CNWRA94-005

DRILLO CODE: A MODULE FOR SIMULATION OF HUMAN INTRUSION SCENARIOS, MODEL DESCRIPTION, AND USER GUIDE

Iterative Performance Assessment Phase 2

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ABSTRACT

This user guide describes the DRILLO code, its structures, the associated simulation model, and instructions for its use. The DRILLO code has been used in the Iterative Performance Assessment (IPA) Phase 2 exercise to simulate the human intrusion scenario for the proposed high-level waste (HLW) at the Yucca Mountain site. The code models the drilling event as a random process and then assesses the consequences of the drilling in terms of the release of radioactivity to the geologic media and accessible environment.

The DRILLO code, which consists of two modules, can be run in two modes. It can be run either under the Total-System Performance Assessment (TPA) code or in a standalone mode. In the TPA mode, DRILLO code models occurrence of drilling as a random process and calculates the number of boreholes, time of drilling events (within the next 10,000 yr), and whether a waste canister has been hit by the drill bit. In addition, the code computes the consequences of the drill bit intersecting a waste canister, a contaminated rock, or both. This information is passed to other modules of the TPA code.

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FOREWORD

In accordance with the provisions of the Nuclear Waste Policy Act of 1982, the U.S. Nuclear Regulatory Commission (NRC) has the responsibility of evaluating and granting a license for the first and subsequent, if any, geological repositories for high-level nuclear waste (HLW). This act was amended in 1987 to designate one site in the unsaturated region of tuffaceous rocks of Yucca Mountain in southern Nevada for detailed characterization. To meet its licensing function, the NRC will review the application submitted by the U.S. Department of Energy (DOE). The Center for Nuclear Waste Regulatory Analyses (CNWRA) at Southwest Research Institute (SwRI) is a Federally Funded Research and Development Center (FFRDC) created to support the NRC in its mission of evaluating and licensing the proposed HLW repository. One critical section of the DOE license application will deal with the assessment of the future performance of the repository system, which has to meet certain standards established by regulations.

In order to develop capabilities to review the Performance Assessment (PA) in the DOE license application, the NRC and the CNWRA are engaged in developing and applying PA methods and models to existing data. Later, at the time of the license application review, these methods may be used to conduct independent PA, if the NRC elects to do so. Because of the large space and time scales involved in estimating repository performance, mathematical models encoded as computer codes are the chosen tools for PA. The repository system consists of designed (or engineered) barriers embedded in the natural geological setting. Estimating performance of the total system requires that the behavior of these components be projected under a variety of possible future conditions. This effort is obviously a complex task that requires a variety of calculations. The development of the DRILLO code described in this report is a part of the total performance assessment computer code that performs these calculations.

ACKNOWLEDGMENTS

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1 INTRODUCTION

1.1 REGULATORY AND TECHNICAL BACKGROUND

A very specific regulatory purpose for the conduct of Performance Assessment (PA) is to determine if the geological repository system satisfies the regulatory standards. This determination is done by comparing the estimated values of the regulatory performance measures with the limiting values of the same measures specified in the regulations. Thus, the PA models must be designed to estimate the performance measures. In addition to the regulatory function, PA will also be used to design [by the U.S. Department of Energy (DOE)] and judge the adequacy of [by the U.S. Nuclear Regulatory Commission (NRC)] the site characterization program. To meet these varied objectives, the Total-System Performance Assessment (TPA) code has been developed to provide computational algorithms for estimating values of various performance measures [see Sagar and Janetzke (1993) for the description of the TPA code]. To estimate the performance measures, the TPA code contains a set of Consequence Modules (CMs) that are largely independent computational units. The DRILLO code, which is one of these CMs used to evaluate consequences due to human intrusion events by exploratory drilling in the vicinity of Yucca Mountain (YM).

The primary regulations applicable to the high-level waste (HLW) geological repository were promulgated by the NRC in 10 CFR Part 60—Disposal of High-Level Radioactive Wastes in Geologic Repositories. Two sections of 10 CFR Part 60 pertain specifically to post-closure performance. These sections include Part 60.112—Overall System Performance Objective for the Geologic Repository after Permanent Closure; and Part 60.113—Performance of Particular Barriers after Permanent Closure. Part 60.112 makes reference to satisfying the generally applicable environmental standards for radioactivity established by the Environmental Protection Agency (EPA). These environmental standards were promulgated by the EPA in 40 CFR Part 191 in 1985. However, on litigation, certain provisions of these standards were remanded by a federal court. Proposed revisions of 40 CFR Part 191 were under review in early 1993. In late 1992, the U.S. Congress enacted a new law known as the Energy Policy Act according to which the EPA will develop standards applicable specifically to YM that may be different from those in 40 CFR Part 191. However, for the development of the DRILLO code, the 1985 EPA standards are followed. The DRILLO code will be modified, as necessary, at the appropriate time to account for any changes in the EPA rule.

Three different performance measures are used in Part 191. These measures are: (i) release of radioactivity over the entire accessible environment (AE) boundary (i.e., vertical boundary at 5 km from edge of the repository integrated over areal space) cumulated over a 10,000-yr period (integrated over time) after closure must not exceed specific limits at specified probability levels (Part 191.13—Containment Requirements), where the preferred method of representing this performance measure is through a Complementary Cumulative (Probability) Distribution Function (CCDF); (ii) dose to humans in the first 1,000 yr after repository closure must not exceed specified limit (Part 191.15—Individual Protection Requirements—this requirement has no probability attached to it); and (iii) concentration of alpha-, beta-, and gamma-emitting radionuclides must not exceed specified limits (Part 191.16—Groundwater Protection Requirements—there is no probability attached to this requirement). While the first performance measure is to consider all future credible scenarios, the other two apply only to undisturbed performance.

In addition, three other performance measures are used in 10 CFR Part 60.113 to define performance of individual barriers (in contrast to the total system). These performance measures are: (i) life of the waste package must exceed specified limits [Part 60.113(a)(ii)(A)—Substantially Complete Containment Requirement]; (ii) release from engineered barriers must be less than specified limits [Part 60.113(a)(1)(ii)(B)—Groundwater Release Requirement]; and (iii) Groundwater Travel Time (GWTT) must be greater than specified limits [Part 60.113(a)(2)—Groundwater Travel Time Requirement].

In all, there are six distinct performance measures. In general, the TPA code must accommodate compliance determination by estimation of the three measures related to 40 CFR Part 191 and preferably, but not necessarily, for the other three related to 10 CFR Part 60.113. Figure 1-1 depicts schematically the six performance measures and lists the generic steps for their assessment. The steps for the assessment of the six performance measures include model conceptualization of process, assembly of data suitable for input to the mathematical models for calculating consequences, sensitivity and uncertainty analysis, and regulatory compliance assessment. The NRC and CNWRA are developing regulatory definitions for the performance measure of 60.113 and the corresponding complementary determination methods. Performance measures computed in the Phase 2 TPA are examples only to demonstrate a concept. Whether such compliance determination will be accomplished through the TPA is a decision not yet made. In any event, the Phase 2 methods are not intended to be regulatory guidance and should not be taken to be such guidance.

1.2 TOTAL-SYSTEM PERFORMANCE ASSESSMENT CODE BACKGROUND

To estimate the performance measures, the TPA code contains a set of CMs that are computationally independent units, with their execution controlled by an Executive Module (Exec) (Sagar and Janetzke, 1993). The Exec acts as the manager and ensures that CMs are executed in the desired sequence and that appropriate values of the common parameters are passed to the CM. The Exec of the TPA directs data flow between different subprocesses and controls their execution. Figure 1-2 shows schematically the organization of Version 2.0 of the TPA code. The shaded parts of Figure 1-2 represent the Exec. A data flow diagram indicating intermodule communication interfaces is shown in Figure 1-3. This figure also shows all CMs of the TPA, including the DRILLO code, which consists of two modules.

1.3 PURPOSE OF SOFTWARE

The objective of the DRILLO modules is to provide computational algorithms for estimating consequences due to human intrusion events by exploratory drilling in the TPA simulations. The code simulates drilling scenarios as a random process. Specifically, the DRILLO simulation will determine the number of waste packages failed by the drilling and the amount of radionuclide released to the geologic media and to the AE. The results from the DRILLO simulations are then used by other TPA CMs to calculate aqueous and gaseous radionuclide source terms, human individual or population dose, and the total amount of radioactivity released directly to the AE.

1.4 REPORT CONTENT

A brief description of the conceptual and mathematical models embodied in the DRILLO software is presented in Chapter 2. It also describes the assumptions made and the limitations of the model. Features of the software are described in Chapter 3, which includes a detailed description of the

