BLT-MS (Breach, Leach, and Transport-Multiple Species) DATA INPUT GUIDE

A COMPUTER MODEL FOR SIMULATING RELEASE OF CONTAMINANTS FROM A SUBSURFACE LOW-LEVEL WASTE DISPOSAL FACILITY

Manuscript Completed: November 1996
Date Published: November 1996

Prepared by
T. M. Sullivan, R. J. MacKinnon,* R. R. Kinsey,
A. Aronson, M. Divadeenam

Brookhaven National Laboratory
P.O. Box 5000
Upton, NY 11973

*Ecodynamics Research Associates, Inc.
P.O. Box 9229
Albuquerque, NM 87103

R. E. Cady, NRC Project Manager

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Prepared for
Division of Regulatory Applications
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001
NRC Job Code A3276

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ABSTRACT

The BLT-MS computer code has been developed, implemented, and tested. BLT-MS is a two-dimensional finite element computer code capable of simulating the time evolution of concentration resulting from the time-dependent release and transport of aqueous phase species in a subsurface soil system. BLT-MS contains models to simulate the processes (water flow, container degradation, waste form performance, transport, and radioactive production and decay) most relevant to estimating the release and transport of contaminants from a subsurface disposal system. Water flow is simulated through tabular input or auxiliary files. Container degradation considers localized failure due to pitting corrosion and general failure due to uniform surface degradation processes. Waste form performance considers release to be limited by one of four mechanisms: rinse with partitioning, diffusion, uniform surface degradation, or solubility. Radioactive production and decay in the waste form are simulated. Transport considers the processes of advection, dispersion, diffusion, radioactive production and decay, reversible linear sorption, and sources (waste forms releases). To improve the usefulness of BLT-MS a pre-processor, BLTMSIN, which assists in the creation of input files, and a post-processor, BLTPLOT, which provides a visual display of the data have been developed. This document reviews the models implemented in BLT-MS and serves as a guide to creating input files for BLT-MS.

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EXECUTIVE SUMMARY

The objective of the source term evaluation project is to provide a suite of models capable of predicting radionuclide release rates from low-level radioactive waste disposal facilities. Six models have been produced thus far under this program. These models all simulate container performance, waste form performance, and advective-dispersive transport in porous media. Two of these models, DUST (Disposal Unit Source Term) [Sullivan, 1993] and BLT (Breach, Leach, and Transport) [Sullivan and Suen, 1989] are single-species, single-solute codes. DUST is a one-dimensional finite-difference model which was developed to permit rapid simulation of a large number of simple cases and is extremely useful for screening studies to determine, for example, the radionuclide released from the facility at the highest rate. BLT is a two-dimensional finite-element model designed to permit more detailed analyses taking into account the effects of geometry and material anisotropy due to different facility designs and hydrogeologic conditions. A third model GETAR (Gas Evolution Transport and Reaction) [Yim, 1994] was developed to examine release of gas phase contaminants, e.g., ^{14}C , ^3H , ^{222}Rn . It is a one-dimensional, multiple solute code capable of analyzing production of gases due to biodegradation and their subsequent transport out of the disposal facility.

Although DUST and BLT are applicable to a wide range of LLW performance assessment problems, they can only calculate the release and aqueous phase transport of a single chemical species during a simulation. In some applications, this limitation precludes adequate assessment of potentially important processes of radioactive production due to decay and geochemical interactions between the various radionuclides, chemicals in the aqueous phase, and the surrounding porous media. To better address these problems, DUST and BLT have been extended to include sequential and branched chain decay wherein a parent may produce two progeny radionuclides. The resulting codes are DUST-MS (Disposal Unit Source Term - Multiple Species) and BLT-MS (Breach, Leach, and Transport - Multiple Species). To address geochemical interactions, BLT-EC (Breach, Leach, and Transport - Equilibrium Chemistry) has been developed [MacKinnon, et al., 1995]. Further documentation of BLT-EC including guidance on how to use the code will be discussed in a subsequent document.

