1.276E+01	293	1.273E+01
171	1.298E+01	212	1.286E+01	253	1.281E+01	294	1.279E+01
172	1.290E+01	213	1.289E+01	254	4.328E+00	295	1.275E+01
173	1.292E+01	214	1.285E+01	255	1.278E+01	296	1.270E+01
174	6.342E+00	215	2.475E+00	256	1.280E+01	297	1.271E+01
175	6.395E+00	216	2.552E+00	257	1.286E+01	298	1.470E+01
176	9.369E+00	217	4.287E+00	258	1.481E+01	299	1.272E+01
177	1.291E+01	218	1.292E+01	259	1.615E+01	300	1.272E+01
178	1.294E+01	219	1.295E+01	260	1.709E+01	301	1.586E+01
179	1.290E+01	220	1.288E+01	261	1.407E+00	302	3.433E+00
180	2.364E+00	221	1.385E+00	262	2.644E+00	303	4.873E+00
181	2.395E+00	222	1.358E+00	263	2.598E+00	304	6.105E+00
182	4.076E+00	223	2.567E+00	264	4.480E+00	305	6.331E+00
183	1.206E+00	224	2.569E+00	265	6.944E+00	306	7.374E+00
184	6.787E-01	225	6.863E-01	266	6.758E+00	307	1.004E+01
185	1.307E+00	226	6.774E-01	267	6.439E-01	308	5.051E-01
186	6.334E-01	227	1.336E+00	268	5.931E-01	309	3.980E-01
187	2.193E-02	228	2.209E-02	269	1.196E+00	310	7.577E-01
188	2.299E-02	229	2.298E-02	270	2.143E+00	311	1.249E+00
189	1.272E-01	230	1.290E-01	271	2.447E+00	312	1.730E+00
190	9.010E-04	231	1.312E-03	272	2.075E-02	313	1.596E-02
191	1.008E-03	232	1.141E-03	273	2.027E-02	314	1.328E-02
192	1.398E-03	233	1.210E-03	274	1.177E-01	315	8.793E-02
193	2.178E-04	234	7.182E-05	275	1.233E-03	316	1.843E+00
194	1.918E-04	235	1.732E-04	276	8.622E-04	317	2.404E+00
195	0.000E-01	236	1.129E-05	277	1.294E-03	318	3.612E+00
196	1.311E+01	237	1.900E+01	278	6.254E-05	319	9.149E-04
197	1.307E+01	238	1.687E+01	279	1.655E-04	320	5.333E-04
198	1.303E+01	239	1.541E+01	280	2.016E-06	321	1.034E-03
199	1.306E+01	240	1.729E+01	281	1.913E+01	322	2.358E-05
200	1.309E+01	241	1.856E+01	282	1.990E+01	323	8.079E-05
201	1.300E+01	242	1.530E+01	283	1.884E+01	324	1.726E-05
202	1.306E+01	243	1.805E+01	284	1.679E+01	325	1.265E+01
203	1.302E+01	244	1.825E+01	285	1.710E+01	326	1.266E+01
204	1.297E+01	245	1.636E+01	286	1.779E+01	327	7.310E+00
205	1.298E+01	246	6.649E+00	287	9.893E+00	328	7.350E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 48 of 51)

```
***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER   100.0     YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER  1   COMP-1,  MG/LIT .....

... OUTPUT FOR NODES  329 TO  445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...
```

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	9.964E+00	359	1.825E+00	389	2.498E-04	419	9.353E-06
330	1.266E+01	360	8.027E-05	390	2.513E-05	420	1.813E-02
331	1.267E+01	361	0.000E-01	391	1.329E-01	421	5.316E-02
332	1.265E+01	362	6.053E-05	392	1.422E-01	422	1.788E-02
333	1.268E+01	363	1.265E+01	393	3.757E-01	423	1.832E-03
334	1.267E+01	364	1.265E+01	394	1.429E-04	424	0.000E-01*
335	1.267E+01	365	7.425E+00	395	0.000E-01	425	0.000E-01*
336	1.269E+01	366	7.521E+00	396	4.961E-05	426	0.000E-01*
337	2.861E+00	367	1.015E+01	397	1.506E-01	427	3.415E-03
338	3.183E+00	368	1.266E+01	398	4.014E-01	428	1.504E-04
339	5.042E+00	369	3.260E+00	399	1.466E-01	429	0.000E-01*
340	3.180E+00	370	3.302E+00	400	1.456E-02	430	0.000E-01*
341	3.203E+00	371	5.179E+00	401	5.294E-03	431	0.000E-01*
342	5.053E+00	372	1.773E+00	402	7.995E-03	432	0.000E-01*
343	2.831E-01	373	1.025E+00	403	1.094E-02	433	4.647E-03
344	1.724E-01	374	1.863E+00	404	3.030E-02	434	2.315E-05
345	3.073E-01	375	9.945E-01	405	7.957E-04	435	0.000E-01*
346	4.640E-01	376	1.932E+00	406	2.494E-04	436	0.000E-01*
347	8.157E-01	377	8.657E-02	407	2.197E-03	437	0.000E-01*
348	9.653E-03	378	3.426E-02	408	1.330E-02	438	0.000E-01*
349	5.046E-03	379	5.775E-02	409	1.520E-02	439	5.253E-03
350	4.666E-02	380	8.102E-02	410	4.364E-02	440	0.000E-01
351	6.303E-01	381	2.029E-01	411	6.190E-05	441	0.000E-01*
352	7.750E-01	382	4.496E-03	412	6.518E-05	442	0.000E-01*
353	1.444E+00	383	7.702E-04	413	0.000E-01	443	0.000E-01*
354	3.462E-04	384	1.268E-02	414	1.655E-02	444	5.490E-03
355	4.162E-04	385	1.026E-01	415	1.732E-02	445	0.000E-01*
356	3.670E-04	386	1.217E-01	416	5.017E-02		
357	8.799E-01	387	3.153E-01	417	1.178E-05		
358	9.530E-01	388	0.000E-01	418	0.000E-01		

```
CONSTITUENT COMP-1 DIAGNOSTICS
      MAXIMUM VALUE IS          1.990E+01
      MAXIMUM CHANGE IS         1.487E+00 AT NODE  310, MAXIMUM FRACTIONAL CHANGE IS      3.269E+01
      MAXIMUM CORRECTION IS     2.948E-02 AT NODE  383, MAXIMUM FRACTIONAL CORRECTION IS  1.635E+01
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
  2.5472E-03 AT ELEMENT    72 FOR MATERIAL TYPE CANIST
  4.0447E-05 AT ELEMENT    87 FOR MATERIAL TYPE PCKNG
  2.0338E-01 AT ELEMENT    15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-1 PRESENT IN THE SIMULATION ENVIRONMENT IS  2.975E-01 GRAMS.
```