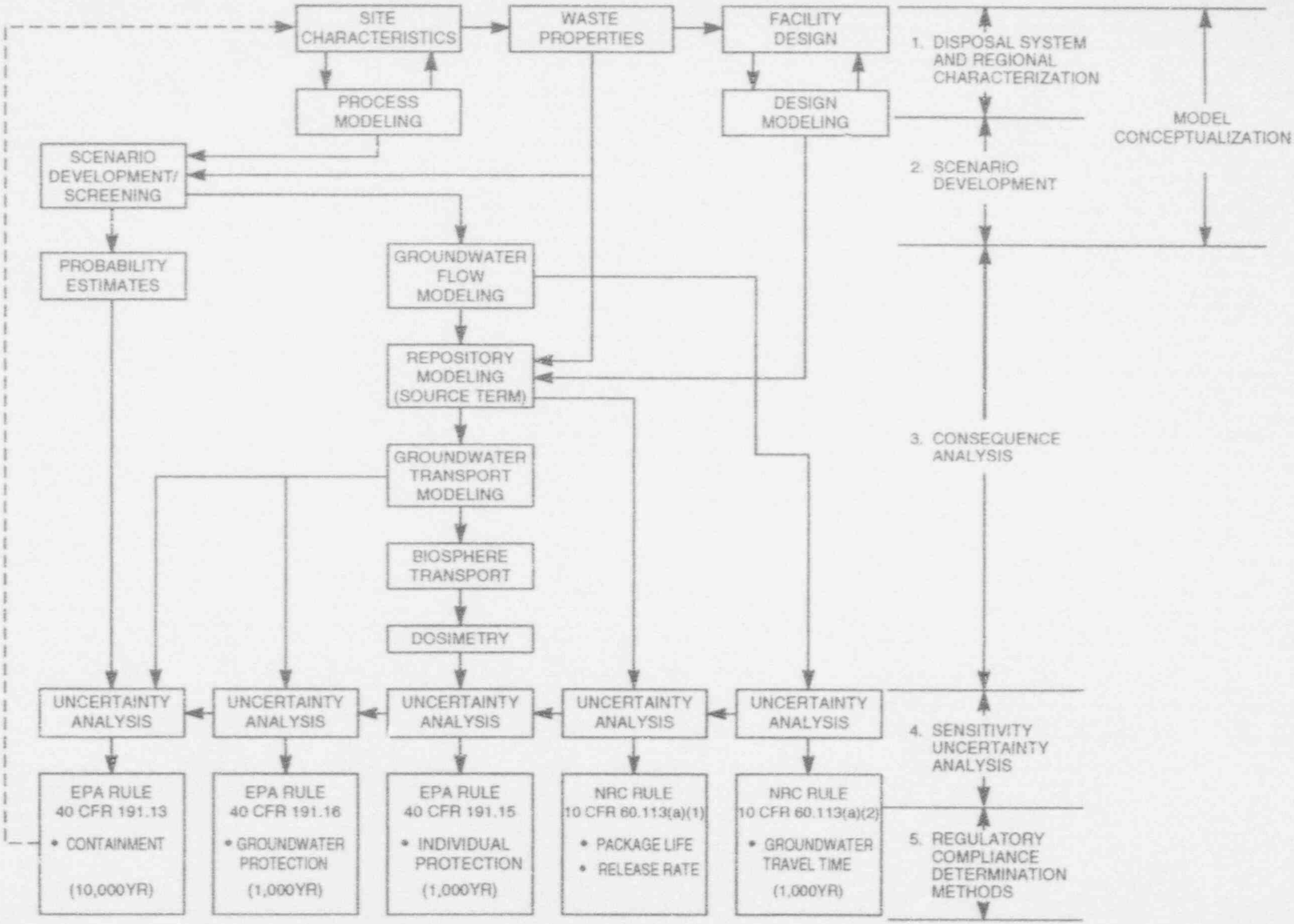

Figure 1-1. Regulatory performance measures

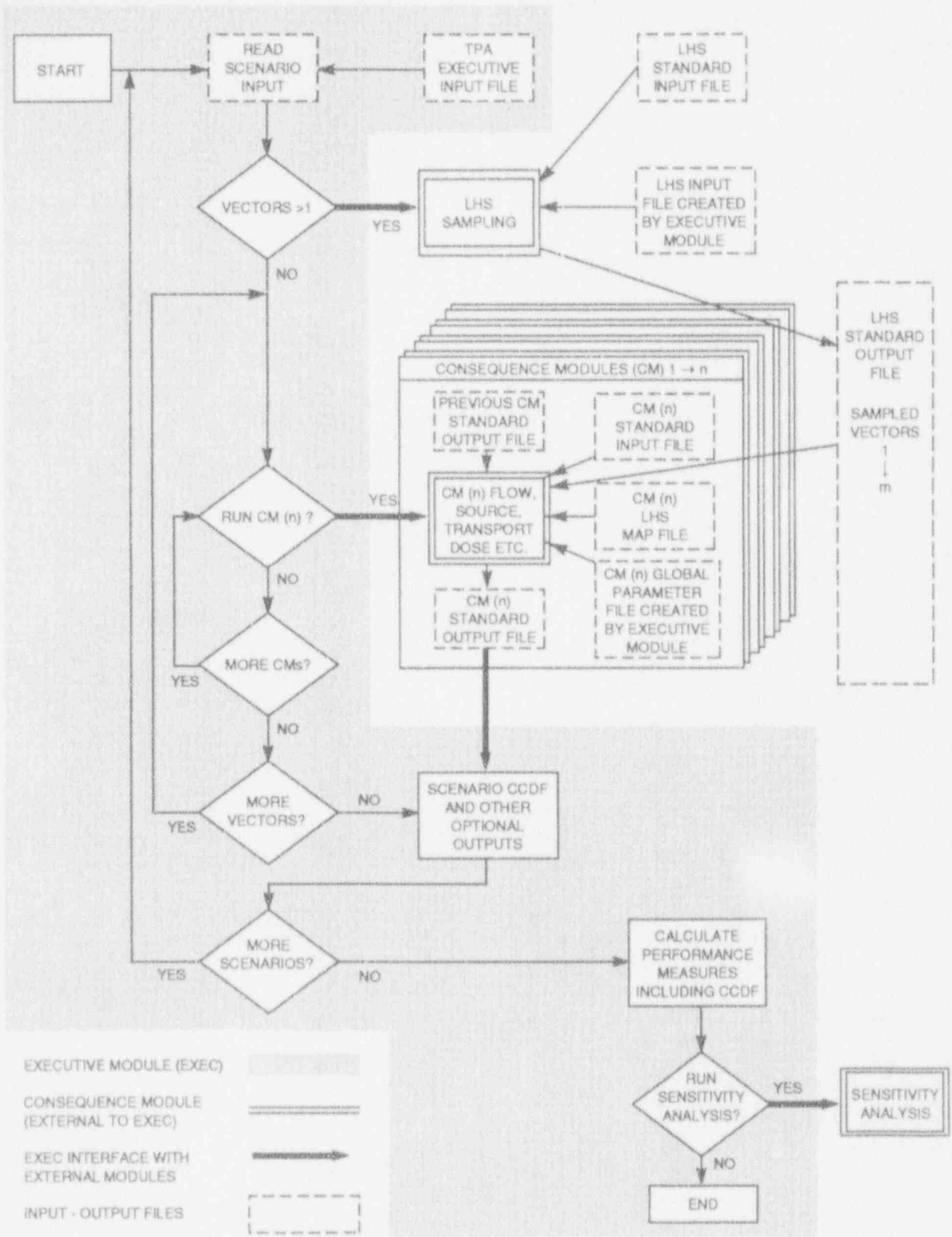

Figure 1-2. Organization of the TPA computer code

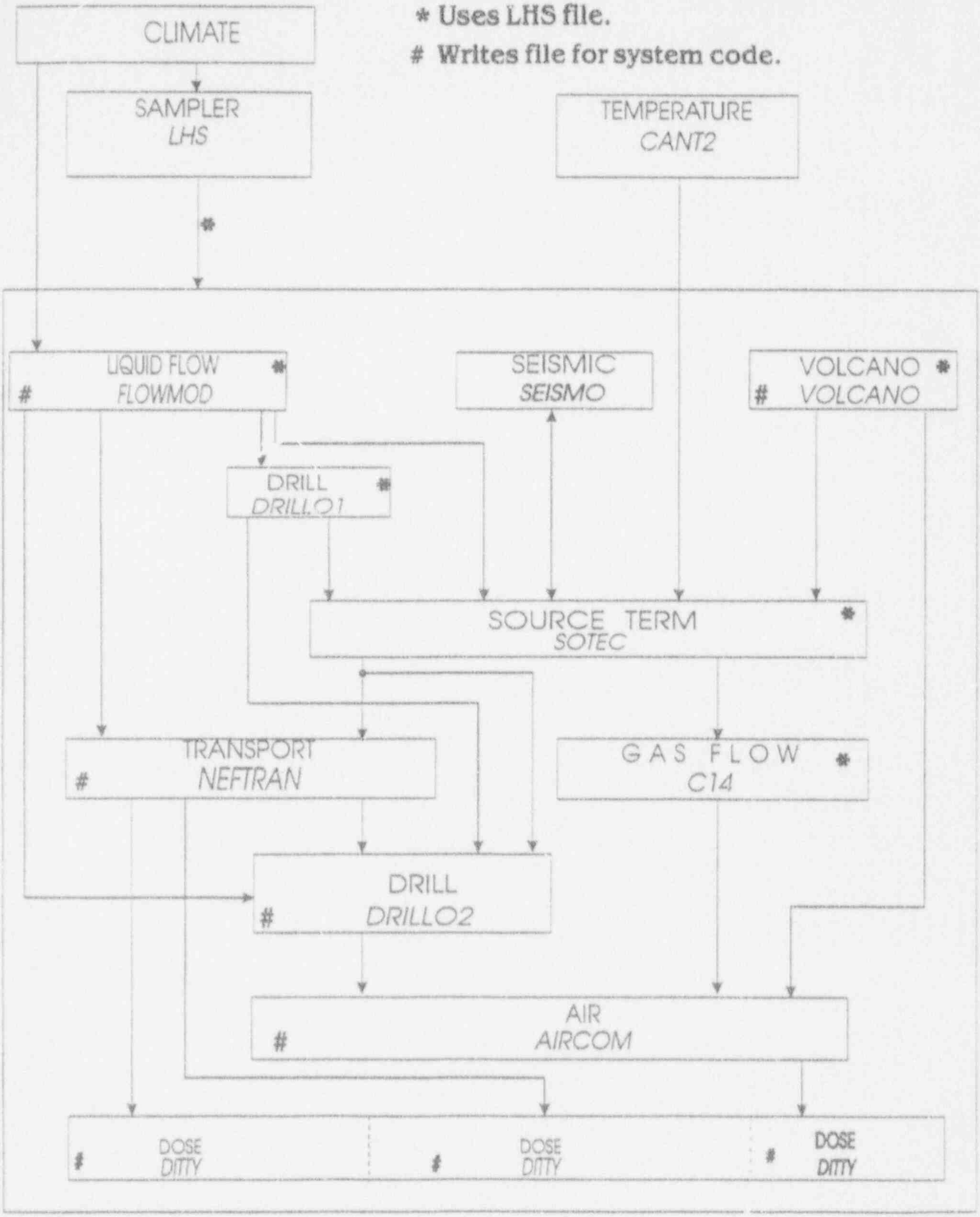

Figure 1-3. TPA system flow diagram

software capabilities and code structure. Chapter 4 contains the input instructions for the DRILLO code. Chapter 5 describes the outputs. The verification and validation status is discussed in Chapter 6. Chapter 7 gives the references. Sample problems are given in the text of the report. Appendix A lists DRILLO code error messages.

2 MODEL DESCRIPTION

2.1 OVERVIEW

The DRILLO computer code is designed to model the effects of human intrusion by drilling on the performance of the potential repository in YM. The code considers the scenario of the release of radionuclides to the geologic media and AE due to drilling operations that violate the integrity of the canisters in the repository. This scenario is predicated on the assumption that the active and passive institutional controls preventing violation of the repository are lost, and, thereby, drilling operations at the site of the repository become a potential failure mode for the repository.

The philosophy used in the design of this component of the TPA code is that of representing a complex scenario using a simple analysis that resolves the essence of the process. This is accomplished here by simplifying the geometry of the repository into two major regions, the engineered barrier system (EBS) and the rock column (RC), and by reducing the multidimensionality of the problem to a single dimension. Radionuclides are modeled as residing in one of three compartments: (i) EBS, (ii) RC, or (iii) the AE.

The human intrusion scenario is stipulated to consist of drilling in and around the proposed repository site. The premise is that, at various times starting 100 years after closure and extending through the 10,000-yr regulatory period for the repository; one or more boreholes are drilled from the surface of YM, penetrating down into the region of the repository. This would then create the potential for the removal of radionuclide material to the ground surface either directly from waste canisters or from the surrounding contaminated rock. In the scenario, it is assumed that: (i) 20th century drilling technology is being used; (ii) if a borehole intersects any portion of a waste canister, then its integrity is lost; and (iii) that if a fraction of the material is excavated and transported directly to the ground surface through the drill string in the drilling fluids.

The DRILLO computer code performs two primary computations. The first is the prediction of three parameters: (i) the location of the boreholes; (ii) the time of the drilling events; and (iii) whether or not a waste canister has been hit by the drill bit. These calculations are made assuming the process to be random, as defined in Codell et al. (1992). In this scenario, the drill bit may either directly hit and penetrate only rock that may be contaminated, or both hit a canister and penetrate contaminated rock. Radioactive material may then be brought to the surface in either of these cases. The prediction of canister impacts and event times are then used in the TPA source term module (i.e., SOTEC).

The second primary computation is the prediction of the consequences of the drill bit intersecting a waste canister, contaminated rock, or both. A drill bit directly hitting a waste package and/or penetrating contaminated rock is assumed to lift a portion of the radionuclide inventory to the ground surface. The magnitude of the quantity of material deposited on the ground surface is then predicted by DRILLO, which is used by TPA code to calculate direct release to the AE. A small percentage of this material is then assumed to be particulates, which become airborne. This information is then provided to other TPA modules (i.e., AIRCOM) for the calculation of human dose.

In the remainder of this section, complete details of the mathematical models and the assumptions upon which they are based, representing the processes of the human intrusion scenario due to drilling, are presented.

2.2 MODELED REGIONS

DRILLO subdivides the repository system into three compartments. These are the EBS, the RC, and the AE. Each of these compartments is a control volume in which radionuclide material may reside. Figure 2-1 illustrates the relationships between these three compartments. In general, radionuclide material is produced and decayed within the compartment, and is transported into and out of the compartment by fluid motion. In this version of the code, only liquid transport, not gaseous transport between compartments is considered.

The EBS is defined to be the compartment in which the waste canisters are placed. Initially, radionuclide material will be present only in the EBS. The EBS is further subdivided into seven regions in which the number of waste canisters may vary from region to region. The nuclear material in each of these seven regions is then allowed to decay and migrate out of the EBS into the RC through both advective and diffusive processes. The initial inventory of nuclear material is assumed to be the same for every canister in each of the regions, but the number of canisters in each region is allowed to be different. However, as described below, the rate of migration of radionuclides out of each EBS region into the underlying RC may be different.

The three-dimensional (3D) geometry of the EBS is represented here as a two-dimensional (2D) surface area through which the boreholes will penetrate. The areal description of the EBS is then defined through a set of panels or 4 node, 2D elements. Figure 2-2 illustrates the relationship between the 3D structure of the EBS and its 2D representation. For each region of the EBS, a set of N panels with four nodes (defining its shape and extent) are input. These data consist of (x,y) coordinates and node connectivity data, similar in concept to a finite element grid description. Each panel then, is a quadrilateral of arbitrary shape. Its corresponding area is then computed by subdividing the element into two triangular elements. Using the definitions illustrated in Figure 2-3, the area of the panels or element polygons is computed by

$$\begin{aligned} \text{Panel Area} &= 0.5 * \left[\left(|V_1| * |V_2| \right)^2 - \left(V_1 \cdot V_2 \right)^2 \right]^{1/2} \\ & 0.5 * \left[\left(|V_3| * |V_4| \right)^2 - \left(V_3 \cdot V_4 \right)^2 \right]^{1/2} \end{aligned} \qquad (2\text{-}1)$$

where * refers to multiplication of the vector magnitudes and · denotes the dot product. Each quadrilateral area is then summed on a per-region basis to compute the total area of the region. These region areas are then summed to give the total cross-sectional area of the EBS compartment.

The RC compartment represents the rock strata underlying the EBS regions. Each of the seven EBS regions has an underlying RC region associated with it. The RC compartment extends down from the EBS to the saturated zone beneath YM. Nuclear material may be transported from the EBS to the RC as illustrated in Figure 2-1. The rate and nature of such transfer is provided by the SOTEC code. The waste material deposited in the RC may then decay further and consequently be transported out to the AE, again by fluid motion. The rate of transport of nuclear material from the RC to the AE is dictated by the flow rate of groundwater through the unsaturated zone. These flow rate data are provided to DRILLO from the FLOWMOD module of the TPA code. The cross-sectional area of each RC region is the same as its overlying EBS region. The RC is then connected directly to the AE by the interface to the saturated zone beneath each RC region and also to the ground surface through drill boreholes.