The objective of this document is to provide the necessary information to understand and apply the BLT-MS code to problems in subsurface disposal of wastes. BLT-MS is a two-dimensional finite element computer code capable of simulating the time evolution of concentration resulting from the time-dependent release and transport of aqueous phase species in a subsurface soil system. It has the following features:

- Container degradation models; BLT-MS simulates local corrosion (only a small fraction of the container area is breached) and general corrosion (entire container is assumed to fail when corrosion thickness reaches the corrosion allowance). BLT-MS permits simulation of multiple containers (currently dimensioned as 100) with up to 20 different sets of container failure parameters. This permits an easy method to simulate the different failure times expected from the different containers.
- Waste form leaching models; BLT-MS simulates four processes that can control release from the waste form. The processes are: surface rinse upon contact with water subject to equilibrium partitioning, diffusion, uniform degradation, and solubility limited release. BLT-MS simulates one waste form for each container, multiple (currently dimensioned as 20) waste form release parameters are allowed. In addition each waste form may have a unique inventory. This allows a method to simulate the range of waste forms that may potentially occur in disposal.
- Radionuclide transport model; BLT-MS considers advection, dispersion, diffusion, radioactive decay and production, equilibrium chemical partitioning, waste form sources, and external sources and sinks.
- Simulation of up to 10 radionuclides during the calculation each with unique waste form release and transport properties.
- Simulation of chain decay with branching in the waste form prior to release and during transport.

BLT-MS, in addition to the capability of simulating multiple species and radioactive ingrowth within a single simulation, has a number of other improvements over its predecessor, BLT. These include:

- a pre-processor, BLTMSIN, which guides the user through creating an input file,
- improved treatment of how the sources are incorporated into the transport equation,
- improved treatment of the rinse release model with partitioning,
- improved treatment of the uniform degradation model,
- improved methods of specifying the finite element geometry, and
- improved post-processor, BLTPLOT, which can be used to visualize the data and generate a paper copy .

This report provides:

- the theory and governing equations used to simulate release from the waste form and transport in the porous media.
- the results of a number of verification studies that demonstrate BLT-MS is capable of accurately predicting transport with chain decay, and ingrowth of progeny in the waste form prior to release.
- a detailed discussion of the input requirements and formatting requirements.
- an overview on how to use BLTMSIN, a menu-driven pre-processor that is useful in creating input files used by BLT-MS.
- a discussion of the output files generated by BLT-MS.
- information on the use of BLTPLOT a menu-driven post-processor that is capable of generating a graphical or hard copy display of the information generated by BLT-MS.

1 INTRODUCTION

1.1 Background

The U.S. Nuclear Regulatory Commission (NRC) issued the regulation 10 CFR Part 61, "Licensing Requirements for Land Disposal of Radioactive Waste" [Federal Register, 1982]. A requirement found in 10 CFR PART 61 states that "proposed disposal site, disposal facility design, land disposal facility operations (including equipment, facilities and procedures), disposal site closure and post-closure institutional control is adequate to protect the public health and safety . . ." In the post-closure period, protection of the public is judged by requiring that releases which may occur must be demonstrated with reasonable assurance not to exceed an equivalent dose of "25 millirems to the whole body, 75 millirems to the thyroid, and 25 millirems to any other organ of any member of the public." This requires the quantitative assessments of the potential impacts of a low-level radioactive waste (LLW) disposal facility on the public. In particular, estimation of the dose to the maximally exposed individual is required.

The quantitative projection of the dose to man is accomplished through a performance assessment. A performance assessment integrates all of the processes and events that influence the potential for exposure to radioactivity disposed of in the LLW facility. Therefore, the performance assessment for the groundwater pathway would include models to project the flow of water into and through the disposal facility as a function of time, the release of radioactive contaminants from the waste forms, the transport of the contaminants from the facility through the vadose zone and aquifer to the biosphere and exposure to the contaminants through ingestion (drinking water, food grown with contaminated water, etc.) and direct exposure.

A key component of any performance assessment is the source term. The source term is defined as the radionuclide release rate from the disposal facility. In general, the release can occur in the gas or liquid phase. In this report the focus is on release to the liquid phase. Often, there is confusion over the definitions of inventory and source term. Inventory is the mass disposed and is one component that determines the source term. The source term refers to a more general concept and is influenced by the inventory as well as the physical and chemical processes that influence the release and transport of the contaminants out of the facility.