LISTING D-6. Output Report File for Test Case Two. (Sheet 49 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 100.0 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 1 TO 164 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
1	0.000E-01*	42	5.384E-02	83	0.000E-01	124	1.114E+00
2	0.000E-01*	43	1.771E-02	84	2.912E-05	125	1.646E+00
3	0.000E-01*	44	1.479E-02	85	7.266E-01	126	3.013E-01
4	0.000E-01*	45	4.443E-02	86	1.333E+00	127	3.740E-01
5	0.000E-01*	46	4.803E-02	87	7.589E-01	128	6.823E-01
6	0.000E-01*	47	1.059E-02	88	7.532E-01	129	1.152E-02
7	0.000E-01*	48	3.077E-02	89	1.338E+00	130	1.461E-02
8	0.000E-01*	49	3.798E-02	90	1.330E+00	131	9.171E-02
9	0.000E-01*	50	5.397E-03	91	6.143E-01	132	5.193E-04
10	0.000E-01*	51	1.391E-02	92	1.051E+00	133	5.697E-04
11	0.000E-01*	52	2.246E-02	93	1.221E+00	134	1.252E-03
12	0.000E-01*	53	3.534E-04	94	1.353E+00	135	5.260E-05
13	0.000E-01*	54	4.377E-04	95	1.368E+00	136	1.043E-04
14	0.000E-01*	55	5.852E-03	96	7.870E-01	137	4.777E-06
15	0.000E-01*	56	4.292E-05	97	3.732E-01	138	5.259E+00
16	1.516E-03	57	1.259E-04	98	5.995E-01	139	4.213E+00
17	5.566E-03	58	2.887E-05	99	8.365E-01	140	4.150E+00
18	5.738E-03	59	1.262E-06	100	1.478E-01	141	5.256E+00
19	5.798E-03	60	0.000E-01	101	2.217E-01	142	5.258E+00
20	1.576E-03	61	2.345E-05	102	3.890E-01	143	4.215E+00
21	1.350E-03	62	1.414E-01	103	6.489E-03	144	5.251E+00
22	4.925E-03	63	3.815E-01	104	8.793E-03	145	5.254E+00
23	5.350E-03	64	3.961E-01	105	5.899E-02	146	2.777E+00
24	1.016E-03	65	4.065E-01	106	1.744E-04	147	3.186E+00
25	3.639E-03	66	1.501E-01	107	3.643E-04	148	4.233E+00
26	4.368E-03	67	1.209E-01	108	8.268E-04	149	1.321E+00
27	5.790E-04	68	3.177E-01	109	7.842E-05	150	1.474E+00
28	1.878E-03	69	3.554E-01	110	4.835E-05	151	2.251E+00
29	2.716E-03	70	8.153E-02	111	1.053E-05	152	4.292E-01
30	6.507E-05	71	2.020E-01	112	3.130E+00	153	4.714E-01
31	1.301E-04	72	2.644E-01	113	2.157E+00	154	8.752E-01
32	8.212E-04	73	3.818E-02	114	2.117E+00	155	1.578E-02
33	9.530E-06	74	8.347E-02	115	3.075E+00	156	1.798E-02
34	2.394E-05	75	1.398E-01	116	3.094E+00	157	1.124E-01
35	5.245E-06	76	2.508E-03	117	2.137E+00	158	7.995E-04
36	0.000E-01	77	3.180E-03	118	3.119E+00	159	7.475E-04
37	0.000E-01	78	2.621E-02	119	3.073E+00	160	1.448E-03
38	3.755E-06	79	1.051E-05	120	1.609E+00	161	4.525E-05
39	1.679E-02	80	2.503E-04	121	2.208E+00	162	1.154E-04
40	5.114E-02	81	2.962E-04	122	2.740E+00	163	1.305E-05
41	5.253E-02	82	6.806E-05	123	8.644E-01	164	5.259E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 50 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 100.0 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 165 TO 328 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
165	5.259E+00	206	5.246E+00	247	3.350E+00	288	5.220E+00
166	5.256E+00	207	5.237E+00	248	4.318E+00	289	5.223E+00
167	5.257E+00	208	5.241E+00	249	5.228E+00	290	5.220E+00
168	5.258E+00	209	3.243E+00	250	5.232E+00	291	5.220E+00
169	5.252E+00	210	3.318E+00	251	5.228E+00	292	5.224E+00
170	5.252E+00	211	4.303E+00	252	5.228E+00	293	5.221E+00
171	5.254E+00	212	5.237E+00	253	5.232E+00	294	5.221E+00
172	5.245E+00	213	5.242E+00	254	2.426E+00	295	5.224E+00
173	5.248E+00	214	5.237E+00	255	5.228E+00	296	5.218E+00
174	3.164E+00	215	1.548E+00	256	5.228E+00	297	5.217E+00
175	3.192E+00	216	1.594E+00	257	5.233E+00	298	5.243E+00
176	4.200E+00	217	2.389E+00	258	5.249E+00	299	5.215E+00
177	5.246E+00	218	5.238E+00	259	5.270E+00	300	5.215E+00
178	5.249E+00	219	5.243E+00	260	5.292E+00	301	5.258E+00
179	5.245E+00	220	5.238E+00	261	9.959E-01	302	2.062E+00
180	1.481E+00	221	9.716E-01	262	1.660E+00	303	2.709E+00
181	1.504E+00	222	9.584E-01	263	1.633E+00	304	3.166E+00
182	2.279E+00	223	1.615E+00	264	2.504E+00	305	3.272E+00
183	8.583E-01	224	1.609E+00	265	3.464E+00	306	3.657E+00
184	5.354E-01	225	5.438E-01	266	3.388E+00	307	4.492E+00
185	9.221E-01	226	5.390E-01	267	5.191E-01	308	4.264E-01
186	5.012E-01	227	9.521E-01	268	4.862E-01	309	3.499E-01
187	1.932E-02	228	1.987E-02	269	8.787E-01	310	6.059E-01
188	2.034E-02	229	2.055E-02	270	1.419E+00	311	9.249E-01
189	1.269E-01	230	1.296E-01	271	1.571E+00	312	1.198E+00
190	7.310E-04	231	1.012E-03	272	1.929E-02	313	1.616E-02
191	6.010E-04	232	9.077E-04	273	1.911E-02	314	1.433E-02
192	1.673E-03	233	1.557E-03	274	1.203E-01	315	9.351E-02
193	1.439E-04	234	5.067E-05	275	9.845E-04	316	1.272E+00
194	1.327E-04	235	1.146E-04	276	7.718E-04	317	1.581E+00
195	1.435E-05	236	2.997E-05	277	1.555E-03	318	2.162E+00
196	5.260E+00	237	5.321E+00	278	5.093E-05	319	8.279E-04
197	5.259E+00	238	5.295E+00	279	1.205E-04	320	5.734E-04
198	5.257E+00	239	5.277E+00	280	1.952E-05	321	1.274E-03
199	5.257E+00	240	5.295E+00	281	5.332E+00	322	2.950E-05
200	5.259E+00	241	5.313E+00	282	5.334E+00	323	8.046E-05
201	5.252E+00	242	5.271E+00	283	5.326E+00	324	2.021E-05
202	5.253E+00	243	5.307E+00	284	5.285E+00	325	5.215E+00
203	5.255E+00	244	5.306E+00	285	5.292E+00	326	5.217E+00
204	5.246E+00	245	5.277E+00	286	5.318E+00	327	3.639E+00
205	5.250E+00	246	3.327E+00	287	4.430E+00	328	3.656E+00