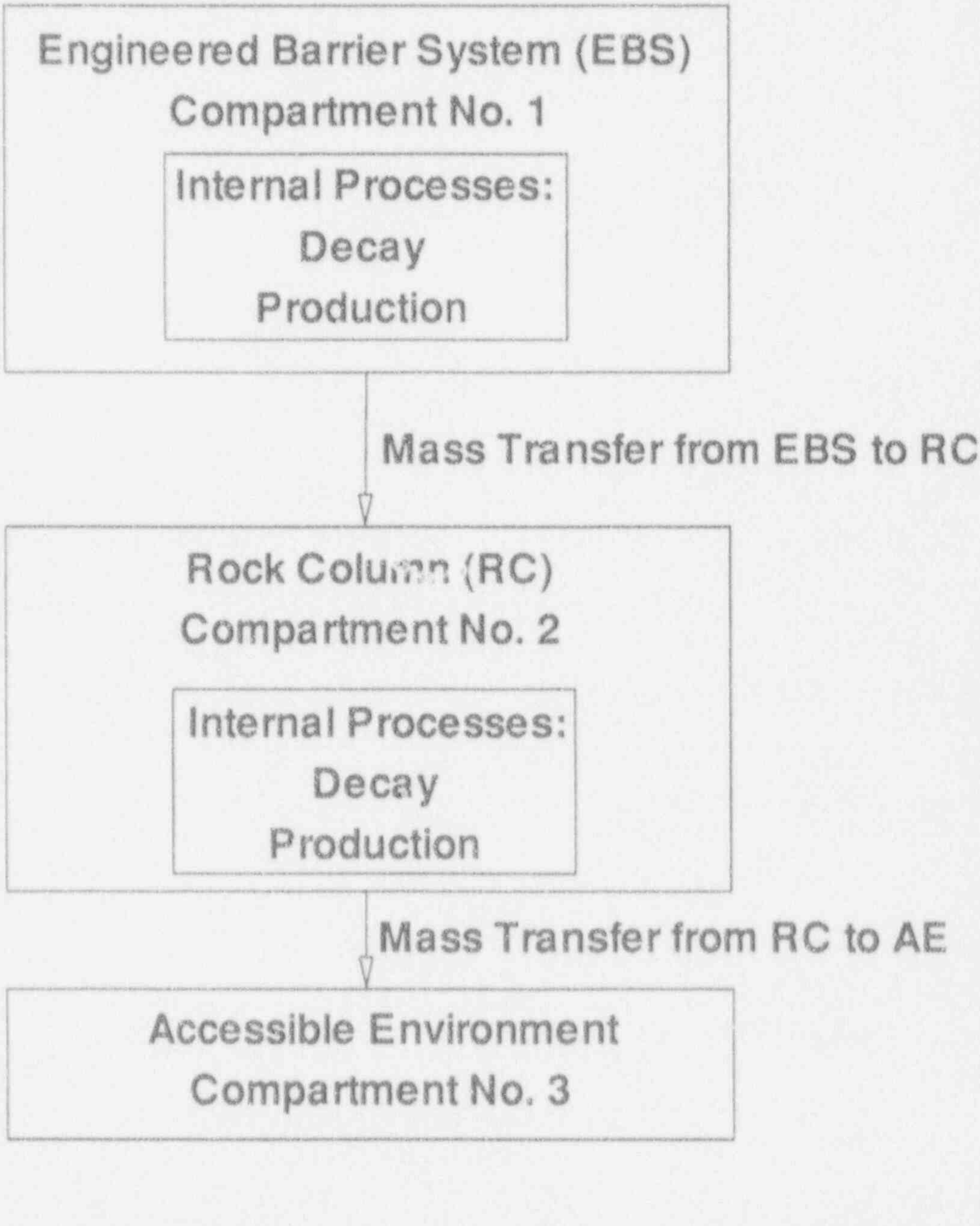

Figure 2-1. Schematical representation of the regions modeled in DRILLO

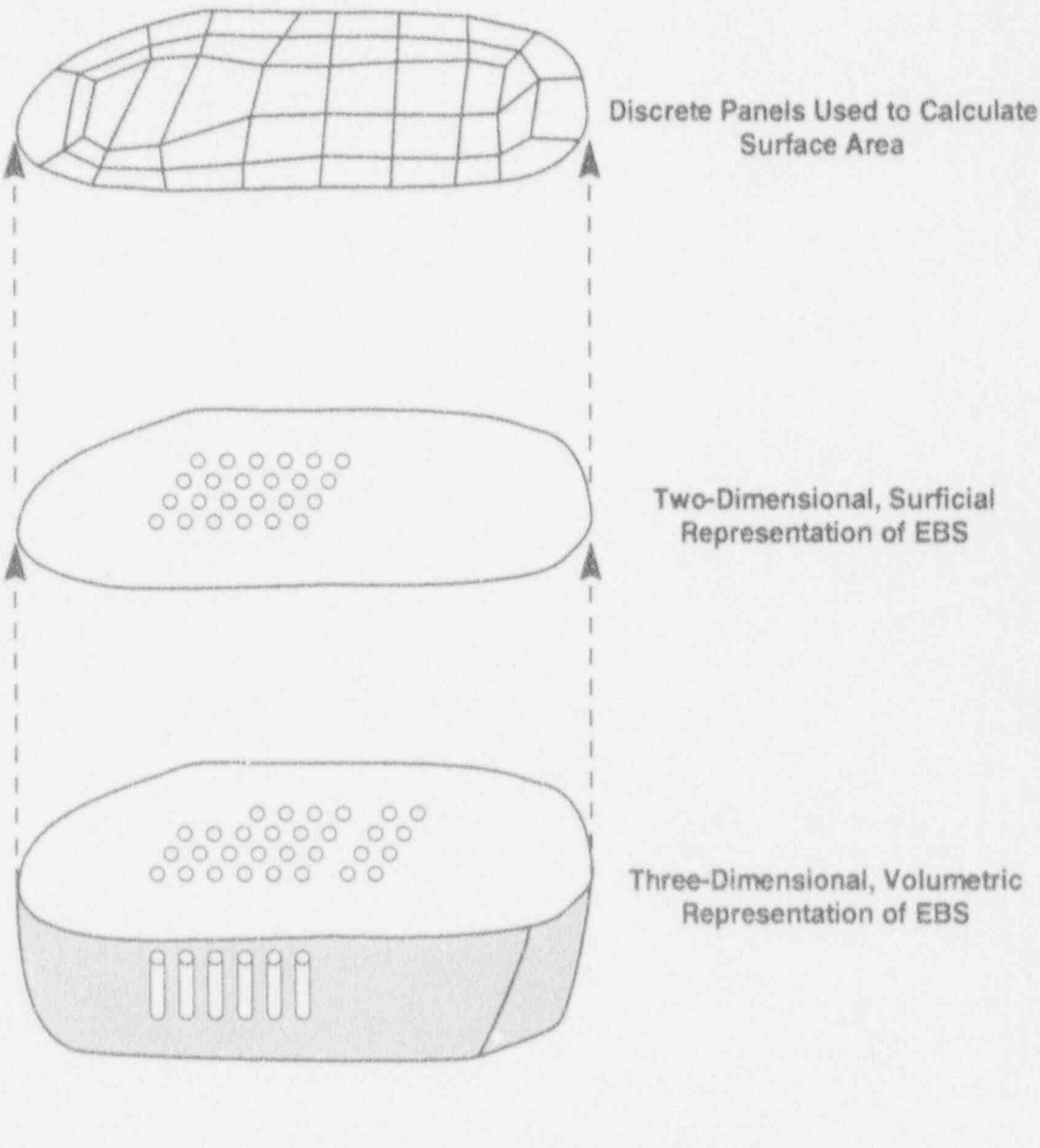

Figure 2-2. Relationship between 3D structure of EBS and its 2D model

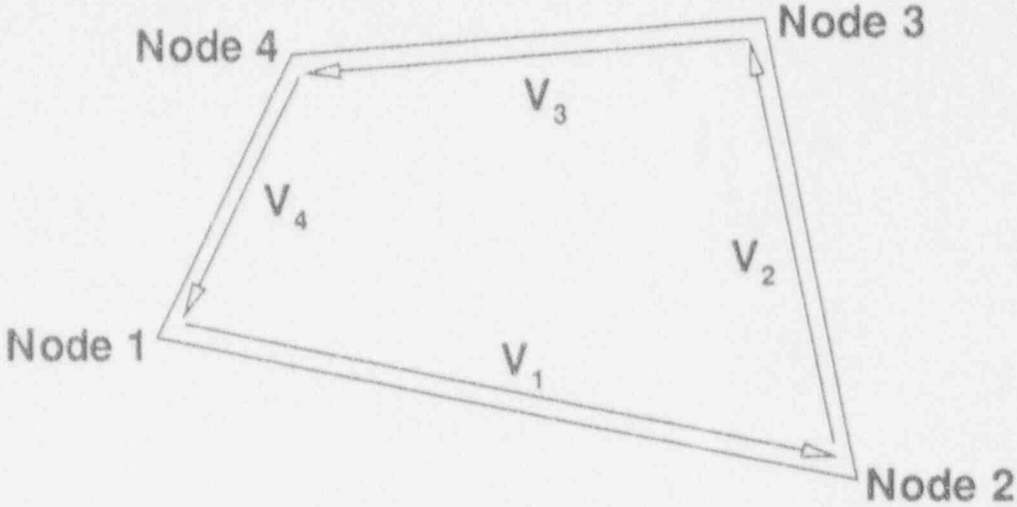

Figure 2-3. Definition of terms used in the computation of surface panel areas

The AE compartment represents regions outside of the EBS and RC. The AE is defined to begin at 5 km from the perimeter of the EBS, and is also represented by the saturated zone beneath the RC. Drilling outside of the perimeter of the EBS could exhume waste material from the RC; however, the consequences of such releases, in terms of dose, are assumed here to be negligible, because the waste will be very dilute as lateral diffusion is expected to be the primary mechanism for lateral transport, and this is an extremely slow process. Exhumation of radionuclides from the saturated "footprint" is also possible, but is neglected here.

2.3 RELEASE MECHANISMS

Surface release occurs under two circumstances. In the first case, the drill bit directly intersects a waste canister. The waste materials are then lifted to the surface by entrainment in the drilling fluids or by contamination of the drill string. It is assumed that the drill bit can penetrate a waste canister, that the waste canisters are vertically emplaced, and that even partial intersections with a waste canister result in complete failure of the waste canister, enabling its subsequent release of its contents. Given an inventory of radionuclides (the method for determining this inventory is discussed herein) at the time of the drilling event, DRILLO computes the quantity of material deposited on the ground surface through the drilling process. Thus, for each nuclide j in the inventory of a canister in a region of the EBS, the quantity of nuclide j deposited on the ground surface due only to a canister hit is

$$Q_{EBS}\,(i,j,k) = I_{EBS}\,(i,j) * (Radius^2/Radcan^2) \tag{2-2}$$

where $Q_{EBS}\,(i,j,k)$ is the amount of nuclide j, in chain number i, released from drill borehole k. $Q_{EBS}\,(i,j,k)$ is in units of curies. $I_{EBS}\,(i,j)$ is the inventory in a canister of nuclide j, in chain number i, at the instant of the drilling event in the EBS region, and again, this is measured in curies. *Radius* is the radius of the kth drill borehole, and *Radcan* is the radius of the waste canister, where the ratio of the squares of these terms is not allowed to exceed 1.

It is assumed here that all canisters in all seven EBS regions undergo the same decay and production process, so that at any instant in time, there is no difference between EBS regions in terms of the character of the radionuclide inventories in a canister. However, due to different flux rates out of each EBS region, there will be a different, total, or gross radionuclide inventory in each EBS region. Data from the TPA consequence module, SOTEC, provide the efflux rates for each nuclide (i,j) from each EBS region as a function of time. These data are then used to modify the total inventory of nuclear material in a given EBS region at an instant in time. Details of the SOTEC code are given in Sagar et al. (1992).

Specifically, the initial inventory of radionuclides in a canister are allowed to decay over the elapsed time from emplacement to the drilling event. This temporally adjusted inventory in a canister, at the instant of the drilling event, is then multiplied by the number of canisters in the particular region of the EBS. This gives the maximum possible gross inventory in the EBS region at the time of the drilling event. During this period of time, radionuclide material may also be transported out of the EBS region. This material is then allowed to decay as well, giving a magnitude for the amount of radionuclides transported out of the EBS at the moment of the drilling event. The final total inventories of nuclear material in an EBS region, at the instant of the drilling event, is then calculated as

$$IT_{EBS}\,(i,j) = IM_{EBS}\,(i,j) - I_{EFFLUX}\,(i,j) \tag{2-3}$$

where $IM_{EBS}\,(i,j)$ is the maximum possible inventory in the EBS region, and $I_{EFFLUX}\,(i,j)$ is the inventory of materials transported out of the EBS region during the elapsed time.

The effective or average inventory per canister is then computed as

$$I_{EBS}\,(i,j) = IT_{EBS}\,(i,j)/CANPZ(m) \tag{2-4}$$

where $CANPZ(m)$ is the number of canisters in a particular EBS region, m. It is this averaged inventory that is used in Eq. (2-2) to calculate the release.

If a drill borehole does not hit a waste canister in the EBS, then no waste materials are released to the ground surface from this compartment. It is assumed that there is no contaminated rock in the EBS and that the only source of waste materials in the EBS comes from the waste canisters.

In the second case, the drill bit may or may not intersect a waste canister, but does pass through rock that has been contaminated by migrating radionuclides. Similar to the first case, contaminated rock from the RC is lifted to the surface by the drilling fluid or the drill string. Further, as in the EBS, radionuclides are allowed to decay and migrate into and out of the RC. These inventories are computed for each of the drilling events, the details of which will be discussed in this report. It is assumed that these radionuclides are uniformly distributed in the RC region. This means that the consequence of excavating contaminated rock in an RC region from a single borehole is equal to the total inventory in the RC region at the time of the drilling event, multiplied by the ratio of the area of the borehole to the area of the region of the EBS overlying the RC. In DRILLO, the equation for the magnitude of the quantity of nuclear material deposited on the ground surface from a borehole penetrating contaminated rock is

$$Q_{RC}\ (i,j,k) = I_{RC}\ (i,j) * \left[B_{area} / EBSZ_{area}(m)\right] \tag{2-5}$$

where $Q_{RC}\ (i,j,k)$ is the amount of nuclide j, in chain number i, released by borehole k, measured in curies. $I_{RC}\ (i,j)$ is the inventory of nuclide j, in chain number i, in the RC associated with a specific region of the EBS. B_{area} is the cross-sectional area of the borehole, and $EBSZ_{area}(m)$ is the cross-sectional area of the m^{th} EBS region.

Similar to the EBS inventories, a distinction is made between the inventories of radionuclides in each RC region. This is done by computing the release rate of nuclides from the RC to the AE on a per-region basis, and the input rate of nuclides from the EBS to the RC. Specifically, this is done by using data from NEFTRAN, FLOWMOD, and SOTEC. For each RC region, the concentration of radionuclides, as a function of time, in the RC is input from NEFTRAN, and the groundwater flux, as a function of time, from the RC to the AE is input from FLOWMOD. The product of these two quantities gives the magnitude of the efflux of nuclear material from each RC region into the AE. As previously discussed, on a per-EBS-region basis, the amount of radionuclide inventory leaving a specific EBS region, as a function of time, is input to DRILLO from SOTEC. This provides a source of nuclear material for the underlying RC. Thus, for each drilling event, the migration of nuclear material into the RC, from the EBS, the migration of nuclear material from the RC into the AE, and the decay of the nuclear material within the RC are all accounted for. Details of the NEFTRAN code are given in Olague et al. (1991).