The aqueous phase release of the radionuclides from the facility is controlled by water flow, access of water to the waste forms, release of the radionuclides to the water, and migration of the radionuclides. These processes are influenced by facility design, precipitation, hydrology, geochemistry, and waste form and container performance characteristics. All of these processes can play an important role in estimating the source term.

A schematic diagram of a hypothetical low-level waste disposal unit is displayed in Figure 1.1. The salient features of this system are the cover system used to divert water flow away from the waste containing region, an engineered barrier structure which provides an additional barrier to water flow, and structural stability to minimize the possibility of subsidence, waste containers (as many as several thousand containers with differing volumes, designs, and materials of construction per disposal facility are possible), and waste forms of differing physical and chemical characteristics in each container. The inventory may include over 200 different radionuclides.

The BLT-MS (Breach, Leach, Transport - Multiple Species) code has been developed to simulate the major processes that control release to the groundwater resulting from subsurface disposal of low-level waste. BLT-MS is based on the BLT computer code [Sullivan and Suen, 1989]. Similar to BLT, it has models to represent container performance, waste form leaching, and radionuclide transport. In addition, BLT-MS can simulate radioactive production and decay in the waste form as well as during transport. Water flow is handled through tabular input, or auxiliary files created by hydrological codes. It has been designed with the objective of being flexible enough to handle the wide variety of conditions that may potentially exist. However, to allow for special cases and to permit easy modification of the models within the code, a modular code structure has been used.

Figure 1.1 Schematic Diagram of a LLW Disposal Unit

1.2 An Overview of BLT-MS

An objective in developing the BLT-MS code was to produce a tool that could, based on mechanistic principles, simulate a wide variety of situations that may be encountered in low-level waste disposal. The expected output from BLT-MS is the rate of release from the disposal facility. This information is used as input to other codes with the ultimate objective being to obtain an estimate of the dose that could potentially occur due to waste disposal.

BLT-MS is a two-dimensional finite element computer code capable of simulating the time evolution of concentration resulting from the time-dependent release and transport of aqueous phase species in a subsurface soil system. An overview of the processes considered in BLT-MS is presented in Table 1.1. BLT-MS has the following features:

- Water flow rate and moisture contents which influence container degradation, waste form leaching, and transport are input variables.
- Container degradation models. BLT-MS simulates local degradation (only a small fraction of the container area is breached) and general degradation (the entire container is assumed to fail when the container thickness is consumed by degradation processes). BLT-MS permits simulation of multiple (currently dimensioned as 20) sets of container failure parameters. This permits an easy method to simulate the different failure times expected from the different containers.
- Waste form leaching models. BLT-MS simulates four processes that can control release from the waste form. The processes are: surface rinse upon contact with water subject to equilibrium partitioning, diffusion, uniform degradation, and solubility limited release. BLT-MS permits simulation of multiple

(currently dimensioned as 20) waste form release parameters. In addition each waste form may have a unique inventory. This allows a method to simulate the range of waste forms that may potentially occur in disposal.

- Radionuclide transport model which considers advection, dispersion, diffusion, radioactive decay and production, equilibrium chemical partitioning, waste form sources, and external sources and sinks.
- Simulation of up to 10 radionuclides during the calculation each with unique waste form release and transport properties.
- Simulation of chain decay with branching in the waste form prior to release and during transport.

Each of these models will be discussed in detail in section 2 of this report.

Table 1.1 Overview of Process Models Considered in BLT-MS

<p style="text-align: center;">CONTAINER DEGRADATION</p> <p>Model: Local failure (partial failure) General failure (time to failure)</p> <p>Output: Fraction of the container that is breached as function of time</p>
<p style="text-align: center;">WASTE FORM RELEASES</p> <p>Model: Rinse release subject to partitioning Diffusion controlled release Uniform degradation release Solubility limited release Chain decay</p> <p>Output: Waste form mass release rate per unit volume for the transport equation.</p>
<p style="text-align: center;">TRANSPORT</p> <p>Model: 2-dimensional finite element simulation of: Advection, dispersion, diffusion, linear sorption, radioactive production and decay, first order degradation in the liquid and solid phases, and sources (waste forms as well as external source)</p> <p>Output: Time evolution of concentration at each spatial location in the modeled domain</p>

The computational approach that implements the models presented in Table 1.1 has the following procedures within each time step:

- update the water flow rates and moisture contents based on input, if necessary.
- calculate container performance.
- calculate radioactive production and decay in each waste form.
- if container failure has occurred, calculate waste form release rates for each contaminant in each container.