LISTING D-6. Output Report File for Test Case Two. (Sheet 51 of 51)

***** FINITE ELEMENT MODEL FOR CONTAMINANT TRANSPORT ANALYSIS *****

SAMPLE PROBLEM, DIFFUSION FROM A HEATED CANNISTER

...RESULTS AFTER 100.0 YEARS - DYNAMIC SIMULATION...
..... CONCENTRATIONS FOR CONSTITUENT NUMBER 2 COMP-2, MG/LIT .....

... OUTPUT FOR NODES 329 TO 445 ... THE SYMBOL * DENOTES A SPECIFIED VALUE ...

NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION	NODE NUMBER	CONCENTRATION
329	4.483E+00	359	1.276E+00	389	2.275E-04	419	9.245E-06
330	5.216E+00	360	7.210E-05	390	1.897E-04	420	2.332E-02
331	5.218E+00	361	5.108E-06	391	1.377E-01	421	6.138E-02
332	5.215E+00	362	4.227E-05	392	1.456E-01	422	2.297E-02
333	5.216E+00	363	5.214E+00	393	3.411E-01	423	2.895E-03
334	5.215E+00	364	5.214E+00	394	1.186E-04	424	0.000E-01*
335	5.214E+00	365	3.685E+00	395	0.000E-01	425	0.000E-01*
336	5.215E+00	366	3.719E+00	396	3.514E-05	426	0.000E-01*
337	1.818E+00	367	4.540E+00	397	1.533E-01	427	5.102E-03
338	1.977E+00	368	5.214E+00	398	3.612E-01	428	2.841E-04
339	2.792E+00	369	2.018E+00	399	1.498E-01	429	0.000E-01*
340	1.976E+00	370	2.037E+00	400	1.955E-02	430	0.000E-01*
341	1.991E+00	371	2.855E+00	401	7.819E-03	431	0.000E-01*
342	2.801E+00	372	1.247E+00	402	1.133E-02	432	0.000E-01*
343	2.611E-01	373	7.972E-01	403	1.489E-02	433	6.732E-03
344	1.719E-01	374	1.298E+00	404	3.740E-02	434	2.670E-05
345	2.827E-01	375	7.769E-01	405	1.462E-03	435	0.000E-01*
346	4.056E-01	376	1.338E+00	406	5.455E-04	436	0.000E-01*
347	6.498E-01	377	9.333E-02	407	3.455E-03	437	0.000E-01*
348	1.108E-02	378	4.230E-02	408	1.770E-02	438	0.000E-01*
349	7.262E-03	379	6.596E-02	409	1.996E-02	439	7.495E-03
350	5.327E-02	380	8.930E-02	410	5.160E-02	440	0.000E-01
351	5.268E-01	381	1.989E-01	411	7.424E-05	441	0.000E-01*
352	6.286E-01	382	5.716E-03	412	6.823E-05	442	0.000E-01*
353	1.051E+00	383	1.972E-03	413	4.028E-05	443	0.000E-01*
354	4.340E-04	384	1.647E-02	414	2.142E-02	444	7.809E-03
355	4.298E-04	385	1.099E-01	415	2.234E-02	445	0.000E-01*
356	6.692E-04	386	1.273E-01	416	5.839E-02		
357	7.003E-01	387	2.928E-01	417	1.716E-05		
358	7.483E-01	388	6.126E-05	418	0.000E-01		

CONSTITUENT COMP-2 DIAGNOSTICS
MAXIMUM VALUE IS 5.334E+00
MAXIMUM CHANGE IS 1.936E+00 AT NODE 320, MAXIMUM FRACTIONAL CHANGE IS 1.173E+01
MAXIMUM CORRECTION IS 1.500E-01 AT NODE 356, MAXIMUM FRACTIONAL CORRECTION IS 1.207E+00
APPROXIMATE MAXIMUM PECLET NUMBERS ARE
2.5472E-03 AT ELEMENT 72 FOR MATERIAL TYPE CANIST
4.0447E-05 AT ELEMENT 87 FOR MATERIAL TYPE PCKNG
2.0338E-01 AT ELEMENT 15 FOR MATERIAL TYPE HOST

THE AMOUNT OF THE CONSTITUENT COMP-2 PRESENT IN THE SIMULATION ENVIRONMENT IS 1.499E-01 GRAMS.

APPENDIX E

JOB CONTROL

The job control streams used to run the two example problems of Appendix D are duplicated there for completeness (see Listings D-2 and D-5). However, neither of the example problems uses all possible files. Therefore, a fully illustrative generic job control stream for a CHAINT simulation as run in a PRIME operating environment is shown below.

```
DELETE DAYFILE
DELETE REPORT.OUT
DELETE PLOT.IS5
DELETE MASFLX.IS7
COMO DAYFILE
DATE
OPEN INPUT. DAT 1  1
OPEN REPORT. OUT 2  2
OPEN INITIAL. IS1 3  1
OPEN VELOCITY. IS2 4  1
OPEN RESTART. IS3 5  1
OPEN RESTART. IS4 6  2
OPEN PLOT. IS5 7  2
OPEN GEOMETRY. IS6 10  1
OPEN MASFLX. IS7 11  2
OPEN WORKSPACE 14  3
SEG XQT>#CHAINT
CLOSE WORKSPACE
DELETE WORKSPACE
COMO -END
LOGOUT
```

The single most important aspect here is the correspondence of logical unit numbers and access rights to the various files. This correspondence is summarized in table E-1.

Table E-1. Summary of CHAINT External Files.