The total amount of radionuclides released to the ground surface is the sum of the quantity released by a canister hit and the quantity released by contaminated rock removal for all drilling events. That is

$$Release(i,j) = \sum_{k=1}^{Nbor} \left[Q_{EBS}\ (i,j,k) + Q_{RC}\ (i,j,k)\right] \tag{2-6}$$

where $Release(i,j)$ is the amount of nuclide j, in chain number i, released due to all boreholes. $Nbor$ is the total number of boreholes occurring during the 10,000-yr life of the repository. Note that Q_{EBS} is taken to be zero unless a canister hit is simulated. The time at which the release occurs is taken to be the time of the earliest drilling event. These data are then output to AIRCOM for prediction of human dose.

2.4 RADIONUCLIDE INVENTORIES

As discussed previously, the radionuclide inventories in all canisters in all regions of the EBS are assumed to decay at the same rate. However, due to different rates of transport of nuclear material between the EBS and RC and the RC and AE, for each region, the inventories at an instant in time will be different in the seven regions of the repository. DRILLO calculates the radionuclide inventory, as a function of time, for each EBS and RC region. The inventory in an EBS region is equal to the initial emplaced inventory modified by decay and production and reduced by the flux and cumulative release to the RC. The SOTEC module of the TPA code predicts the flux and release to the RC for each region as a function of time. Application of the Bateman equations to this initial emplaced inventory and to the SOTEC output data yields the current inventory in an EBS region. The inventory in the corresponding RC region is the cumulative flux in (given by SOTEC), modified by decay and production and reduced by the cumulative flux out to the AE (given by NEFTRAN). In this manner, the inventories, at the instant of a drilling event in a given region of the repository are calculated.

The equation for the time variation of the inventory in either the EBS or the RC compartment is described by an ordinary differential equation:

$$dI_j/dt = -\lambda_j I_j + \lambda_{j-1} I_{j-1} + M_j(t) \tag{2-7}$$

where I_j is the inventory of nuclide j, in the given compartment λ_j is the decay constant for nuclide j, and $M_j(t)$ is the rate of mass injection or removal of nuclide j. The solution of this equation with $M_j(t) = 0$ and with initial conditions $I_j(0) = I_{0j}$ yields the Bateman equation whose solution is designated by

$$I_j(t) = B_j\left(t;\ \lambda_j, I_{0j}, I_{j-1}\right) \tag{2-8}$$

As a series of coupled, linear, ordinary differential equations, the solution for this simplified set of equations gives the inventory of nuclide I_j, in terms of the initial inventory of nuclide I_{0j}, and the sum of the inventories of the parent nuclides in the chain, if any.

The solution of Eq. (2-7) for the compartmental inventories, with an arbitrary time function representing mass injected and removed, may then be represented as a superposition of the chain decay problem of Eq. (2-8) and the solution to the Bateman equations for a mass source term applied over a finite time interval. Then, for an EBS region, the inventory of nuclide, j, at time, t, is

$$I_j\,(t) = B_j\left(t;\ I_{0k}, \lambda_k\right) - \sum_{l=1}^{L} B_j\left[(t-t_l);\ \Delta t_l F_{kl}, \lambda_k\right] \quad k = 1, \ldots j \tag{2-9}$$

where F_{kl} represents the flux of nuclear material out of the EBS region over time increment l. In a RC region, there is no initial inventory, thus Eq. (2-9) reduces to

$$I_j(t) = \sum_{l=1}^{L} B_j\left[\,(t-t_l);\ \Delta t_l F_{kl}, \lambda_k\right] \quad k = 1, \ldots j \tag{2-10}$$

where F_{kl} represents the net flux of nuclear material to the RC region.

The initial inventories for a canister are input data to DRILLO. These data consist of the number of nuclides, the name of the nuclide, the number of nuclear chains, the nuclide's initial inventory in terms of curies, and the nuclide's decay rate. The net flux data are provided to DRILLO from SOTEC, NEFTRAN, and FLOWMOD, as previously discussed.

2.5 PROBABILITIES

For a given number of drilling events, three different random numbers are generated for each borehole. These are the time of the drilling event, the region of the repository into which the borehole penetrates, and whether a drill bit has hit a canister. The values for these random numbers may be read from the LHS Global Data Input File of the TPA code if DRILLO is being run as part of the TPA code. In standalone mode, these numbers are calculated within DRILLO using a random-number generator.

The time of a drilling event for a borehole, k, is a random number which may range in value from 100 to StpT (StpT is a variable representing the duration of the simulation and defaults to 10,000 yr). When DRILLO is operated as part of the TPA code, these n times (where n is the total number of drilling events) are read from the LHS input file in units of years. If DRILLO is run in a standalone mode, then n random numbers between 0 and 1 are sampled from a uniform distribution and then multiplied by the length of the regulatory period.

The procedure for determining the region of the EBS into which a borehole falls is a combination of a random number and a transformation that maps the normalized area of the repository to a one-dimensional (1D) data set. As discussed previously, the cross-sectional area of each region of the EBS is calculated. Each area is then normalized by the total area of the repository. These normalized areas are used to create a series of intervals that form a number line ranging from 0 to 1. That is

$$interval(0) = 0.0$$
$$interval(1) = EBSZ_{area}(1) / TOTAL_{area}$$
$$interval(m) = interval(m-1) + EBSZ_{area}(m) / TOTAL_{area}$$

where m ranges from 2 to the number of EBS regions. The EBS region into which the borehole penetrates is then determined by comparing a random number between 0 and 1 to the intervals defined above, or

if $interval(i-1) < R(k) \leq interval(i)$, then borehole k lies in EBS region i

where $i=1$, ... the maximum number of EBS regions, and $R(k)$ is a random number between 0 and 1.

The probability of a canister hit is based on the assumption that the canisters are uniformly distributed within the region of the repository; and that the canisters are vertically emplaced. For any drilling event over a region of the repository, any one of the $CANPZ(m)$ canisters in the EBS region, m, may be hit. It is further implied in this analysis that only one canister may be hit by a single borehole and that all canisters are available for drill bit impact for each drilling event. The probability of hitting a canister in an EBS region, m, during a drilling event, k, is then calculated as

$$P_h(m) = [CANPZ(m) * A_p] / EBSZ_{area}(m)$$
$$A_p = \pi \ (Radius + Radcan)^2 \qquad (2\text{-}11)$$

where *radius* represents the drill bit radius, *Radcan* is canister radius, and A_p is the conservative estimate of the intersection area of a drill bit with canister. With both $P_h(m)$ and the region, *m*, of penetration of borehole, *k*, known, a canister hit is defined to occur if a random number (ranging from 0 to 1), called the hit indicator, is less than or equal to the probability of a hit in that region. Symbolically, this is represented as

if $hit(k) \leq P_h(m)$, then $H(k) = 1$, a hit is registered
if $hit(k) > P_h(m)$, then $H(k) = 0$, no hit registered

where *hit(k)* is the hit indicator, which is a random number, and *H(k)* is the hit register, which is 1 for a canister hit and 0 for a canister miss.

3 DRILLO SOFTWARE DESCRIPTION

3.1 SOFTWARE CAPABILITIES AND SALIENT FEATURES

The DRILLO computer code consists of two modules which are run independently of each other, sharing data through data files stored on disk. These two modules are the DRILLO1 and DRILLO2 codes. DRILLO1 calculates the three parameters for the drilling scenario. As previously discussed, these three parameters are the time of the drilling event, the region of the repository into which the borehole penetrates, and whether a drill bit has hit a canister. DRILLO2 calculates the consequences to the AE of hits by boreholes on canisters and/or of the removal of contaminated rock by a borehole, in terms of total release of nuclides to the ground surface.

DRILLO1 and DRILLO2 may be run as part of the TPA code. In this mode of operation, DRILLO1 and DRILLO2 interact with the other modules in the TPA code through data files. Figures 3-1 and 3-2 display schematically the interactions between DRILLO and the other modules of the TPA code. In particular, DRILLO1 supplies SOTEC data on the total number of canister hits in an EBS region and the earliest time of the drilling events in an EBS region. DRILLO1 then reads data from files created by the TPA Exec code and FLOWMOD. The TPA Exec code provides DRILLO1 with sample data for the number of drilling events (*Nbor*), the radius of the boreholes (*Radius*), and for each borehole, a region number [*R(k)*] and a hit indicator number [*hit(k)*]. TPA Exec also supplies data on the independent parameters of the number of EBS regions (*m*), the waste canister radius (*Radcan*), and the number of canisters per EBS region [*CANPZ(m)*]. Complete details of the DRILLO1 Parameter Map File (DR1MAP.DAT) and the Global Data Temporary Input File TPA_DR1.DGD are given in Sagar and Janetzke (1993). FLOWMOD provides data on the total cross-sectional area of each EBS region and the depth of the unsaturated zone beneath each region of the EBS.

DRILLO2 reads input data from DRILLO1, SOTEC, NEFTRAN, FLOWMOD, and the TPA Exec code. DRILLO1 supplies information on the radius of the borehole, the radius of the waste canisters, the total number of drilling events, and, for each borehole, data on the time of the event, the region number for the borehole, and the hit designator number. In addition, DRILLO1 supplies for each region of the EBS, data on the number of canisters emplaced, the depth of the unsaturated layer, and the cross-sectional area of the EBS regions. SOTEC supplies data on the temporal distribution of the flux of radionuclides from each region of the repository. NEFTRAN supplies data on the temporal distribution of the concentration of nuclides in the RC underlying each EBS region. FLOWMOD supplies data on the magnitude of the flux of groundwater from the RC to the AE. The TPA Exec code provides data to DRILLO2 through the TPA_DR2.DGD data file, whose complete description is given in Sagar and Janetzke (1993).

DRILLO1 and DRILLO2 may both be run as standalone programs. Figures 3-1 and 3-2 display the necessary input files for each code in order for them to be run as standalone programs. The details of these data sets are presented in Section 4 of this report.

3.2 SOFTWARE LIMITATIONS

The DRILLO codes have no specific computational limitations. The codes are currently executable on CRAY, VAX, and SiliconGraphics machines. The source codes are written in standard FORTRAN 77 syntax. It is assumed, however, that the existence of various input files (schematically