- calculate the transport of each contaminant over the time step.

The solution procedure used in BLT-MS will be discussed in more detail in section 3 of this report.

BLT-MS, in addition to the capability of simulating multiple species and radioactive ingrowth within a single simulation, has a number of other improvements over its predecessor, BLT. These include:

- a pre-processor, BLTMSIN, which guides the user through creating an input file,
- improved treatment of how the sources are incorporated into the transport equation,
- improved treatment of the rinse release model with partitioning,
- improved treatment of the uniform degradation model, and
- improved post-processor, BLTPLOT, which can be used to visualize the output data and generate a paper copy of concentration contour plots, system maps, and x-y plots of leaching data, concentration, or flux at specified locations.

These improvements will be described in later sections of the report.

1.3 User Requirements

To effectively apply BLT-MS the code user will need a fundamental understanding of the physical and chemical processes that influence release and transport of radioactive materials in subsurface systems. These processes will be described in detail in section 2 of this report. In addition, a basic understanding of finite element methods is also needed. A number of references on the finite element method exist [Finlayson, 1980] and implementation of the finite element methods in the FEMWASTE code is discussed in [Yeh, 1982].

Misuse of computer codes occurs frequently. The chances of misapplication of the code can be minimized through developing an understanding and familiarity with BLT-MS, its capabilities and limitations, prior to application on a field scale problem. This can be achieved in part through use of some of the test problems supplied with the code and examination of the output generated by the code.

1.4 Computer Requirements

BLT-MS is written in standard FORTRAN 77 and can be compiled on most PC and work station systems with only minor alterations (i.e., change in OPEN statements, etc.). The majority of development and testing of BLT-MS have been performed on DOS-BASED PC's. However, the code has been compiled on a number of workstations (SUN, IBM, and Hewlett Packard). As configured, BLT-MS requires, as a minimum, a 386-based PC machine with a math coprocessor and at least 8 MB of RAM. The memory requirement is large because of the size of the arrays in BLT-MS. Much smaller configurations can be obtained by redimensioning the arrays in BLT-MS.

1.5 Report Outline

The objective of this document is to provide the necessary information to understand and apply the BLT-MS code to problems in subsurface disposal of wastes. Section 2 provides the theory and governing equations used to simulate release and transport. Section 2 has a brief discussion of water flow, followed by more detailed discussions of container performance, waste form leaching including the process of ingrowth, and contaminant transport. Section 3 discusses the coupling between major process models and assumptions that are used in the code. Section 4 presents the results of a

number of verification studies that demonstrate BLT-MS is capable of accurately predicting transport with chain decay, and ingrowth of progeny in the waste form prior to release. Section 5 provides an overview on how to use BLTMSIN a pre-processor that is useful in creating input files used by BLT-MS. Section 6 gives a detailed discussion of the input requirements and formatting requirements. Although most data are read using list directed read statements which removes the need to align values in certain columns, the input file is highly structured. This structure and detailed examples on how to create an input file are supplied in this section. Section 7 discusses the output files generated by BLT-MS. In addition to the main output file, a number of auxiliary output files containing information on waste form releases, waste form mass balances, and the concentration and flux at various specified points in the modeled domain are generated. Section 8 presents information on the use of BLTPLOT a post-processor that is capable of generating a graphical or hard copy display of the information generated by BLT-MS. Section 9 provides a summary and conclusion of the material contained in this report.

2 BLT-MS MATHEMATICAL MODEL DESCRIPTION

Subsurface release and transport of radionuclides from a low-level waste disposal facility involves estimation of the rate of water flow through and around the facility, container performance, waste form performance, and radionuclide transport. A flow chart of the major processes and events is presented in Figure 2.1. This section of the report describes the conceptual models, major assumptions, and governing equations used to represent each of these processes.