LUN[a]	File type[b]	Access	Description
5	Sequential Formatted	Read Only	Principal Input
6	Sequential Formatted	Write Only	Output Report
IS1	Sequential Formatted	Read Only	Initial Conditions
IS2	Sequential Binary	Read Only	Velocity Input
IS3	Sequential Binary	Read Only	Restart Input
IS4	Sequential Binary	Write Only	Restart Output
IS5	Sequential Binary	Write Only	Concentration Plots
IS6	Sequential Binary	Read Only	Geometry Input
IS7	Sequential Binary	Write Only	Mass Flux Plots
16	Direct Access Binary	Read and Write	Solver Scratch Area

[a]LUN = IS1 through IS7 are user specified.
[b]File type is determined internally by CHAINT.

9 2 1 2 4 1 7 1 3 7 1

APPENDIX F

DIAGNOSTIC MESSAGES

The CHAINT computer code has evolved to the current version (2.1) over a number of years and has been tested with a variety of problems. It is therefore expected to provide trouble-free operation. However, for a computer program of such complexity, it is possible that difficulties may be encountered in its application. Moreover, any such problems are likely to arise from a lack of familiarity with the various features and input formats. Hence, CHAINT has the additional capability of diagnosing some possible input errors and a few run-time errors and generating appropriate warning/error messages.

The possible diagnostic messages as printed by CHAINT are reproduced in table F-1 along with possible causes and/or corrective user action. Furthermore, since the input to CHAINT is in fixed format, the foremost remedial action is simply an exhaustive search of the inputs for incorrect data formatting. If unresolvable difficulties are encountered in the application of CHAINT to a well-posed problem, please contact the authors.

9 1 1 2 4 1 7 1 8 7 2

Table F-1. CHAINT Diagnostics. (sheet 1 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
I) PROGRAM CONTROL (CARD TYPES B, C, D)	
TOO MANY CONSTITUENTS REQUESTED. LIMIT IS n. ERROR STOP IN ROUTINE INPUT.	Either reduce the number of constituents or increase the limit (MQL).
TOO MANY ELEMENTS REQUESTED. LIMIT IS n. ERROR STOP IN ROUTINE INPUT.	Either reduce the size of the input geometry or increase the element limit (MAXE).
TOO MANY NODES REQUESTED. LIMIT IS n. ERROR STOP IN ROUTINE INPUT.	Either reduce the size of the input geometry or increase the node limit (MAXP).
TOO MANY MATERIAL TYPES REQUESTED. LIMIT IS n. ERROR STOP IN ROUTINE INPUT.	Either reduce the number of required material types or increase the material type limit (MAXMAT).
** WARNING, TOO MANY CONSTITUENTS ** * HAVE BEEN REQUESTED FOR THE MASS * * FLUX CALCULATIONS. THIS WILL BE RE- * * DUCED TO THE NUMBER OF CONSTITU- * * ENTS PRESENT. *	Reduce the number of mass flux constituents. (NCFLX must not be greater than NQAL.)
INCONSISTENT VELOCITY AND FILE UNIT SPECIFICATIONS. 1) VELOCITY FIELD TYPE <2, AND A VELOCITY FILE IS SPECIFIED, OR 2) VELOCITY FIELD TYPE >1, BUT NO VELOCITY FILE IS SPECIFIED. ERROR STOP IN ROUTINE INPUT.	Either change the velocity field type or specify a logical unit for an external velocity file.
MASS FLUX CONSTITUENTS HAVE BEEN REQUESTED, BUT NO MASS FLUX FILE HAS BEEN SPECIFIED. ERROR STOP IN ROUTINE INPUT.	Either specify a logical unit for an external mass flux file or set NCFLX to zero.
A MASS FLUX FILE HAS BEEN SPECIFIED, BUT THE NUMBER OF MASS FLUX CONSTITUENTS IS ZERO. ERROR STOP IN ROUTINE INPUT.	Either specify the number of mass flux constituents or reset the logical unit for the mass flux file to zero.
** WARNING, THE WEIGHTING FACTOR IS ** * OUT OF THE SUGGESTED RANGE (1 TO 2) * * IT WILL BE RESET TO 1.8. *	Check the valve of the weighting factor, θ (see section 2.5).
II) TIME STEPPING (CARD TYPE E)	
** WARNING, ZONING WILL NOT BE ** * PERFORMED IN DEFERENCE TO BOUND- * * ARY NODES. *	An active node zone cannot be used with Dirichlet boundary conditions.
ERROR IN TIME STEP INPUT, LINE NUMBER n BOUNDARY NODES ARE NOT USED, ZONING MUST BE SPECIFIED. ERROR STOP IN ROUTINE INPUT.	Check the zone input on card type E. A zone must be specified if the default boundary condition is used everywhere.
TOO MANY TIME STEPPING DEFINITION CARDS ARE PRESENT IN THE INPUT DATA FILE. THE PROGRAM LIMIT IS n. ERROR STOP IN ROUTINE INPUT.	Either reduce the number of time step cards or increase the limit (NTT).

Table F-1. CHAINT Diagnostics. (sheet 2 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
III) MATERIAL PROPERTIES (CARD TYPE F)	
ERROR IN ROCK PROPERTIES INPUT, MATERIAL TYPE n IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Change the indicated material type in the input geometry.
ERROR IN ROCK PROPERTIES INPUT. DATA FOR MATERIAL TYPE n IS NOT PRESENT. ERROR STOP IN ROUTINE INPUT.	Either supply data for the indicated material type or correct the material type numbers in the input data set.
** WARNING, FRACTURES OF ZERO WIDTH ** * FOUND. * ** MATERIAL TYPE n FRACTURE WIDTH SET ** * TO 1.0. *	Fracture aperature must be strictly positive. The default is one length unit.
IV) CONSTITUENT PROPERTIES (CARD TYPE H1)	
ERROR IN CONSTITUENT PROPERTIES INPUT. CONSTITUENT NUMBER n IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Either correct the constituent number or increase the limit on the number of constituents (MQL).
ERROR IN CONSTITUENT PROPERTIES INPUT. CONSTITUENT n aa-xxx, HAS CONSTITUENT m AS A DAUGHTER. THE DECAY CHAIN MUST BE ENTERED FROM TOP TO BOTTOM.	One of the daughter constituents is numbered lower than the current constituent. Renumber the constituents in the decay chain.
ERROR IN CONSTITUENT PROPERTIES INPUT. DATA FOR CONSTITUENT n IS NOT PRESENT.	Either supply data for this constituent or correct the constituent numbers in the input data set.
THE NUMBER OF DAUGHTER PRODUCTS EXCEEDS TWO FOR CONSTITUENT n AS A RESULT OF DROPPING OUT CONSTITUENT m. ERROR STOP IN ROUTINE INPUT.	CHAINT handles decay chains of at most two daughters per nuclide. The current decay chain is probably in error (cf. section 3.6).
CONSTITUENT m HAS TOO MANY PARENTS. MAXIMUM ALLOWED IS n. ERROR STOP IN ROUTINE LOAD1.	Check the decay chain input and/or increase the limit on the number of parents (MAXPAR).
** WARNING, MOLECULAR DIFFUSIVITY ** * VALUES LESS THAN OR EQUAL TO ZERO * * WERE RESET TO 3.0 E-02. *	Check the values of molecular diffusivity.
V) RETARDATION FACTORS (CARD TYPE H2)	
** WARNING, SORPTION IS LESS THAN ZERO ** * FOR CONSTITUENT n MATERIAL TYPE m * * (aaaaaaaa). THIS WILL BE SET TO 0.0. *	Correct the value of sorption for the indicated constituent and material type.
VI) GEOMETRY FILE (CARD TYPES I, J)	
GEOMETRY HAS n ELEMENTS. THIS DOES NOT MATCH THE NUMBER GIVEN IN THE PROBLEM SPECIFICATION DATA. ERROR STOP IN ROUTINE INPUT.	Correct the geometry or the number of elements on the problem specification card (card type B).