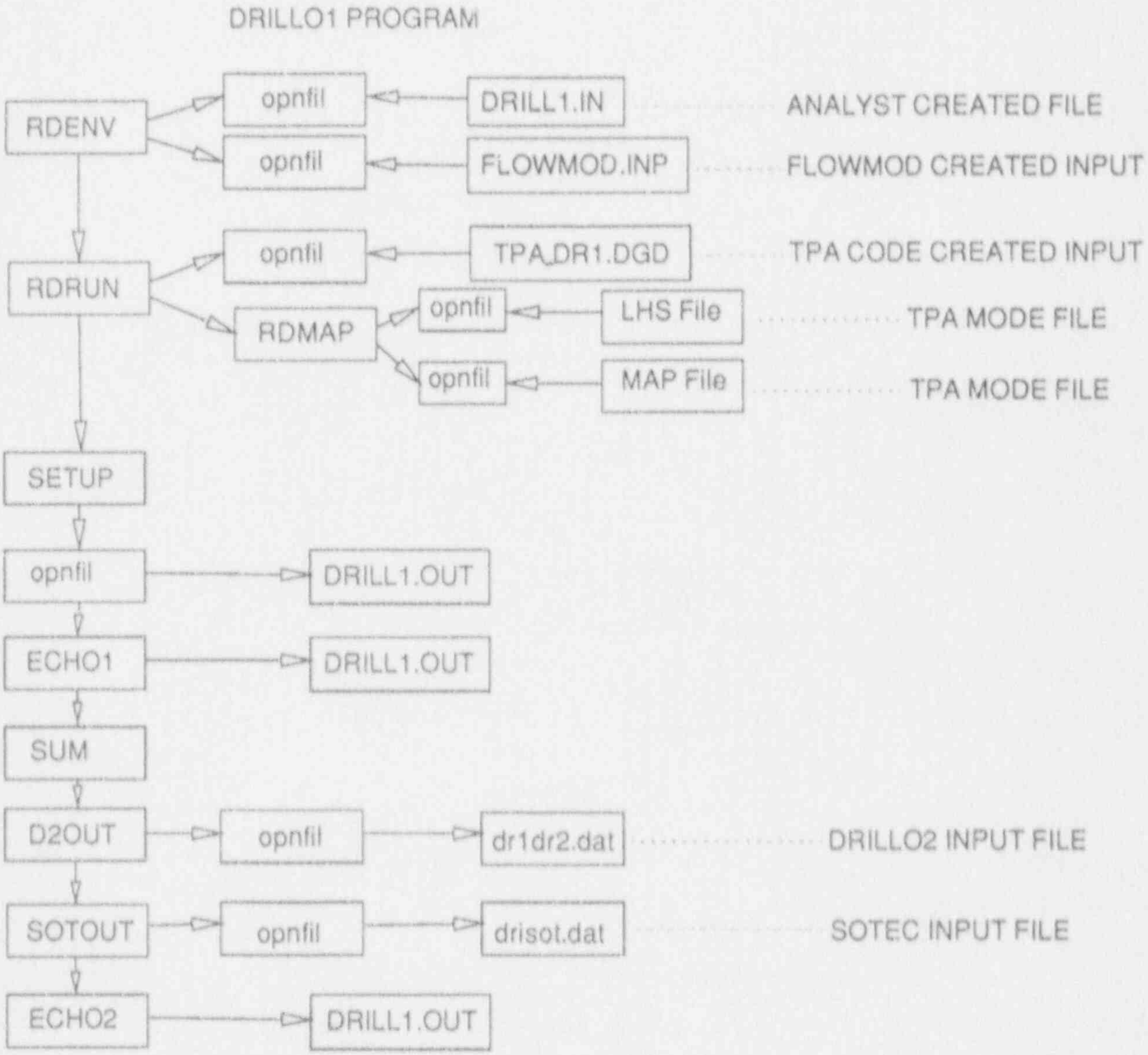

Figure 3-1. Call sequence and input files for DRILLO1 program

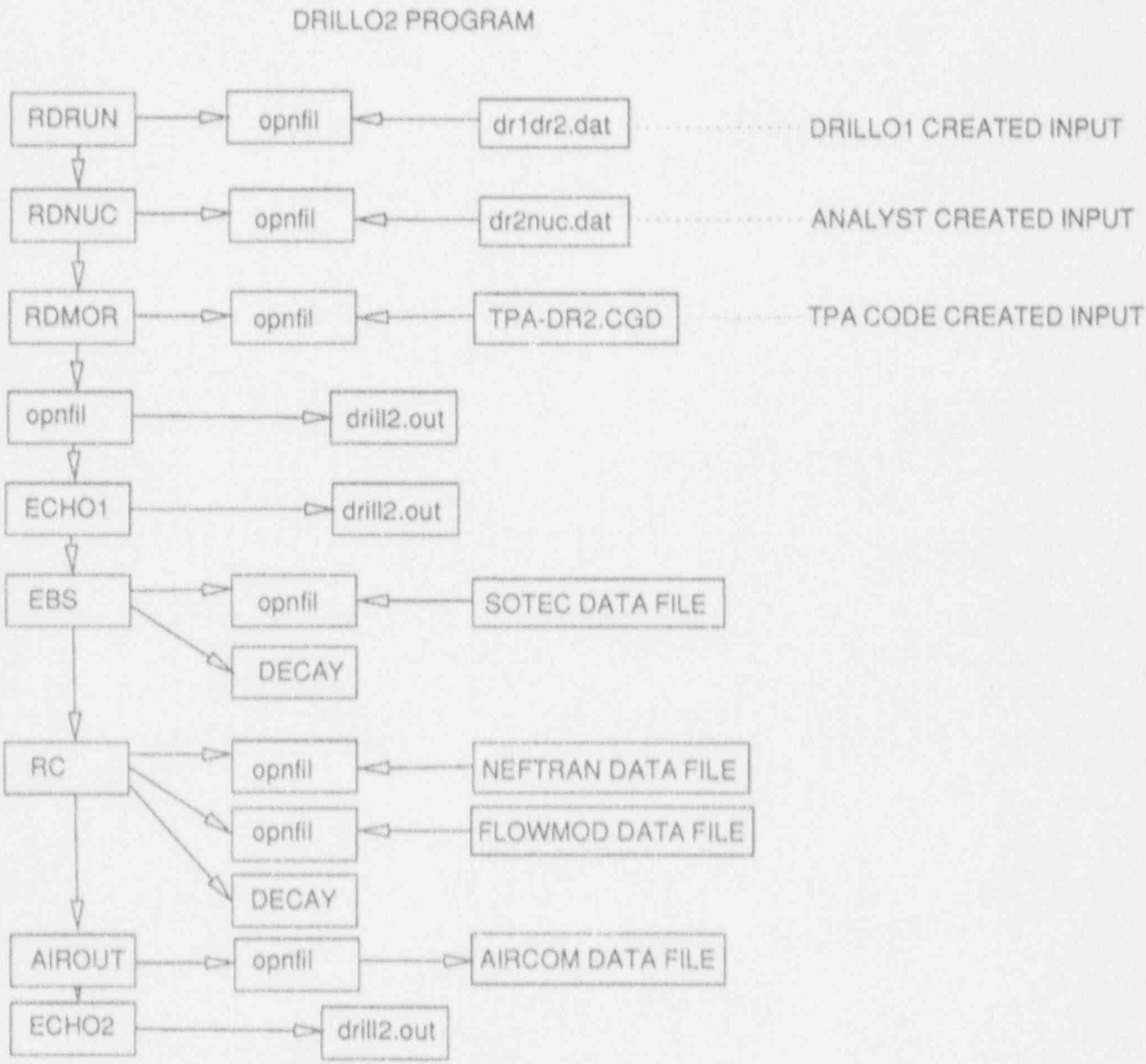

Figure 3-2. Call sequence and input files for DRILLO2 program

shown in Figures 3-1 and 3-2 and discussed in Section 4) are verified by the analyst prior to executing the appropriate module.

3.3 HARDWARE REQUIREMENTS AND INSTALLATION PROCEDURES

The DRILLO1 computer code requires minimal hardware resources. The largest arrays are dictated by the product of the number of EBS regions and the number of layers in the unsaturated zone. Execution times are on the order of seconds, and the disk files created are only a few kilobytes in size.

The DRILLO2 computer code requires more hardware resources than DRILLO1. Here, the largest arrays are 4-indices arrays whose size is the product of the maximum number of time values in the SOTEC radionuclide flux time history file, the maximum number of nuclides, the maximum length of the nuclide decay chain, and the maximum number of EBS regions (for further details refer to Section 3.8). Execution times range from minutes on VAXes to seconds on CRAYs and the disk files created are several kilobytes in size.

The primary source files are maintained as FORTRAN preprocessor input files. The preprocessor is called preFOR and is discussed in Section 3.4.1 of Sagar and Janetzke (1993). Once the preFOR files are copied to disk, an operating procedure may be written to automatically generate the executable files.

3.4 USER SUPPORT

For technical assistance, the user may contact either:

Mr. Ron Janetzke
Center for Nuclear Waste Regulatory Analyses
Southwest Research Institute
P. O. Drawer 28510
San Antonio, TX 78228-0510
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(210) 522-3318

- or -

Dr. Christopher J. Freitas
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e-mail: cfreitas@swri.edu
(210) 522-2137

3.5 CODE STRUCTURE

This section describes the purpose of each subroutine used in DRILLO1 and DRILLO2.

3.5.1 DRILLO1

DRILLO1 calculates the three parameters for the drilling scenario and provides the results of these calculations to DRILLO2 and other TPA consequence modules, as discussed previously. These three parameters are the time of the drilling event, the region of the repository into which the borehole penetrates, and whether or not a drill bit has hit a canister. Figure 3-1 displays the calling sequence of the subroutines that make up the DRILLO1 code. These subroutines are discussed in the following sections.

3.5.1.1 Subroutine RDENV

Subroutine RDENV reads in the data defining the geometry of the repository, the depth of the unsaturated layers underlying each EBS region, and two simulation parameters (i.e., the simulation duration in years and the radius of the waste canisters). Two input files are accessed by RDENV. These are DRILL1.IN and flowmod.inp. A sample DRILL1.IN file and a sample flowmod.inp file are given in Section 4.1.

3.5.1.2 Subroutine RDRUN

Subroutine RDRUN reads in the TPA input file TPA_DR1.DGD if DRILLO1 is being run as part of the TPA code. If DRILLO1 is being run in standalone mode, then subroutine RDRUN calculates a series of random numbers for the time of the drilling event, the region number for the borehole, and a hit indicator number for the borehole. These random numbers are generated for the Nbor boreholes. Also initialized at this point is the radius of the boreholes (a constant value for all boreholes), the duration of the simulation, and the number of canisters per EBS region.

The description of the TPA_DR1.DGD file is given in Section 3.3.15 of Sagar and Janetzke (1993) and in Section 4.1 of this report.

3.5.1.3 Subroutine RDMAP

Subroutine RDMAP reads in data from the LHS file and the parameter map file DR1MAP.DAT of the TPA Exec code. The DR1MAP.DAT file provides the location of sampled variables in the LHS file which are specific to DRILLO1. A description of the DR1MAP.DAT file is given in Section 4.1 of this report. The primary data read in are the number of drilling events, the radius of the boreholes, the time of the drilling events, the region number for each borehole, and the hit indicator for a given borehole.

3.5.1.4 Subroutine SETUP

Subroutine SETUP calculates the cross-sectional area of each EBS region and the total cross-sectional area of the EBS. If DRILLO1 is being run in TPA mode then the area data read from the FLOWMOD output file (read in by subroutine RDENV) are used here rather than those calculated. These area data are then normalized and cast in the form of a series of intervals, the total of these intervals equaling 1. Next, the region number of each borehole is determined. Then the probability of a canister hit is calculated for each EBS region. From this information, the hit register value is determined for each borehole. Now, all the key parameters for each borehole have been established; that is, the time of the drilling event, the EBS region of the drilling event, and whether a canister has been intersected.

3.5.1.5 Subroutine ECHO1

Subroutine ECHO1 prints out the initial input data for the EBS geometry and the RC depth. In addition, it prints out, for each borehole, the time of the drilling event (in years), the region indicator (a random number between 0 and 1), the region number (a number between 1 and 7), the hit indicator (a random number between 0 and 1), and the hit register (either 1 for a hit or 0 for a miss). Also, for each region of the EBS, the total number of canisters and the probability of a hit are output. All these data are written to the file drill1.out.

3.5.1.6 Subroutine SUM

Subroutine SUM determines the total number of canister hits per EBS region and then determines the earliest time at which one of these events occurred in a given EBS region.

3.5.1.7 Subroutine D2OUT

Subroutine D2OUT creates a data file which is then read as an input file by DRILLO2. The data file is named dr1dr2.dat. These data include for each borehole, the time of the drilling event, the region number, and the hit register value. Also included are data for each EBS region, which are the number of emplaced canisters, the depth of the unsaturated layer, and the zone cross-sectional area.

3.5.1.8 Subroutine SOTOUT

Subroutine SOTOUT creates a data file which is then read as an input file by SOTEC. The data file is named dr1sot.dat. These data include, for each EBS region, the total number of canister hits and the time of occurrence of the earliest drilling event in the region. These are the cumulative hit data for an EBS region.

3.5.1.9 Subroutine ECHO2

Subroutine ECHO2 writes the cumulative hit data for each EBS region to drill1.out.

3.5.1.10 Subroutine RAN1

Subroutine RAN1 is a random-number generator. RAN1 is used only in standalone mode. In TPA mode, the location of the random numbers are read from the MAP file and then the actual random number data read from the LHS input file. The subroutine used here comes from Numerical Recipes (Press et al., 1988) and returns a uniform random deviate between 0.0 and 1.0.

3.5.1.11 Subroutine DIST

Subroutine DIST computes the length of the sides of a polygon/panel which describes the surface area of the EBS regions. The distance between two points (x_1,y_1) and (x_2,y_2) is calculated as

$$\text{Distance} = SQRT\left[\left(x_2 - x_1\right)^2 + \left(y_2 - y_1\right)^2\right] \tag{3-1}$$

3.5.1.12 Subroutine DOT

Subroutine DOT computes the dot product of two vectors. The result of this calculation is used in the computation of the polygon areas.

3.5.1.13 Subroutine opnfil

Subroutine opnfil opens a formatted file on the unit specified with the attributes provided in the argument list. This subroutine first determines the availability of the requested unit and file. If either is already in use, then processing is terminated and control is returned to the calling routine. Otherwise, the desired operation is performed.

3.5.2 DRILLO2

DRILLO2 calculates the consequences of the drilling events predicted by DRILLO1 in which boreholes penetrate the repository and remove nuclide materials to the ground surface. DRILLO2 determines the inventories in the EBS region and the associated RC at the time of these drilling events. Based on this inventory, the amount of nuclide material released to the ground surface by each borehole is computed. Figure 3-2 displays the calling sequence of the subroutines that make up the DRILLO2 code.

3.5.2.1 Subroutine RDRUN

Subroutine RDRUN reads the input data file dr1dr2.dat, which is created by DRILLO1. This file contains information on the run mode (TPA or standalone), the duration of the simulation, the radius of the boreholes, the radius of the canisters, and the number of boreholes. Then, for each borehole, the time of the drilling event, the region number of the borehole, and the hit designator for the borehole are read in. Then, for each EBS region, the number of emplaced canisters, the depth of the unsaturated layer, and the cross-sectional area of each EBS region are read in.

3.5.2.2 Subroutine RDNUC

Subroutine RDNUC reads the initial radionuclide inventories from the data file dr2nuc.dat. These data are only used when DRILLO2 is run in standalone mode, otherwise these data are overwritten by similar data in the TPA_DR2.DGD data file. Contained in the dr2nuc.dat data file are the number of nuclide chains, the length of each chain, and, for each member of a nuclide chain, the name of the nuclide, its half-life, and its initial inventory on a per-canister basis.

3.5.2.3 Subroutine RDMOR

Subroutine RDMOR reads the sample run data file TPA_DR2.DGD, if the simulation is running in TPA mode. If the TPA_DR2.DGD file exists, then the names of three additional input files and one output file are read in. These files contain data from or for SOTEC, NEFTRAN, FLOWMOD, and AIRCOM. Additional data are also read in from the TPA_DR2.DGD file; that is, the vector number pointing to the correct location for sample data in the LHS input file, the duration of the simulation, the length of the waste canisters, the total number of emplaced canisters in the repository, the thousands of metric tons-heavy metals for the repository, the number of nuclide chains, the length of these nuclide chains, then for each member of the chain, the name of the nuclide, its total initial inventory (for the entire repository), and the nuclide half-lives. Based on the total inventory of nuclide (i,j) for the repository, the inventory per canister is calculated in this subroutine and is measured in curies per canister.

If TPA_DR2.DGD does not exist, then the three additional input filenames and one output filenames are defaulted to sotnef.dat, nefdr2.dat, flotpa.dat, and dr2air.dat, respectively. The vector number, the duration of the simulation, and the canister length are then defaulted to 1, 10,000, and 3, respectively.

3.5.2.4 Subroutine ECHO1

Subroutine ECHO1 prints out the initial input data to the file drill2.out. These data consist primarily of the borehole data, region data, and initial radionuclide inventory data per canister.

3.5.2.5 Subroutine EBS

Subroutine EBS computes the radionuclide inventory in the EBS region at the instant of a drilling event. As discussed in Section 2, the inventory of a nuclide in the EBS is a function of the decay rate of the nuclide and the transport of the nuclide out of the EBS region.

Subroutine EBS reads data from one supporting file. This file contains data from SOTEC, specifically data for the time history of the flux of nuclide (i,j) from the EBS region.

The calculation of the EBS inventory then proceeds by cycling through each borehole. If the borehole intersects a canister, then the inventory of nuclide (i,j) is solved for using the Bateman equation and accounting for flux from the EBS region. These inventories are then normalized by the number of canisters within the EBS region. It is this final per-canister inventory that is then calculated to be released by the drilling event and is stored in the variable $Q_{EBS}(i,j,k)$, where k is the borehole number.