Figure 2.1 Major Processes Involved in BLT-MS Simulations of Release and Transport

Prior to proceeding to the model description a brief description of the finite element approach is provided. This is necessary to provide the framework for the model calculations in BLT-MS.

A general approach to modeling a low-level waste disposal system would first define a conceptual model of the system and its behavior. Based on this conceptual model, appropriate data on inventory, waste forms, containers, and transport properties would be collected. The geometry of the different regions (engineered barriers, cover systems, waste containing region, soil layers, location of the water table, etc.) would be defined. Based on this information assumptions would be made to simplify the system into a form amenable for numerical simulation. For BLT-MS, these assumptions would potentially include homogenizing the wastes and containers into a few types with specific release properties, assuming uniform transport properties for certain regions in the modeled domain, and reducing the three-dimensional disposal system into a two-dimensional representation.

The finite element approach discretizes the domain to be modeled into a series of regions, finite elements. An example of a finite element grid is presented in Figure 2.2. The modeled region is subdivided into a number of quadrilateral regions. The size and shape of the regions are selected to fit the finite elements to the dimensions of the problem and to provide the desired level of numerical accuracy in the solution. As the finite element size becomes larger, numerical dispersion can become a problem. In BLT-MS, the corner points of the finite element regions are called node points and each element has four node points. Concentrations are calculated in BLT-MS at the node points.

Figure 2.2 BLT-MS: Example Finite Element Grid

The finite element grid represents the transport domain of the BLT-MS calculation. Waste form sources are associated with an element and mass released from the waste form is injected at certain node points of the finite element (Figure 2.3). The method of entering waste form sources into the transport equation depends on the flow rate through the finite-element and is presented in section 2.4.3. However, waste form processes are independent of the transport processes, i.e., diffusion in the waste form is independent of diffusion in the porous media. This distinction is important when attempting to model large (greater than the finite element size) waste forms and when using the rinse with partition model (section 2.3.1).

Figure 2.3 Graphical Display of Waste Form Release to Specific Nodes in a Finite Element Based on the Darcy Flux Vector

2.1 Water Flow Simulation

In source term assessment, the objective of the water flow simulation is to obtain the flow rate and moisture content in the region under simulation. BLT-MS can accept these values from two sources: 1) as part of the input file and b) from an auxiliary file. For each point in the modeled domain, the auxiliary file can have a series of velocities and moisture contents to represent their time evolution.

The foundation for modeling groundwater flow is based on the physics of fluid flow through porous media. Soil can be viewed as a solid matrix with a network of pores and channels through which fluid flows. It is impractical to describe the flow at this level of detail (< 0.001 m) when attempting to simulate flow over tens or hundreds of meters. Therefore, a continuum approach is used in which fine details are averaged over a larger spatial domain.

The governing equation for groundwater flow is formulated based on Darcy's Law for flow through porous media and conservation of mass. Darcy's law states that the volumetric flow rate (or flux) is proportional to the hydraulic gradient and the cross-sectional area.

$$V_d = -K \nabla H \quad (2.1)$$

where

V_d	=	Darcy flux,
K	=	hydraulic conductivity, and
H	=	pressure head which is the sum of the gravitational head and the suction head.

The mass balance equation obtained using Darcy's law to specify the flux is:

$$S \frac{\partial H}{\partial t} = \nabla \cdot K \cdot \nabla H + Q \quad (2.2)$$

where

S	=	specific storativity, the additional volume of water stored in the porous medium, per unit rise of hydraulic head, per unit volume of porous medium, and
Q	=	external source or sink due to injection or withdrawal of water.

Equation 2.2 is the fundamental equation for groundwater flow in porous media. A number of excellent discussions of the process of flow as well as methods for solving Eqn. 2.2 are available [Freeze and Cherry, 1979; National Research Council, 1990]. In low-level waste disposal, the facility is usually located in the unsaturated zone. This makes solution of Eqn. 2.2 numerically challenging because the hydraulic conductivity is a non-linear function of the suction head. The hydraulic conductivity is highest when the porous media is saturated and decreases as the pores become less filled with water. In the unsaturated zone, a small change in suction head can lead to several orders of magnitude change in conductivity. If the porous medium is saturated, the suction head is zero and the hydraulic conductivity no longer varies with changes in head and Eqn. 2.2 is linear.