Table F-1. CHAINT Diagnostics. (sheet 3 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
GEOMETRY HAS n NODES. THIS DOES NOT MATCH THE NUMBER GIVEN IN THE PROBLEM SPECIFICATION DATA. ERROR STOP IN ROUTINE INPUT.	Correct the geometry or the number of nodes on the problem specification card (card type B).
** WARNING, POSITIVE DIRECTION FOR ** * FRACTURE VELOCITIES IS DEFINED BY * * NODE ORDERING. *	This warning is always printed when fracture elements are present and the fluid velocities are defined locally as a function of material type.
ERROR IN NODE SPECIFICATIONS. THE HIGHEST NODE NUMBER IN THE GEOMETRY IS m. THIS EXCEEDS THE MAXIMUM NODE LIMIT OF n. ERROR STOP IN ROUTINE INPUT.	Correct the input geometry.
ERROR IN ELEMENT m MATERIAL TYPE n IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Eliminate or change the indicated material type.
THE CHOICE OF AXISYMMETRIC COORDINATES IS INCOMPATIBLE WITH THE GEOMETRY LIMITS. X MINIMUM (<0) = y X MAXIMUM (=0) = z. ERROR STOP IN ROUTINE INPUT.	Check the input geometry. All r-coordinates must be non-negative and r-maximum must be strictly positive.
ERROR ENCOUNTERED READING GEOMETRY FILE. ERROR STOP IN ROUTINE INPUT.	An unspecified error has occurred while reading the input binary geometry file. Check the geometry file for correctness.
VII) INITIAL CONDITIONS (CARD TYPES L1, L2)	
THE RESTART FILE HAS m_1 NODES AND n_1 CONSTITUENTS. THE CURRENT PROBLEM HAS m_2 NODES AND n_2 CONSTITUENTS. CHANGING THESE NUMBERS ON RESTART IS NOT PERMITTED. ERROR STOP IN ROUTINE INPUT.	Check for correct restart file, and correct number of constituents and nodes on the problem specification card.
ERROR IN THE INITIAL CONDITION INPUT, CONSTITUENT NUMBER m IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Check the initial condition data.
ERROR IN THE INITIAL CONDITION INPUT, NODE NUMBER m IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Check the initial condition data.
NODE k AT LINE m CONSTITUENT n IS DUPLICATED IN THE INITIAL CONDITION LIST. ERROR STOP IN ROUTINE INPUT.	Check the initial condition data.
ERROR ENCOUNTERED READING BINARY RESTART FILE. ERROR STOP IN ROUTINE INPUT.	An unspecified error occurred while reading the binary input restart file. Check the completion status of the predecessor run.
ERROR READING INITIAL CONDITION DATA FROM FILE UNIT m. ERROR STOP IN ROUTINE INPUT.	Initial condition data on the specified file is in error, possibly format or record length.

Table F-1. CHAINT Diagnostics. (sheet 4 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
VIII) BOUNDARY CONDITIONS (CARD TYPE N)	
ERROR IN BOUNDARY CONDITION INPUT, NODE NUMBER m IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Check the boundary condition data for nodes numbered greater than NP.
NODE m IS DUPLICATED AT LINE n OF THE INPUT BOUNDARY NODE LIST. ERROR STOP IN ROUTINE INPUT.	Check the boundary condition data.
** WARNING, ELEMENT m CONSISTS SOLELY ** * OF BOUNDARY NODES *	All nodal values in element m are fixed and will not change during the course of computation.
IX) DARCY VELOCITY (CARD TYPES 01, 02)	
ERROR IN VELOCITY INPUT, MATERIAL TYPE m IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Check the velocity input data.
** WARNING, MATERIAL TYPE m HAS A ** * NON-ZERO FRACTURE WIDTH. THE NON- * * ZERO y VELOCITY WILL BE IGNORED IN * * FRACTURE ELEMENTS. *	The fracture width is only used for line elements, while the y-velocity is only used for planar elements.
ERROR IN VELOCITY INPUT, MATERIAL TYPE m HAS A NON-ZERO FRACTURE WIDTH, A NON-ZERO Y VELOCITY, AND ZERO X VELOCITY. THIS CREATES ZERO FLOW IN LINE ELEMENTS OF THIS MATERIAL TYPE. ERROR STOP IN ROUTINE INPUT.	CHAINT uses only x velocities for fracture elements. Check the input velocities for material type m.
** AXISYMMETRIC COORDINATES HAVE ** * BEEN CHOSEN. THE x VELOCITIES WILL * * BE SCALED BY ONE OVER THE x COORDI- * * NATE AT ALL GAUSS POINTS. *	This message appears only if axisymmetric coordinates are chosen and velocities are specified by material type.
X) MASS FLUX DATA (CARD TYPES P1, P2, P3)	
** CONSTITUENT m IS INACTIVE AND WILL ** * BE DROPPED FROM THE FLUX * * CALCULATIONS. *	Check the constituent selection m card type G.
** NO ACTIVE CONSTITUENTS FOR MASS ** * FLUX FILE. THIS FILE WILL NOT BE * * WRITTEN. *	Check the constituent selection m card type G.
ERROR IN MASS FLUX SPECIFICATIONS. THE NUMBER OF MASS FLUX ELEMENTS IS OUT OF RANGE. THE MAXIMUM ALLOWED IS m. ERROR STOP IN ROUTINE INPUT.	Either decrease the number of mass flux elements or increase the limit (MAXFLX).
ERROR IN MASS FLUX SPECIFICATIONS. ELEMENT NUMBER m IS OUT OF RANGE. ERROR STOP IN ROUTINE INPUT.	Check the element numbers of the mass flux elements.