3.5.2.6 Subroutine RC

Subroutine RC computes the radionuclide inventory in the RC region at the instant of a drilling event. As discussed in Section 2, the inventory of a nuclide in the RC is a function of the decay rate of the nuclide and the net transport of the nuclide in the RC region.

Subroutine RC reads data from two supporting files. The first file contains data from NEFTRAN, specifically, data for the time history of the concentration of nuclide (i,j) in the RC region. The second file contains data from FLOWMOD, specifically data for the magnitude of the groundwater flux through the RC region.

The calculation of the RC inventory then proceeds by cycling through each borehole. For each borehole, the inventory of nuclide (i,j) at the instant of the drilling event is solved for using the Bateman equation and accounting for flux into and out of the RC region. This then provides the total inventory of nuclide (i,j) in the RC region, and the released amount is calculated by scaling the total inventory by the ratio of the borehole cross-sectional area to the RC region cross-sectional area. These data are then stored in the variable Q_{RC} *(i,j,k)*, where *k* is the borehole number.

3.5.2.7 Subroutine DECAY

Subroutine DECAY solves the Bateman equations with the resulting inventory of time, initial inventory, nuclide half-life, the number of chains, and the number of members in the chain. The resulting inventory is then returned as the output of this routine.

3.5.2.8 Subroutine AIROUT

Subroutine AIROUT sums the releases due to all drilling events occurring during the simulation period and applies them at the time of the earliest drilling event. The releases are summed for each nuclide (*i,j*). These data are then output to a separate data file which is then read by AIRCOM.

3.5.2.9 Subroutine ECHO2

Subroutine ECHO2 writes the summary information on the inventory of each nuclide (*i,j*) (in the EBS and RC) at the instant of each drilling event to drill2.out.

3.5.2.10 Subroutine opnfil

Subroutine opnfil opens a formatted file on the unit specified with the attributes provided in the argument list. This subroutine first determines the availability of the requested unit and file. If either is already in use, processing is terminated and control is returned to the calling routine. Otherwise, the desired operation is performed.

3.6 INSTRUCTIONS FOR CODE MAINTENANCE

The program preFOR (Janetzke and Sagar, 1991) is a preprocessor for FORTRAN codes. It is designed to provide flexibility in developing and maintaining FORTRAN codes. Included in preFOR are various utility modules to find the length of strings, fix tabs, perform I/O, etc. When invoked, preFOR will prompt the user for an input filename. The input file is a FORTRAN source code in which preFOR commands have been embedded. The program will then prompt the user for an output filename. The output file produced by preFOR is a standard FORTRAN file that may be compiled. Details of the preFOR command set and its use are documented in Janetzke and Sagar (1991).

3.7 ARRAY SIZES IN DRILLO1

The arrays in the DRILLO1 computer code are sized based on five parameters: maxBor, maxP, maxZn, maxNd, and maxLy. All but two of the resulting arrays are single-index arrays (based on one of these parameters). One of the two array represents the polygons defining the surface area of the EBS regions [which has a size of (maxP,4,2)], and the other array represents the layer heights in the unsaturated layers in the RC [which has a size of (maxZn,maxLy)]. The five index parameters are defined:

maxBor	=	maximum number of boreholes
maxP	=	maximum number of panels or polygons describing the surface area of an EBS region
maxZn	=	maximum number of EBS regions
maxNd	=	maximum number of nodes describing the surface area of the entire repository
maxLy	=	maximum number of unsaturated layers in an RC region

3.8 ARRAY SIZES IN DRILLO2

The arrays in the DRILLO2 computer code are sized based on five parameters as well: maxBor, maxnuc, maxmem, maxtim, and maxZn. The resulting arrays are single index arrays (based on one of these parameters), double-index arrays (based on either the combination maxnuc, maxmem or maxtim, maxZn), triple index arrays (based on maxnuc, maxmem, or maxBor), and quadruple-index arrays (based on maxtim, maxnuc, maxmem, or maxZn). The five index parameters are defined as:

maxBor	=	maximum number of boreholes
maxnuc	=	maximum number of radionuclide chains
maxmem	=	maximum number of nuclide chain members
maxtim	=	maximum number of history data points
maxZn	=	maximum number of EBS regions

3.9 UNITS IN DRILLO

All units in DRILLO (DRILLO1 and DRILLO2) are metric [i.e., meter (length), kilogram (mass), and year (time)], except for radiation, which is in terms of curies, and initial radionuclide inventories, which are in metric tons-heavy metal (mthm).

4 INSTRUCTIONS FOR DATA INPUT

As already discussed, DRILLO may be run as a standalone program or as part of the TPA code. In either case, the analyst must create at least one input data file. Other input data files must also exist for proper operation of DRILLO; however, these additional data files are created by other TPA consequence modules or the TPA code itself.

The proper operational modes for DRILLO are:

(i) as part of the TPA code, in which DRILLO1 is executed using inputs from other TPA modules, then DRILLO2 is executed with inputs from DRILLO1 and other TPA modules

(ii) as a standalone program, in which DRILLO1 is executed using data files previously created by other TPA modules or the analyst, then DRILLO2 is executed with inputs from DRILLO1 and previously created files from other TPA modules or the analyst

(iii) as two standalone programs with the properly specified input data files

4.1 INPUT DATA FILES FOR DRILLO1

DRILLO1 requires as many as five different input data files. Only one of these files is created by the analyst; the remaining four are created by other TPA consequence modules or the TPA code itself.

4.1.1 Description of the drill1.in Input File

The drill1.in input file for DRILLO1 is created by the analyst. This data file is required for both standalone operation and TPA mode operation. It contains the following information:

Line 1:	Title
Line 2:	Simulation duration in years; variable name = StpT
Line 3:	Radius of the waste canisters in meters; variable name = RadCan
Line 4:	Descriptive header
Line 5:	Number of nodes describing repository area; variable name = NNODE
Line 6:	Descriptive header
Group 1:	Node number, x coordinate, y coordinate; variable names = N, X(i), Y(i)
Line 7:	Descriptive header
Line 8:	Number of panels describing repository area and number of repository zones; variable names = Nrect, Nzone
Line 9:	Descriptive header
Group 2:	Panel number, corner-one node number, corner-two node number, corner-three node number, corner-four node number, and zone number of panel; variable names = N, C(1), C(2), C(3), C(4), Zone(i)

Example of drill1.in data file:

INPUT FILE TO DRILLO1

```
10000.0 Duration of Simulation (years)
0.4 Radius of waste canisters (meters)
Coordinates of nodes used to build panel rectangles
43                    Number of nodes
   I          X           Y       (x,y in meters)
   1         0.0         0.0
   2       -36.8      -208.9
   3       -46.6      -264.1
   4      -111.1      -630.4
   5      -185.2     -1050.6
   6      -259.3     -1470.8
   7      -333.4     -1891.1
   .      ......      .......
   42       14.9     -3252.4
   43      -21.8     -3460.4
Node/Panel connectivity table
 17     7   Number of panels, number of zones
 I   C1   C2   C3  C4  Zone
 1   25    3   27  26   1
 2    3    4   29  28   1
 3    4    5   31  30   2
 4    5    6   33  32   3
 5    6    7   35  34   3
 6    7    8   37  36   3
..   ..   ..   ..  ..  ..
16  13    14    4   2   2
17  12    13    2   1   7
```

4.1.2 Description of the flowmod.inp Input File

The flowmod.inp data file is created by the FLOWMOD module of the TPA code and must be present for DRILLO1 to operate in either standalone or TPA modes. These data that are read from the flowmod.inp data file are the number of repository regions or zones, the number of unsaturated layers in the RC, the cross-section area of each region of the repository, and the depth of each unsaturated layer in the RC.

Example of flowmod.inp data file: (the boldface lines are read by DRILLO1)

THE TIME TO END THE SIMULATION IN YEARS

```
   1.0E4
NUMBER OF AREAS, MAX # OF LAYERS, AND MAX # OF UNSATURATED LAYERS
    7     7    7
INFILTRATION (M/YR)  FOR THIS REALIZATION
    1.0E-3
SATURATED GRADIENT FOR THIS REALIZATION (ZEROS INDICATE LAYERS NOT PRESENT)
  .0026   .0026   .0026   .0026   .0026    .0026    .0026
DISPERSION LENGTH (M) USED FOR ALL NEFTRAN LEGS
     10.0
THE NUMBER OF CHAINS AND THE NUMBER OF ISOTOPES
    2    5
THE NUMBER OF ISOTOPES PER CHAIN
  3    2
```

```
ISOTOPE INFORMATION - 3 LINES PER ISOTOPE
LN 1 NAME, AT# , P#1, P#1, FRC F1, FRC F2, INV(CI), HLIFE(Y), EPA WGT
LINE 2 MATRIX KDS (M**3/KG)  PER LAYER
LINE 3 FRACTURE RDS  PER LAYER
NP237  237   0    0   1.0   0.0     2.17E4     2.14E6     1.0
     .005     .005     .0027     .006     .003     .006     .003
     1.0      1.0      1.0      1.0      1.0      1.0      1.0
U233   233   1    0   1.0   0.0     2.66       1.62E5     1.0
     .002     .02     .005     0.0     .0015     .002     .0015
     1.0      1.0      1.0      1.0      1.0      1.0      1.0
TH229  229   2    0   1.0   0.0     1.96E-3    7.34E3     1.0
    .47     .18     .18     .18     .18     .34     .18
     1.0      1.0      1.0      1.0      1.0      1.0      1.0
PU240  240   0    0   0.0   0.0     3.15E7     6.[illegible]8E3     1.0
    .2     .2     .066     .15     .007     .1     .007
     1.0      1.0      1.0      1.0      1.0      1.0      1.0
U236   236   1    0   1.0   0.0     1.54E4     2.39E7     1.0
    .002     .02     .005     0.0     .0015     .002     .0015
     1.0      1.0      1.0      1.0      1.0      1.0      1.0
TOPO SPRING  PERM. (M**2), POR., BETA, & MAT GRN DENSITY(KG/M**3)
     1.94e-18    .11        1.8      2580.
     3.24e-16   1.1E-5        4.2
CAL HILLS VITRIC PERM. (M**2), POR, BETA, & MAT GRN DENS(KG/M**3)
     2.75E-14        .45       3.87     2370.
     9.72E-16       4.6E-5        4.2
CAL HILLS ZEO PERM. (M**2), POR, BETA, & MAT GRN DENS(KG/M**3)
    1.94E-18          .28         1.6        2230.
     9.72E-16        4.6E-5        4.2
PROW PASS PERM. (M**2), POR, BETA, & MAT GRN DENS(KG/M**3)
    4.53E-16          .24          2.64    2590.
    6.48E-17       1.3E-5        4.2
U. CRATER FLAT PERM. (M**2), POR, BETA, & MAT GRN DENS(KG/M**3)
   4.53E-18        .24          2.0       2270.
   9.72E-16      4.6E-5        4.2
BULL FROG  PERM. (M**2), POR, BETA, & MAT GRN DENS(KG/M**3)
    6.48E-17        .25        3.00      2630.
    6.48E-17      1.3E-5        4.2
M. CRATER FLAT PERM. (M**2), POR, BETA, & MAT GRN(KG/M**3)
   4.53E-18        .24          2.0       2270.
   9.72E-16      4.6E-5        4.2
********THIS INFORMATION USES BOREHOLE USW H5 *****PART #1
INLET AND OUTLET AREAS (SQUARE METERS) FOR AREA #1
  1.27E6     2.62E5
AREA #1 UNSATURATED LAYER LENGTHS (M)  - ZEROS INDICATE LAYERS NOT PRESENT
  60.      70.      40.      30.      60.      0.0      0.0
SATURATED LENGTHS (M)  -  ZEROS INDICATE LAYERS NOT PRESENT
  1500.   0.0   2000.   1250.   0.0   0.0   0.0
********THIS INFORMATION USES BOREHOLE USW G4 *****PART #2
INLET AND OUTLET AREAS (SQUARE METERS) FOR AREA #2
  1.44E6     2.62E5
AREA #2 UNSATURATED LAYER LENGTHS (M)  - ZEROS INDICATE LAYERS NOT PRESENT
  60.     0.0     130.     0.0     0.0     0.0     0.0
SATURATED LENGTHS (M)  -  ZEROS INDICATE LAYERS NOT PRESENT
  1500.   0.0   2000.   1250.   0.0   0.0   0.0
********THIS INFORMATION USES BOREHOLE UE 25 A#1 *****PART #3
INLET AND OUTLET AREAS (SQUARE METERS) FOR AREA #3
 1.48E5      2.62E5
AREA #3 UNSATURATED LAYER LENGTHS (M)  - ZEROS INDICATE LAYERS NOT PRESENT
  60.     0.0     70.     0.0     0.0     0.0     0.0
SATURATED LENGTHS (M)  -  ZEROS INDICATE LAYERS NOT PRESENT
  1500.   0.0   2000.   1250.   0.0   0.0   0.0
********THIS INFORMATION USES BOREHOLE USW G1 *****PART #4
```

```
INLET AND OUTLET AREAS (SQUARE METERS) FOR AREA #4
  2.18E5     2.62E5
AREA #4 UNSATURATED LAYER LENGTHS (M)  - ZEROS INDICATE LAYERS NOT PRESENT
   60.      20.      140.      0.0      0.0      0.0      0.0
SATURATED LENGTHS (M)  -  ZEROS INDICATE LAYERS NOT PRESENT
  1500.   0.0   2000.   1250.   0.0   0.0   0.0
********THIS INFORMATION USES BOREHOLE H6 *****PART #5
INLET AND OUTLET AREAS (SQUARE METERS) FOR AREA #5
  1.99E5     2.62E5
AREA #5 UNSATURATED LAYER LENGTHS (M)  - ZEROS INDICATE LAYERS NOT PRESENT
  60.      70.      0.0      60.0      0.0      0.0      0.0
SATURATED LENGTHS (M)  -  ZEROS INDICATE LAYERS NOT PRESENT
  1500.   0.0   2000.   1250.   0.0   0.0   0.0
********THIS INFORMATION USES BOREHOLE USW H3 *****PART #6
 INLET AND OUTLET AREAS (SQUARE METERS) FOR AREA #6
  7.86E5     2.62E5
AREA #6 UNSATURATED LAYER LENGTHS (M)  - ZEROS INDICATE LAYERS NOT PRESENT
   60.      140.      0.0      0.0      90.      100.      40.
SATURATED LENGTHS (M)  -  ZEROS INDICATE LAYERS NOT PRESENT
  1500.   0.0   2000.   1250.   0.0   0.0   0.0
********THIS INFORMATION USES BOREHOLE USW H4 *****PART #7
INLET AND OUTLET AREAS (SQUARE METERS) FOR AREA #7
  1.34E6     2.62E5
AREA #7 UNSATURATED LAYER LENGTHS (M)  - ZEROS INDICATE LAYERS NOT PRESENT
  60.      30.      100.      20.      0.0      0.0      0.0
SATURATED LENGTHS (M)  -  ZEROS INDICATE LAYERS NOT PRESENT
  1500.   0.0   2000.   1250.   0.0   0.0   0.0
```