Solution of Eqn. 2.2 yields the distribution of pressure head in the modeled domain and is not of direct concern to simulation of contaminant transport. Therefore, the calculated pressure head distribution is used in Eqn. 2.1 to obtain the Darcy flux. The Darcy flux is the volumetric flow rate per unit area of the porous medium and is not the seepage velocity,

the rate that water moves through the pores. The seepage velocity, V_s , is obtained by dividing the Darcy flux by the moisture content, θ .

$$V_s = \frac{V_d}{\theta} \quad (2.3)$$

Similar to hydraulic head, the moisture content is a non-linear function of pressure head. Knowledge of the pressure head permits an estimation of the moisture content in the vadose zone. In the saturated zone, the moisture content is the porosity.

In general, solution of the equation for hydraulic head can be a difficult numerical task. For low-level waste disposal, the task is often extremely difficult because of the use of multi-layered covers with markedly different hydrological properties and concrete engineered barriers.

To overcome the difficulties in obtaining a numerical solution, the unit gradient approximation is often used. This approximation states that the flow through the system is one-dimensional (in the z-direction) and the hydraulic gradient is unity. With this assumption, the Darcy flux can be obtained by estimating the hydraulic conductivity. As an upper bound to flow, the flux is limited to the minimum of the natural recharge rate or the saturated hydraulic conductivity of the most resistive flow layer in the cover or engineered barrier. The moisture content for each material is obtained through use of the moisture content versus hydraulic conductivity curve for the material. While the unit gradient approximation may not yield a realistic description of flow in and around a disposal facility, it will provide an upper bound on the flow rate. If it can be demonstrated that the upper bound on flow rate leads to a conservative estimate on release rates, then the approximation can be useful. However, it is not always possible to demonstrate this, particularly when production of progeny is a concern.

BLT-MS uses a two-dimensional finite element representation of the subsurface system to simulate transport. As such, the input of velocities must be provided at the nodal points that are simulated. BLT-MS is currently structured to accept input from an auxiliary file created by the computer code FEMWATER, version 1 [Yeh, 1987]. The interface between FEMWATER and BLT-MS is identical to that between FEMWATER and BLT. A detailed description on how to create FEMWATER input files and the coupling between FEMWATER and BLT can be found in the input guide prepared for the BLT code [Sullivan and Suen, 1989].

A more recent version of FEMWATER, version 2, has been released. Version 2 has improved numerical solution techniques for the non-linear equations and should provide more accurate estimates of water flow velocities. However, the input and output requirements have undergone substantial modification since version 1. Therefore, the output file is not directly useable in BLT-MS. This can be overcome by either writing a post-processor for the FEMWATER version 2 output file, or by altering the statements in BLT-MS that read the output file. In general, any water flow code could be used to calculate velocities provided a post-processor was developed to manipulate the data to the form required by BLT-MS.

Time-dependent flow rates can be simulated in BLT-MS through the auxiliary file created by FEMWATER. The auxiliary file can have several sets of flow velocities at various times. BLT-MS has the capability to read the auxiliary file to get the flow rate at various times. Flow is assumed to vary linearly in time between the two time points of the velocity fields.

2.2 Container Degradation (Breach)

In source term assessment, the objective of the container performance modeling is to determine how long the container protects the waste form from being contacted by water. The parameter of importance is the fractional area of the container that has failed. Once the container fails, water can contact the waste form. The time-dependent estimate of the fraction of the container that has failed is estimated through the models in the code. BLT-MS has two general categories

of container degradation models: general degradation models in which the container fails completely exposing the entire waste form to water at the time of failure, and local degradation models which permit only a fraction of the container to fail and thereby only expose a small fraction of the waste to water.

The majority of containers used in low-level waste disposal are made out of carbon steel. However, other materials are used, particularly for high integrity containers (HIC's) which are used for class B and C wastes. These materials include several different stainless steel alloys including Ferallium a duplex stainless steel, high-density polyethylene, cement, and combinations of materials (e.g., high-density polyethylene container placed inside a cement overpack).