Table F-1. CHAINT Diagnostics. (sheet 5 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
** WARNING, ELEMENT m IS A LINE ELEMENT BETWEEN ELEMENTS k AND n AND IS NOT IN THE FLUX SURFACE ELEMENT LIST. NO FLUX WILL BE CALCULATED FOR THIS ELEMENT. **	This indicates that a line element is included in mass flux surface, but is not specified as part of the surface. Check the input geometry and flux surface of correctness.
FLUX SURFACE ELEMENTS m AND n ARE NOT CONNECTED. CONTIGUOUS ELEMENTS IN THE FLUX SURFACE LIST MUST BE CONNECTED. ERROR STOP IN ROUTINE SURFAC.	Check the input geometry and flux surface for correctness.
** WARNING, ELEMENT m IN THE FLUX SURFACE LIST IS NOT CONNECTED TO TWO OTHER ELEMENTS IN THE LIST, AND IS NOT ON THE GEOMETRY BOUNDARY. THE FLUX SURFACE MAY END INTERNALLY TO THE GEOMETRY AT NODE n. **	Check the input geometry and flux surface for correctness.
** WARNING, ELEMENT m HAS TWO OR MORE MID-SIDE NODES ON THE GEOMETRY BOUNDARY. THE FLUX SURFACE MUST END AT THIS ELEMENT, AND IS AMBIGUOUSLY DEFINED. **	Check the flux surface for correctness.
TOO MANY NODES ARE CONNECTED TO THE MASS FLUX SURFACE. THE CURRENT VALUE IS m WHILE THE MAXIMUM ALLOWED IS n. ERROR STOP IN ROUTINE SURFAC.	Either reduce the size of the mass flux surface or increase the limit (MAXPF).
XI) GEOMETRY DATA READ ERRORS	
ERROR READING GEOMETRY ELEMENT RECORDS. ERROR STOP IN ROUTINE INPUT.	Error reading element/connectivity records.
ERROR READING GEOMETRY NODE COORDINATES. ERROR STOP IN ROUTINE INPUT.	Error reading the nodal coordinate list. Check the geometry file.
XII) VELOCITY INPUT FILE	
VELOCITY FILE INCOMPATIBILITY. THE INPUT VELOCITY FILE HAS m NODES, WHILE THE CURRENT PROBELM HAS n NODES. ERROR STOP IN ROUTINE HEADR.	Check for the correct input velocity file.
VELOCITY FILE INCOMPATIBILITY. THE INPUT VELOCITY FILE HAS m MATERIAL TYPES, WHILE THE CURRENT PROBLEM HAS n MATERIAL TYPES. ERROR STOP IN ROUTINE HEADR.	Check for the correct input velocity file.
** WARNING, THE CHAINT INPUT POROSITIES DO NOT MATCH THE VALUES READ FROM THE EXTERNAL VELOCITY FILE. THOSE READ FROM THE INPUT DATA FILE (SEE PRINT FILE) WILL BE USED. **	Check the porosities in the input data file against those used for the corresponding MAGNUM-2D run.

Table F-1. CHAINT Diagnostics. (sheet 6 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
** WARNING, THE CHAINT INPUT FRACTURE ** * WIDTHS DO NOT MATCH THE VALUES * * READ FROM THE EXTERNAL VELOCITY * * FILE. THOSE READ FROM THE INPUT DATA * * FILE (SEE PRINT FILE) WILL BE USED. *	Check the fracture widths in the input data file against those used for the corresponding MAGNUM-2D run.
ERROR OR END OF FILE ENCOUNTERED UPON INPUT VELOCITY FILE HEADER READ. ERROR STOP IN ROUTINE HEADR.	Check for the correct input velocity file. Also check the completion status of the predecessor run.
THE INPUT VELOCITY FILE BEGINS AT TIME x, WHICH EXCEEDS THE SIMULATION INITIAL TIME. ERROR STOP IN MAIN ROUTINE.	Check for the correct input velocity file. Check the start time for the current run and the corresponding MAGNUM-2D run.
VELOCITY FILE RESTART ERROR. RESTART DATA HAS m NODES AND n ELEMENTS. ERROR STOP IN ROUTINE RDVEL.	Mismatching numbers of nodes and/or elements.
RESTART DATA HAS m MATERIAL TYPES. THIS EXCEEDS THE PROGRAM MAXIMUM OF n OR IS FEWER THAN THE CURRENT PROBLEM REQUIRES. ERROR STOP IN ROUTINE RDVEL.	Possible mismatching material types.
ERROR OR PREMATURE END OF FILE ENCOUNTERED WHILE READING INPUT VELOCITY FILE. LAST TIME READ IS t. ERROR STOP IN ROUTINE RDVEL.	Check for correct input velocity file. Check the completion status of the corresponding MAGNUM-2D run.
VELOCITY FILE ENDS PRIOR TO END OF CURRENT SIMULATION. ERROR STOP IN MAIN ROUTINE.	Check for correct input velocity file. Check the simulation completion times for the current run and for the corresponding MAGNUM-2D run.
TIME SKIPPED ON INPUT VELOCITY FILE = t.	This message is merely an acknowledgment of repositioning of the input velocity file for a restarted run. No user action is required.
XIII) SOURCE ELEMENTS (CARD TYPES Q,R,S)	
TOO MANY SOURCE ELEMENTS. INPUT SPECIFIES m SOURCE ELEMENTS. CURRENT PROBLEM HAS ONLY n ELEMENTS. ERROR STOP IN ROUTINE LOAD.	Correct the number of source elements.
TOO MANY SOURCE LOADING TIMES. A TOTAL OF m SOURCE LOADING TIMES HAVE BEEN READ. THIS EXCEEDS THE PROGRAM LIMIT OF n. ERROR STOP IN ROUTINE LOAD.	Either reduce the number of source loading times or increase the limit (MAXSLT).
SOURCE LOAD DATA FOR LESS THAN TWO TIMES HAVE BEEN READ. THIS IS INSUFFICIENT. ERROR STOP IN ROUTINE LOAD.	Check source loading data. Data for at least two times must be present for correct interpolation.
LAST SOURCE LOAD TIME OF t IS LESS THAN CURRENT SIMULATION TIME OF x, LOAD INDEX IS m, NUMBER OF LOAD TIMES IS n. ERROR STOP IN ROUTINE LOAD (ENTRY LOADS).	The time dependent mass source ends prematurely.