4.1.3 Description of the TPA_DR1.DGD Input File

If the DRILLO1 computer code is run in TPA mode, then the input file TPA_DR1.DGD must exist. This data file is created and maintained by the TPA code. If this data file does not exist, then the DRILLO1 code defaults to standalone execution mode. Global data read from this file are as follows:

Line 1: Title
Line 2: LHS output filename
Line 3: LHS map filename
Line 4: Current vector number; variable name = Vnum
Line 5: Simulation duration; variable name = StpT
Line 6: Number of repository zones; variable name = Nzone
Line 7: Radius of waste canisters; variable name = RadCan
Line 8: Number of waste canisters in each repository zone; variable name = CANPZ(i)

Example of TPA_DR1.DGD file:

GLOBAL PARAMETERS FOR DRILLO

```
lhscn1.out
dr1map.dat
1
10000.0
7
0.4
2335   6150   4875   3675   1275   5625   1073
```

4.1.4 Description of the dr1map.dat Input File

The dr1map.dat input file is only required by DRILLO1 when executing in TPA mode. This data file is created and maintained by the analyst who is running the TPA code. The location of sampled parameters specific to DRILLO1 are contained in this file. The VAR column gives the variable name for the sampled parameter. The INDEX column gives the starting address for the variable in the LHS file, and COUNT gives the number of quantities to be read. Complete details of the purpose and implementation of this data file may be found in Sagar and Janetzke (1993). The data contained in the dr1map.dat file are:

Line 1: Title
Line 2: Descriptive header
Line 3: Pointer to the number of boreholes; variable name = Nbor; and number of data points to be read.
Line 4: Pointer to the radius of the boreholes; variable name = radius; and number of data points to be read.
Line 5: Pointer to the set of region numbers; variable name = Regn(i); and number of data points to be read.
Line 6: Pointer to the set of time data for borehole events; variable name = Td(i); and number of data points to be read.
Line 7: Pointer to the set of hit indicators for boreholes; variable name = hit(i); and number of data points to be read.

Example of dr1map.dat file:

DRILLO1 MAP FILE

```
VAR     INDEX   COUNT
Nbor     289      1
radius   290      1
Regn     291     30
Td       321     30
hit      351     30
```

4.1.5 Description of the LHS Input File

The LHS input file is required only when DRILLO1 is run in TPA mode. A complete description of the LHS input file is given in Sagar and Janetzke (1993).

4.2 INPUT DATA FILES FOR DRILLO2

The DRILLO2 computer code requires five different input data files when it is functioning as a standalone program, and it requires six different input data files when it is functioning as part of the TPA code.

4.2.1 Description of the dr1dr2.dat Input File

The dr1dr2.dat data file is normally created by the DRILLO1 code; however, this file may also be created by the analyst if DRILLO2 is being run independently of all other TPA modules. The dr1dr2.dat file contains all of the control parameters for the DRILLO2 simulation. The specific contents of this file are:

Line 1:	Title
Line 2:	Determines whether this is a TPA mode simulation; variable name = TPAmode (is either T or F)
Line 3:	Duration of simulation; variable name = StpT
Line 4:	Radius of boreholes; variable name = radius
Line 5:	Radius of waste canisters; variable name = RadCan
Line 6:	Number of boreholes or drilling events; variable name = Nbor
Line 7:	Descriptive header
Group 1:	Borehole number, time of the drilling event, region number of the borehole, and the hit indicator for the borehole; variable names = n, Td(i), R(i), H(i)
Line 8:	Number of repository regions; variable name = Nzone
Line 9:	Descriptive header
Group 2:	Region number, number of waste canister in region, depth of the unsaturated layer beneath the EBS region, and the cross-sectional area of the repository region; variable names = n, CANPZ(i), TOTRCH(i), Zarea(i)

Example of dr1dr2.dat file:

```
BORE HOLE INFORMATION FROM DRILLO1 TO DRILLO2

                    F : TPA mode?
     10000.00 : Simulation stop time
                               0.10 : Radius of boreholes
                               0.40 : Radius of waste canisters
                                 10 : Number of bore holes
  borehole #    time of drill   Region #    hit #
       1          2841.3           1           0
       2          6087.9           3           1
       3          6669.0           6           0
       4          1387.2           4           1
       5           911.9           2           1
       6          2908.5           2           0
       7          1911.9           3           0
       8          3592.2           3           0
       9          3029.1           3           1
      10          4846.5           2           0
                     7 : Number of Repository Zones
  zone #    # of canisters   Unsaturated Depth       Zone Area
    1          4000.0000            260.0000         404596.0313
    2          4000.0000            190.0000        1398660.6250
    3          4000.0000            130.0000        1127967.8750
    4          4000.0000            220.0000         749432.7500
    5          4000.0000            190.0000         296395.2500
    6          4000.0000            430.0000        1281494.2500
    7          4000.0000            210.0000         245109.8750
```

4.2.2 Description of the dr2nuc.dat Input File

The dr2nuc.dat data file is required in all modes of use of DRILLO2; however, its contents are only used when DRILLO2 is run in standalone mode. This data file contains the names of the radionuclides, their half-lives, and their initial inventories. This file represents an analyst-created data set. The contents of the file are:

Line 1: Title
Line 2: The number of radionuclide chains and the length of each chain; variable names = NCHNS, NI(i)
Group 1: Radionuclide name, half-life in years, and initial inventory per canister in curies; variable names = NAMALL(i,j), HLFALL(i,j), Io(i,j). These data have an input format of (A6, 1X, e10.2, 1X, e10.2)

Example of dr2nuc.dat file:

ISOTOPE DATA: NAME, HALFLIFE (YEARS), INITIAL INVENTORY PER CANISTER (CURIES)

```
16  4   5   3   2   5   1   1   1   1   1   1   1   1   1   1
CM246    5.50E+03    6.55E-02
PU242    3.79E+05    3.61E+00
U238     4.51E+09    6.66E-01
.....    ........    ........
C14      5.73E+03    3.26E+00
SE79     6.49E+04    8.50E-01
NB94     2.03E+04    2.69E+00
```

4.3 DESCRIPTION OF THE TPA_DR2.DGD INPUT FILE

If the DRILLO2 computer code is run in TPA mode, then the input file TPA_DR2.DGD must exist. This data file is created and maintained by the TPA code. If this data file does not exist, then the DRILLO2 code defaults to standalone execution mode. Global data read from this file are as follows:

Line 1: Title
Line 2: Name of the input file created by SOTEC
Line 3: Name of the input file created by NEFTRAN
Line 4: Name of the input file created by FLOWMOD
Line 5: Name of the output file created by DRILLO2 for input to AIRCOM
Line 6: Vector number for the sample data
Line 7: Duration of the simulation; variable name = StpT
Line 8: Length of the waste canisters; variable name = CanL
Line 9: Total number of waste canisters in the entire repository; variable name = totcan
Line 10: Unit conversion factor in kilometric tons-heavy metal; variable name = kmthm
Line 11: Number of radionuclide chains; variable name = nchns
Group 1: The length of each chain; variable name = ni(i)
Group 2: Radionuclide name; variable name = namall(i,j)

Group 3: Initial inventory of nuclide (i,j) in entire repository in units of curies / kilometric tons-heavy metal; variable name = Io(i,j)

Group 4: Half-life in years for each nuclide (i,j); variable name = hlfall(i,j)

Example of TPA_DR2.DGD file:

TITLE: TPA temporary file for DRILLO2 global parameters.

```
sotnef.dat
nefdr2.dat
flotpa.dat
dr2air.dat
          1
  10080.0
  0.4700000E+01
  25008.0
     70.0
       16
        4         5         3         2         5         1         1         1
        1         1         1         1         1         1         1         1
  CM246 , PU242 , U238  , U234  , CM245 ,
  AM241 , NP237 , U233  , TH229 , AM243 ,
  PU239 , U235  , PU240 , U236  , PU238 ,
  U234  , TH230 , RA226 , PB210 , CS137 ,
  CS135 , I129  , SN126 , TC99  , ZR93  ,
  SR90  , NI59  , C14   , SE79  , NB94  ,
  0.258E-01  0.160E+01  0.318E+00  0.113E+01  0.126E+00  0.164E+04  0.288E+00
0.254E-04  0.140E-06
  0.155E+02  0.308E+03  0.168E-01  0.508E+03  0.240E+00  0.212E+04  0.113E+01
0.129E-03  0.367E-06
  0.471E-07  0.766E+05  0.350E+00  0.295E-01  0.717E+00  0.123E+02  0.188E+01
0.532E+05  0.356E+01
  0.154E+01  0.381E+00  0.793E+00
  0.473E+04  0.379E+06  0.447E+10  0.240E+06  0.850E+04  0.432E+03  0.214E+07
0.159E+06  0.734E+04
  0.738E+04  0.241E+05  0.704E+09  0.654E+04  0.234E+08  0.877E+02  0.245E+06
0.770E+05  0.160E+04
  0.223E+02  0.300E+02  0.230E+07  0.157E+08  0.100E+06  0.213E+06  0.153E+07
0.291E+02  0.800E+05
  0.573E+04  0.650E+05  0.203E+05
```

4.3.1 Description of the Input File from SOTEC

DRILLO2 requires a data input file that contains information on the release rates from the EBS of radionuclide (*i,j*) at discrete times. SOTEC creates this data file. The file may have an arbitrary name; however, this name must be input to DRILLO2 through the TPA_DR2.DGD file if DRILLO2 is run in TPA mode. Otherwise, this file has a default name of sotnef.dat. The data read in from this file are as follows:

Line 1: Title

Line 2: EBS zone number for which data applies; variable name = IZONUM

Line 3: Number of radionuclides for which data exists, and the number of time steps for the history of releases; variable name = NNBNUC, NTNDF

The following lines are then repeated for each radionuclide:

Line 4: Radionuclide name; variable name = NUCNAM
Group 1: Time of release (in years), and magnitude of release of radionuclide (i,j) in curies/year; variable name = Tnode (l,m), Flux(l,i,j,m)

Lines 1 through 4 and Group 1 are repeated for each zone of the EBS.

Example of SOTEC data file:

```
TITLE: Release rates from SOTEC to NEFTRAN.
        1   is the cell number
       30         250 um nucs, num bins
CM246
      10.000    0.4056539E-03
      50.000    0.4056539E-03
      90.000    0.4056539E-03
     130.000    0.4056539E-03
  ..........    .............
    9890.000    0.4529808E-03
    9930.000    0.4518717E-03
    9970.000    0.4507493E-03
PU242
      10.000    0.2541397E-11
      50.000    0.2541397E-11
      90.000    0.2541397E-11
     130.000    0.2541397E-11
     170.000    0.2541397E-11
     210.000    0.2541397E-11
     .......    .............
```

4.3.2 Description of the Input File from NEFTRAN

DRILLO2 requires a data input file that contains information on the concentration in an RC region of radionuclide (*i,j*) at discrete times. NEFTRAN creates this data file. The file may have an arbitrary name; however, this name must be input to DRILLO2 through the TPA_DR2.DGD file if DRILLO2 is run in TPA mode. Otherwise, this file has a default name of nefdr2.dat. The data read in from this file are as follows:

Line 1: Title
Line 2: RC zone number for which data applies; variable name = IZONUM
Line 3: Number of radionuclides for which data exists; variable name = NNBNUC

The following set of data is read for each radionuclide:

Line 4: Radionuclide name and number of discrete times for concentration data; variable names = NUCNAM, NTNDG
Group 1: Time of release (in years), and magnitude of concentration of radionuclide (i,j) in curies/m^3; variable name = TnodeG (l,m), CCC(l,i,j,m)

Lines 1 through 4 and Group 1 are repeated for each zone of the RC.

Example of NEFTRAN data file:

TITLE: Transfer file for concentrations from NEFTRAN to DRILLO2.

```
    1 Area number.
    5 Number of nuclides.
NP237       50
0.2000E+03 0.0000E+00
0.6000E+03 0.1357E-02
.......... ..........
0.9800E+04 0.1324E-02
0.1000E+05 0.0000E+00
U233        50
0.2000E+03 0.0000E+00
0.4000E+03 0.1868E-05
0.6000E+03 0.4525E-05
.......... ..........
```

4.3.3 Description of the Input File from FLOWMOD

DRILLO2 requires a data input file that contains information on the rate of groundwater flux from a RC region. FLOWMOD creates this data file. The file may have an arbitrary name; however, this name must be input to DRILLO2 through the TPA_DR2.DGD file if DRILLO2 is run in TPA mode. Otherwise, this file has a default name of flotpa.dat. The pertinent data read in from this file are: the sample vector number, the number of RC regions, the number of flow paths in each RC region, and the magnitude of the groundwater flux in a RC region in units of m^3/year.