A considerable data base of information exists on both general and local corrosion of carbon steels [Romanoff, 1957]. Information is also available on the general corrosion rates of stainless steels [Gerhold et al., 1981]. A summary of these data has been included in the BLT Data Input Guide [Sullivan and Suen, 1989]. For other materials, the data base for performance in subsurface systems is more sparse. A detailed examination of the available literature on high density polyethylene has been performed [Cowgill and Sullivan, 1993] with the conclusion that the data available to predict the long-term behavior of high density polyethylene have large uncertainties. Examination of concrete container performance has also received little attention. There is a wealth of information on concrete performance in engineered structures and this could be used as a basis for estimating the time over which concrete protects the wastes from water.

When there are large uncertainties in predicted lifetime, often it is assumed that the container fails at a time near the low end of the range in expected performance. For example, high integrity containers are often assumed to fail at 300 years, their minimum design life.

2.2.1 General Degradation

The general degradation model assumes that the degradation process is constant and independent of time. For corrosion of metals, this can be conservative because the corrosion data in soil systems generally indicate a decreasing rate of corrosion in time [Romanoff, 1957; Gerhold et al., 1981]. The output of the general degradation model is the time at which failure occurs, t_f , and can be determined from the following:

$$t_f = \frac{d}{g} \quad (2.4)$$

where

d	=	degradation allowance thickness (cm) and
g	=	the general degradation rate (cm/s).

Both d and g are input parameters. The degradation thickness is the thickness of the container that is allowed to degrade prior to failure. It is often the container thickness minus a small fraction of the thickness to account for mechanical failure when the container gets too thin to support the overburden.

To simulate failure at the start of the calculation the value of the degradation rate, g, is set to a value much greater than the degradation allowance. The average and range of corrosion rates of carbon steel, 304 stainless steel, and 316 stainless steel are presented in Table 2.1 [Romanoff, 1957; Gerhold et al., 1981].

Table 2.1 Average and range of corrosion rates for carbon steel, 304 stainless steel, and 316 stainless steel.

<u>Material</u>	<u>Average (cm/s)</u>	<u>Range (cm/s)</u>
Carbon Steel	$1.8 \cdot 10^{-10}$	$2.7 \cdot 10^{-11} - 6 \cdot 10^{-10}$
304 Stainless Steel	$8.9 \cdot 10^{-14}$	$3.5 \cdot 10^{-15} - 5.3 \cdot 10^{-13}$
316 Stainless Steel	$4.1 \cdot 10^{-14}$	$8.9 \cdot 10^{-16} - 1.8 \cdot 10^{-13}$

2.2.2 Local Degradation

The objective of the local degradation model is to calculate the fraction of the container that has been penetrated due to degradation as a function of time. The localized failure model generally permits water access to the wastes at earlier times than the general corrosion model. Therefore, it will tend to be more important for short-lived radionuclides which undergo substantial decay prior to release.

The localized failure model in BLT-MS is structured to evaluate pitting corrosion of metallic containers. The data base used to generate the empirical parameters is based on carbon steel data. Stainless steel did not show significant pitting for times up to 14 years in soil systems [Gerhold et al., 1981]. For high density polyethylene containers data are also insufficient to estimate localized corrosion in an empirical manner. For concrete containers, crack formation will occur and permit enhanced water flow through the concrete to the wastes. Concrete degradation models can be used to estimate the rate and extent of crack formation. The models in BLT-MS are not appropriate for cracking of concrete.

The localized corrosion pitting model estimates the area breached based on the maximum pit depth h , corrosion allowance, d , and the number of penetrating pits per container, N_p . The area breached is equal to

$$A_b = N_p \pi (h^2 - d^2) \quad h > d \quad (2.5)$$

$$A_b = 0 \quad h < d$$

In BLT-MS, the area breached calculated in Eqn. 2.5 is limited to the area of the container as an upper bound.

The number of penetrating pits on carbon steel has been estimated to range between 0.05 and 0.5 per cm^2 . For a 55 gallon drum with a surface area of $21,000 \text{ cm}^2$, this indicates the number of penetrating pits should range from 1,100 to 11,000. [Sullivan et al., 1988]

The maximum pit depth, h , is obtained from the data generated by the National Institute of Standards and Technology [Romanoff, 1957] and takes the form:

$$h = k t^n \left[\frac{A}{372 \text{ cm}^2} \right]^a \quad (2.6)$$

where

k = empirical pitting parameter cm/yr^n ,

t	=	corrosion time in years,
A	=	surface area of the container in cm ² ,
a	=	experimentally derived empirical correlation coefficient.