Table F-1. CHAINT Diagnostics. (sheet 7 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
XIV) EXECUTION ERRORS	
NO ACTIVE ELEMENTS FOUND IN GEOMETRY. ERROR STOP IN ROUTINE SETUP.	This can result from all of the nodes in a geometry being either boundary nodes or being outside the current zone limits.
ERROR IN NODE SEQUENCING. m NODES ARE PERMITTED. THIS MANY EQUATIONS SHOULD BE CREATED. n EQUATIONS HAVE BEEN SET UP FOR THIS PROBLEM. ERROR STOP IN ROUTINE SETUP.	An error has occurred in the subroutine which sets up the equation ordering. Check the input geometry for errors.
NO ACTIVE CONSTITUENTS REMAINING. ERROR STOP IN MAIN ROUTINE.	A constituent is dropped from the calculations if its half-life is much smaller that the current time step. All of the constituents have been dropped. Check the time stepping and the constituent half-lives (see section 3.6).
THE NUMBER OF DAUGHTER PRODUCTS EXCEEDS TWO FOR CONSTITUENT m AS A RESULT OF THE DROPPING OUT OF AN INTERMEDIATE CONSTITUENT IN THE DECAY CHAIN. ERROR STOP IN ROUTINE SELECT.	Check the decay chain for correctness.
CONSTITUENT m HAS TOO MANY PARENTS. ERROR STOP IN ROUTINE SELECT.	A constituent has too many parents as a result of an intermediate constituent being dropped. Check the decay chain for correctness. Simplify the decay chain or increase the limit on the number of parents (MAXPAR).
** WARNING, CONSTITUENT m HAS BEEN ** * DROPPED. THE TIME STEP IS TOO LARGE * * RELATIVE TO THE CONSTITUENT DECAY * * RATE. *	This warning is always printed when a constituent is dropped from the calculations due to short half-life.
** WARNING, PECLET NUMBER AT ELEMENT * * m (aaaaaaaa IS x). *	A warning is printed whenever the local value of the Peclet number exceeds one half. This is the point at which upstream weighting is invoked.
NELL = m IS GREATER THAN MAXE (= n). ERROR STOP IN ROUTINE FRONT.	Possible incompatibility between element connectivity and element ordering.
LCOL = m, NELL = n. THE DIFFERENCE (NMAX-NCRIT) IS NOT SUFFICIENTLY LARGE TO PERMIT THE ASSEMBLY OF THE NEXT ELEMENT. EITHER INCREASE NMAX OR LOWER NCRIT. (POSSIBLE GEOMETRY BANDWITH/ORDERING ERROR). ERROR STOP IN ROUTINE FRONT.	Either increase the maximum frontwidth (NMAX), optimize the element numbering, or decrease the problem size. Optimization of element numbering is strongly recommended.
END OF FILE ENCOUNTERED ON WORKSPACE FILE n. ERROR STOP IN ROUTINE RED.	An error has occurred in reading the CHAINT scratch file. Check that this file is open and available, and not used by or for another function.

Table F-1. CHAINT Diagnostics. (sheet 8 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
WARNING-MATRIX SINGULAR OR ILLCONDITIONED, x IS LESS THAN y, EQUATION NUMBER m. ERROR IN FRONT AT LOCATION n. ERROR STOP IN ROUTINE FRONT.	Check for correct (non-zero) values of rock and constituent properties.
BINARY READ SIZE ERROR. ROUTINE BININ MUST BE MODIFIED SO THAT n OR MORE RECORDS CAN BE READ AT ONCE. ERROR STOP IN ROUTINE BININ.	Direct I/O block size is insufficient for scratch file.
BINARY WRITE ERROR. ROUTINE BINOUT MUST BE MODIFIED SO THAT n OR MORE RECORDS CAN BE WRITTEN AT ONCE. ERROR STOP IN ROUTINE BINOUT.	Direct I/O block size is insufficient for scratch file.
XV) SEQUENTIAL BINARY FILE HEADER ERRORS	
ERROR READING BINARY FILE HEADER. THERE ARE TOO MANY BINARY SOURCE FILES FOR THIS RUN. THE CURRENT VALUE IS k. THE PROGRAM LIMIT (MIPF) IS m. FILE UNIT NUMBER n. STOP IN ROUTINE RHEADR.	Increase the parameter MIPF (parameter block PARA.).
** WARNING, BINARY FILE TRACEBACK ** * HEADER FOR FILE UNIT NUMBER k HAS n * * ITEMS. THE PROGRAM LIMIT (MAXSR) IS * * m. *	The binary file specified has too many items in its traceback header. The excess data will be lost, but execution continues.
ERROR ENCOUNTERED READING BINARY FILE HEADER RECORD. FILE UNIT NUMBER m. STOP IN ROUTINE RHEADR.	The program was unable to read the binary file header on the specified unit. The file header is bad or the wrong type of file is being accessed.
PREMATURE END OF FILE ENCOUNTERED READING BINARY FILE HEADER RECORD. FILE UNIT NUMBER m. STOP IN ROUTINE RHEADR.	An end of file was found on the specified unit where a file header was expected.
ERROR ENCOUNTERED READING BINARY FILE TRACEBACK HEADER. FILE UNIT NUMBER m. STOP IN ROUTINE RHEADR.	The program was unable to read the binary file traceback header on the specified unit.
PREMATURE END OF FILE ENCOUNTERED READING BINARY FILE TRACEBACK HEADER. FILE UNIT NUMBER m. STOP IN ROUTINE RHEADR.	An end of file was found on the specified unit where a traceback header was expected. The file header is bad or the wrong type of file is being accessed.
XVI) OTHER I/O ERRORS	
ERROR READING INPUT RESULTS FILE FOR RESTART. RESTART SIMULATION TIME (= x) IS LESS THAT THE END TIME IN THE INPUT RESULTS FILE (= y). STOP IN ROUTINE ENDFL.	The current restarted time is less than the end time on the designated results file.