Example of FLOWMOD data file (boldface lines are read by DRILLO2):

TITLE: Data transfer file for GWTT and FLUX from FLOWMOD to TPA and DRILLO2.

```
          1 Vector.
          7  Number of parts.
          4           4           4           4           2
          4
         24 Total number of paths for repository.
GWTT FOR REPOSITORY PART #    INFILTRATION IS M/YR
          1                     0.600E-03
SHORTEST(YRS), MOST FLUX, AVERAGE, AND FLUX NORMALIZED
      0.306E+05       0.648E+05       0.477E+05       0.602E+05
GWTT FOR REPOSITORY PART #    INFILTRATION IS M/YR
          2                     0.800E-03
SHORTEST(YRS), MOST FLUX, AVERAGE, AND FLUX NORMALIZED
       0.497E+03       0.779E+05       0.392E+05       0.542E+05
GWTT FOR REPOSITORY PART #    INFILTRATION IS M/YR
          3                     0.125E-02
SHORTEST(YRS), MOST FLUX, AVERAGE, AND FLUX NORMALIZED
      0.495E+03       0.495E+03       0.238E+05       0.?15E+05
GWTT FOR REPOSITORY PART #    INFILTRATION IS M/YR
          4                     0.600E-03
SHORTEST(YRS), MOST FLUX, AVERAGE, AND FLUX NORMALIZED
      0.155E+04       0.903E+05       0.459E+05       0.779E+05
```

```
GWTT FOR REPOSITORY PART #    INFILTRATION IS M/YR
        5                        0.600E-03
SHORTEST(YRS), MOST FLUX, AVERAGE, AND FLUX NORMALIZED
     0.114E+05      0.238E+05      0.176E+05      0.224E+05
GWTT FOR REPOSITORY PART #    INFILTRATION IS M/YR
        6                        0.600E-03
SHORTEST(YRS), MOST FLUX, AVERAGE, AND FLUX NORMALIZED
     0.760E+05      0.884E+05      0.822E+05      0.870E+05
GWTT FOR REPOSITORY PART #    INFILTRATION IS M/YR
        7                        0.800E-03
SHORTEST(YRS), MOST FLUX, AVERAGE, AND FLUX NORMALIZED
     0.360E+04      0.658E+05      0.347E+05      0.468E+05
TOTAL
     0.495E+03      0.238E+05      0.416E+05      0.488E+05
```

5 DESCRIPTION OF OUTPUT DATA FILES

DRILLO creates two types of output files; that is, one for user diagnostics and information and one for input to other TPA modules.

5.1 OUTPUT DATA FILES FROM DRILLO1

DRILLO1 creates a user diagnostics and information file called drill1.out. In addition, DRILLO1 creates two output files for use by other TPA code modules. One file, dr1dr2.dat, is created for DRILLO2; and is described in Section 4.2.1 of this report. The other file, dr1sot.dat, is created for SOTEC.

Example of output file dr1sot.dat created by DRILLO1 for SOTEC:

CANISTER HIT DATA FROM DRILL1 TO SOTEC

```
    7
 zone    # cans  time of hit
   1         0           0.0
   2         0           0.0
   3         0           0.0
   4         0           0.0
   5         0           0.0
   6         0           0.0
   7         1           0.0
```

Example of user diagnostics and information file drill1.out:

ECHO OUTPUT FROM DRILLO1 PROGRAM

```
     Nrect =    17

i zone   x1        y1        x2        y2        x3       y3        x4      y4

1   1   -10.9     -61.8     -46.6     -264.1    527.9    -365.5    563.6   -163.1
2   1   -46.6     -264.1    -111.1    -630.4    642.9    -763.3    707.4   -397.1
3   2   -111.1    -630.4    -185.2    -1050.6   763.6    -1217.9   837.7   -797.7
4   3   -185.2    -1050.6   -259.3    -1470.8   727.3    -1644.8   801.4   -1224.6
5   3   -259.3    -1470.8   -333.4    -1891.1   577.6    -2051.7   651.7   -1631.5
6   3   -333.4    -1891.1   -407.5    -2311.3   298.2    -2435.7   372.3   -2015.5
7   4   -407.5    -2311.3   -481.6    -2731.5   51.2     -2825.5   125.3   -2405.3
8   4   -481.6    -2731.5   -555.7    -3151.8   -60.8    -3239.1   13.3    -2818.8
9   4   -555.7    -3151.8   -592.4    -3359.8   -21.8    -3460.4   14.9    -3252.4
10  4   -901.0    -2657.6   -975.1    -3077.8   -555.7   -3151.8   -481.6  -2731.5
11  5   -1091.6   -2190.7   -1165.7   -2610.9   -481.6   -2731.5   -407.5  -2311.3
12  6   -1168.8   -1743.8   -1242.9   -2164.0   -407.5   -2311.3   -333.4  -1891.1
13  6   -1243.3   -1297.3   -1317.4   -1717.6   -333.4   -1891.1   -259.3  -1470.8
14  6   -1323.2   -849.9    -1397.3   -1270.2   -259.3   -1470.8   -185.2  -1050.6
15  2   -1249.1   -429.7    -1323.2   -849.9    -185.2   -1050.6   -111.1  -630.4
16  2   -1174.8   -8.3      -1249.1   -429.7    -111.1   -630.4    -36.8   -208.9
17  7   -1137.9   200.6     -1174.8   -8.3      -36.8    -208.9    0.0     0.0
               T : TPA mode?
     lhscnl.out                                                       : LHS filename
     dr1map.dat                                                       : MAP filename
               1 : lhs vector number
        10000.00 : Simulation stop time
```

0.17 : Radius of boreholes
0.33 : Radius of waste canisters
1 : Number of bore holes

borehole #	time of drill	Region value	Region #	hit value	hit #
1	0.0	0.9946465	7	0.0000000	1

7 : Number of Unsaturated Layers in RC

zone #	layer #	layer heights
1	1	60.000
	2	70.000
	3	40.000
	4	30.000
	5	60.000
	6	0.000
	7	0.000
2	1	60.000
	2	0.000
	3	130.000
	4	0.000
	5	0.000
	6	0.000
	7	0.000
3	1	60.000
	2	0.000
	3	70.000
	4	0.000
	5	0.000
	6	0.000
	7	0.000
4	1	60.000
	2	20.000
	3	140.000
	4	0.000
	5	0.000
	6	0.000
	7	0.000
5	1	60.000
	2	70.000
	3	0.000
	4	60.000
	5	0.000
	6	0.000
	7	0.000
6	1	60.000
	2	140.000
	3	0.000
	4	0.000
	5	90.000
	6	100.000
	7	40.000
7	1	60.000
	2	30.000
	3	100.000
	4	20.000
	5	0.000
	6	0.000
	7	0.000

Number of Canisters per Repository Zone

zone #	number of canisters	probability
1	10000.00	0.00609796
2	20000.00	0.01075613
3	30000.00	0.15698132
4	40000.00	0.14209929
5	50000.00	0.19458319
6	60000.00	0.05911765
7	70000.00	0.04045588

CUMULATIVE HIT RESULTS

zone	# cans	time of hit
1	0	0.0
2	0	0.0
3	0	0.0
4	0	0.0
5	0	0.0
6	0	0.0
7	1	0.0

5.2 OUTPUT DATA FILES FROM DRILLO2

DRILLO2 creates a user diagnostics and information file called drill2.out. In addition, DRILLO2 creates one output file for use by another TPA code module. This file, dr2air.dat, is created for use by DITTY.

Example of output file dr2air.dat created by DRILLO2 for AIRCOM:

ACTIVITY RELEASE DATA FROM DRILLO2

```
    30
CM246
    5
          0.0       0.0
         -1.0       0.0
          0.0       0.1916500E-01
          1.0       0.0
      10080.0       0.0
PU242
    5
          0.0       0.0
         -1.0       0.0
          0.0       0.1188527E+01
          1.0       0.0
      10080.0       0.0
U238
    5
          0.0       0.0
         -1.0       0.0
          0.0       0.2362197E+00
          1.0       0.0
      10080.0       0.0
U234
    5
          0.0       0.0
         -1.0       0.0
```

```
        0.0      0.8393971E+00
        1.0      0.0
    10080.0      0.0
...  .......      ...............
...  .......      ...............
SE79
   5
        0.0      0.0
       -1.0      0.0
        0.0      0.2830180E+00
        1.0      0.0
    10080.0      0.0
NB94
    5
        0.0      0.0
       -1.0      0.0
        0.0      0.5890636E+00
        1.0      0.0
    10080.0      0.0
```

Example of user diagnostics and information file drill2.out:

```
ECHO OUTPUT FROM DRILLO2 PROGRAM

          T : TPA mode?
sotnef.dat                                        : SOTEC Data File
nefdr2.dat                                      : NEFTRAN Data File
flotpa.dat                                      : FLOWMOD Data File
dr2air.dat                                       : DITTY Input File
          1 : lhs vector number
   10080.00 : Simulation stop time
       0.17 : Radius of boreholes
       0.33 : Radius of waste canisters
       4.70 : Length of waste canisters

          1 : Number of bore holes

      borehole #    time of drill    Region #      hit #

       1               0.0             7             1

            7 : Number of repository zones

       zone #     # of canisters    unsat. layer depth     zone area

        1           10000.00              260.0000        1270000.0000
        2           20000.00              190.0000        1440000.0000
        3           30000.00              130.0000         148000.0000
        4           40000.00              220.0000         218000.0000
        5           50000.00              190.0000         199000.0000
        6           60000.00              430.0000         786000.0000
        7           70000.00              210.0000        1340000.0000

      Initial Inventories per Canister

      Chain #          Name            Inventory
          1            CM246           0.072216898
          1            PU242           4.478566647
          1            U238            0.890115082
```

1	U234	3.162987947
2	CM245	0.352687150
2	AM241	4590.531250000
2	NP237	0.806142032
2	U233	0.000071097
2	TH229	0.000000392
3	AM243	43.386116028
3	PU239	862.124145508
3	U235	0.047024950
4	PU240	1421.944946289
4	U236	0.671785057
5	PU238	5934.101074219
5	U234	3.162987947
5	TH230	0.000361084
5	RA226	0.000001027
5	PB210	0.000000132
6	CS137	214411.390625000
7	CS135	0.979686499
8	I129	0.082573578
9	SN126	2.006958008
10	TC99	34.428981781
11	ZR93	5.262316227
12	SR90	148912.343750000
13	NI59	9.964811325
14	C14	4.310620308
15	SE79	1.066458702
16	NB94	2.219689608

EBS INVENTORY

FIRST BOREHOLE OCCURRED AT TIME = 0.0

Borehole = 1 Time of hit = 0.0 Zone = 7

CM246	PU242	U238	U234	
0.191650E-01	0.118853E+01	0.236220E+00	0.839397E+00	
CM245	AM241	NP237	U233	TH229
0.935965E-01	0.121824E+04	0.213935E+00	0.873794E-05	0.171737E-06
AM243	PU239	U235		
0.115139E+02	0.228791E+03	0.124795E-01		
PU240	U236			
0.377357E+03	0.178279E+00			
PU238	U234	TH230	RA226	PB210
0.157480E+04	0.839397E+00	0.958250E-04	0.296193E-07	0.396761E-07
CS137				
0.569007E+05				
CS135				
0.259990E+00				
I129				
0.219135E-01				
SN126				
0.532609E+00				
TC99				
0.913680E+01				
ZR93				
0.139652E+01				
SR90				
0.395185E+05				
NI59				
0.264447E+01				
C14				
0.114396E+01				

```
  SE79
0.283018E+00
  NB94
0.589064E+00

 RC INVENTORY

 FIRST BOREHOLE OCCURRED AT TIME =            0.0

 Borehole =  1   Time of drilling =   0.0   Zone =  7
  CM246           PU242          U238           U234
0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
  CM245           AM241          NP237          U233           TH229
0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
  AM243           PU239          U235
0.000000E+00   0.000000E+00   0.000000E+00
  PU240           U236
0.000000E+00   0.000000E+00
  PU238           U234           TH230          RA226          PB210
 0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
  CS137
0.000000E+00
  CS135
0.000000E+00
  I129
0.000000E+00
  SN126
0.000000E+00
  TC99
0.000000E+00
  ZR93
0.000000E+00
  SR90
0.000000E+00
  NI59
0.000000E+00
  C14
0.000000E+00
  SE79
0.000000E+00
  NB94
0.000000E+00
```

6 VERIFICATION, BENCHMARKING, AND VALIDATION STATUS

The DRILLO codes were verified through a line-by-line analysis and through a debugging step in which the codes were executed line-by-line in a symbolic debugger. The output data were verified for a range of input parameters. The DRILLO codes are managed under procedures set out in the CNWRA Technical Operating Procedure (TOP)-018. The production of this user's manual is one of the requirements of TOP-018. No known codes are suitable for benchmarking the DRILLO codes. Because of the nature of the processes simulated (i.e., both stochastic and occurring over long time periods), validation by comparison to data is not possible.

7 REFERENCES

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APPENDIX A

ERROR MESSAGES

ERROR MESSAGES

A.1 ERROR MESSAGES FROM DRILLO1

Number of zones does not agree with flowmod.inp file
DRILLO1 could not find unsaturated layer data in file flowmod.inp for zone, zone number
DRILLO1 could not find LHS file
DRILLO1 could not find MAP file
VECTOR Number is different in files TPA_DR1.DGD and, LHS filename

A.2 ERROR MESSAGES FROM DRILLO2

Number of repository zones is different in files dr1dr2.dat and, SOTEC filename
DRILLO2 could not match isotope names between files dr2nuc.dat and, SOTEC filename
DRILLO2 could not match isotope names between files dr2nuc.dat and NEFTRAN filename
Number of repository zones is different in files dr1dr2.dat and FLOWMOD filename
DRILLO2 could not find vector number, vector number, in file, FLOWMOD filename
DRILLO2 could not find a time interval for TnodeG in the TnodeF data

Common to both DRILLO1 and DRILLO2 are error messages written by subroutine opnfil, which opens all input/output data files. These error messages are:

OPEN OPERATION INCOMPLETE. CHECK opnfil SOURCE CODE.
Unit is open. Use of OPNFIL requires a closed unit.
File is in use, probably on another unit or by another user.
Requested READ file was not found.
NEW file creation blocked by existing file.
File status request is not valid.