Table F-1. CHAINT Diagnostics. (sheet 9 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
PREMATURE END OF FILE ENCOUNTERED READING INPUT RESULTS FILE FOR RESTART, UNIT NUMBER m. STOP IN ROUTINE ENDFL.	The current restart simulation cannot correctly read the designated results file. Check the completion status of the predecessor run.
ERROR ENCOUNTERED, READING INPUT RESULTS FILE FOR RESTART. UNIT NUMBER m. STOP IN ROUTINE ENDFL.	The current restart simulation cannot correctly read the designated results file. Check for correct results file assignment.
ERROR ON INPUT RESULTS FILE (FOR RESTART). THE FILE HAS m NODES AND k COMPONENTS. THE DATA SET REQUIRES n NODES AND l COMPONENTS. STOP IN ROUTINE ENDFL.	The designated results file has node and component size specifications that are not the same as those for the current restart simulation.
ERROR READING INPUT MASS FLUX FILE FOR RESTART. RESTART SIMULATION TIME (= x) IS LESS THAT THE END TIME ON THE INPUT MASS FLUX FILE (= y). STOP IN ROUTINE ENDFL.	The current restart simulation start time is less than the end time on the designated mass flux file.
PREMATURE END OF FILE ENCOUNTERED, READING INPUT MASS FLUX FILE, UNIT NUMBER m. STOP IN ROUTINE ENDFL.	The current restart simulation cannot correctly read the designated mass flux file.
ERROR ENCOUNTERED, READING INPUT MASS FLUX FILE FOR RESTART, UNIT NUMBER m. STOP IN ROUTINE ENDFL.	The current restart simulation cannot correctly read the designated mass flux file. Check for correct mass flux file assignment.
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE FILE HAS m NODES. THE DATA SET REQUIRES n NODES. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same number of nodes as the current restart simulation. Check for correct mass flux file assignment. Check the node number values for this and the previous run.
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE FILE HAS n MASS FLUX CONSTITUENTS. THE DATA SET REQUIRES m MASS FLUX CONSTITUENTS. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same number of mass flux constituents as the current restart simulation. Check for correct mass flux file assignment. Check the number of mass flux constituents for this and the previous run.
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE VELOCITY FIELD TYPE POINTER IS x. THIS PROBLEM REQUIRES A VALUE OF y. THE VELOCITY FIELD IS CONSTANT WITH TIME. THE PROBLEM REQUIRES VARIABLE VELOCITIES. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same velocity field time dependence as the current restart simulation. Check for correct mass flux file assignment.

Table F-1. CHAINT Diagnostics. (sheet 10 of 10)

MESSAGE[a]	CAUSE/CORRECTIVE ACTION
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE VELOCITY FIELD SOURCE POINTER = x. THE VELOCITY FIELD IS DEFINED EXTERNALLY. THE PROBLEM REQUIRES VELOCITIES DEFINED INTERNALLY. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same velocity field source pointer as the current restart simulation. Check for correct mass flux file assignment.
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE AXISYMMETRIC OPTION VALUE IS m. THE DATA REQUIRES THIS OPTION TO BE n. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same symmetry (axisymmetric/cartesian) as the current restart simulation. Check for correct mass flux file assignment. Check the axisymmetric option pointer for this and the previous run.
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE FILE HAS m MASS FLUX SURFACES. THE DATA SET REQUIRES n MASS FLUX SURFACES. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same number of mass flux surfaces as the current restart simulation. Check for correct mass flux file assignment. Check the number of flux surfaces for this and the previous run.
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE FILE HAS m MATERIAL TYPES. THE DATA SET REQUIRES n MATERIAL TYPES. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same number of material types as the current restart simulation. Check for correct mass flux file assignment. Check the number of material types for this and the previous run.
ERROR ON INPUT MASS FLUX FILE (FOR RESTART). THE FILE HAS m FLUX SURFACE NODES. THE DATA SET REQUIRES n FLUX SURFACE NODES. STOP IN ROUTINE ENDFL.	The designated mass flux file does not have the same number of flux surface nodes as the current restart simulation. Check for correct mass flux file assignment. Check the flux surface definitions (element lists) for this and the previous run.

[a]An error message resulting from error termination during input is generally followed by the line number and card type where the error occurred.

9 2 1 2 4 1 7 1 3 3 2

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APPENDIX G

SOFTWARE ABSTRACT

9 2 1 2 4 1 7 1 8 3 4

FEDERAL INFORMATION PROCESSING STANDARD SOFTWARE SUMMARY

01. Summary date — Yr. 86 Mo. 01 Day 31

02. Summary prepared by (Name and Phone) — Niall W. Kline (509) 376-4634

03. Summary action — New [X] Replacement [ ] Deletion [ ]

Previous Internal Software ID

04. Software date — Yr. 85 Mo. 12 Day 13

05. Software title — Finite Element Chain Decay and Transport Model

06. Short title — CHAINT

07. Internal Software ID — Version 2.1

08. Software type
- [ ] Automated Data System
- [X] Computer Program
- [ ] Subroutine/Module

09. Processing mode
- [ ] Interactive
- [X] Batch
- [ ] Combination

10. Application area

General
- [ ] Computer Systems Support/Utility
- [X] Scientific/Engineering
- [ ] Bibliographic/Textual
- [ ] Management/Business
- [ ] Process Control
- [ ] Other

Specific: Geologic Disposal of High-Level Waste

11. Submitting organization and address

Performance Assessment Group
Rockwell Hanford Operations
P.O. Box 800
Richland, Washington 99352

12. Technical contact(s) and phone (509)376-2996

Robert G. Baca
Rockwell Hanford Operations
P.O. Box 800
Richland, Washington 99352

13. Narrative

The CHAINT computer code is a general purpose, two-dimensional, finite element model of radionuclide mass transport in a fractured porous medium accounting for effects of dissolution, decay, retardation, advection, diffusion and dispersion. CHAINT is a counterpart program to the MAGNUM-2D code, a two-dimensional finite element model of nonisothermal groundwater flow in a geologic medium. Both codes are operational as stand-alone FORTRAN programs. The code and a user's guide are available upon written request.

14. Keywords

Radionuclide, geologic disposal, finite element, groundwater, continuum, porous medium, diffusion, high-level waste

15. Computer manuf'r and model	16. Computer operating system	17. Programing language(s)	18. Number of source program statements
PRIME 750	PRIMOS IV Rev. 19.4	FORTRAN 77	approx. 6000
19. Computer memory requirements	**20. Tape drives**	**21. Disk/Drum units**	**22. Terminals**
N/A	0	up to 10 disk units up to 2.5 megabytes, total	N/A

23. Other operational requirements The CHAINT code is maintained in a virtual memory environment, and the memory usage is application dependent. Array storage allocation is adjustable. A terminal may be required for pre/post-processing.

24. Software availability
- Available [X]
- Limited [ ]
- In-house only [ ]

Written requests should be directed to the technical contact identified in item 12 above.

25. Documentation availability
- Available [X]
- Inadequate [ ]
- In-house only [ ]

Written requests should be directed to the technical contact identified in item 12 above.

26. FOR SUBMITTING ORGANIZATION USE

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Figure G-1. Software Abstract.

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