The constant 372 cm² is a scaling factor and represents the size of the samples in Romanoff's study. All of the parameters necessary for calculating the maximum pit depth can be input directly in BLT-MS, or the code will calculate values based on the following expressions.

Values for the pitting parameter k are determined from the following relationship [Sullivan and Suen, 1989]:

$$k = 0.01458 (10 - \text{pH}) \quad \text{pH} < 6.8$$

$$k = 0.0457 \quad 6.8 < \text{pH} < 7.3$$

$$k = 0.0256(\text{pH} - 5.13) \quad \text{pH} > 7.3$$

If the pH is not known, the user may input a value of 0 for pH and the code will assume a value of 7 is assumed. This provides the minimum value of the pitting parameter. More conservative assumptions could be used, however, pH 7 is the mean value in the studies of Romanoff [Romanoff, 1957].

Values for the empirical constant n depend on the degree of soil aeration. It is known that soil aeration plays an important role in pitting. However, it is not a well defined property. General guidelines for determining aeration can be found in Romanoff [Romanoff, 1957]. In general, aeration factors influence the access of oxygen and moisture to the metal. Aeration characteristics of a soil are dependent on the physical characteristics such as particle size, particle-size distribution, and apparent specific gravity. All of these are related to the size and continuity of the pore space which are also related to drainage. Aeration is a more general concept than drainage, however, as aeration also depends on topographic features, depth to the water table, and amount of rainfall. In general, soils of coarse texture, such as sands, tend to have low water-holding capacity and are characterized by high aeration. Fine textured soils, such as clays, tend to have poor aeration.

There are four general categories of aeration: good, fair, poor, and very poor [Romanoff, 1957]. The average value for n for these categories is 0.26, 0.39, 0.44, and 0.59, respectively. If the clay content of the soil is known, the parameter n may be calculated from [Mughabghab and Sullivan, 1989]:

$$n = n_0 \theta (1 - CL)^{0.4} \quad (2.7)$$

where

n ₀	=	1, 1.5, 2, 2.5, for good, fair, poor, and very poor aeration in the soil,
θ	=	volumetric water content, and
CL	=	fraction of clay in the soil.

Values for the exponent "a" in Eqn. 2.6 depend on the material and the soil. Extensive studies by Logan [Logan, 1939] indicate that for wrought iron and carbon steels "a" ranged from 0.08 to 0.32 with a mean value of 0.15.

2.3 Waste Form Releases (Leach)

The objective of the waste form release models is to estimate the rate of release of radionuclides from the waste form to the water after the container has failed. The release rate depends upon the physical and chemical form of the radionuclides in the wastes. To simulate the range of waste form conditions, BLT-MS has four process models which can be used to estimate the rate of release: rinse with partitioning, diffusion, uniform degradation, and solubility limited release.

Low-level radioactive wastes are generated from a variety of different processes by the nuclear industry, medical industry, universities, government, and private industry. The variety of processes that generate the waste leads to a wide range in the physical and chemical properties of the wastes. In low-level waste management the wastes can be disposed of in many forms including activated metals, cement solidified wastes, lab trash, evaporator bottoms, ion-exchange resins, and other forms. The U.S. NRC's Uniform Low-level Radioactive Waste Manifest lists over twenty different categories of wastes [U.S. Nuclear Regulatory Commission, 1995]. Detailed discussions of the distribution of radionuclides by various waste forms can be found in a number of studies [Yim, 1994; Dehmel et al., 1994; Cowgill and Sullivan, 1993; Roles, 1989].

In obtaining an estimate of release from the waste form, the analyst should first consider all of the different types of wastes and the distribution of radioactive contaminants by waste form. Based on this knowledge of the inventory, the analyst should attempt to define the leaching mechanisms appropriate for each waste type (for example, solidified wastes are often assumed to control release through the diffusion process, activated metals, and waste glass are often treated to release contaminants due to dissolution which is modeled as a constant rate process, etc.). In the absence of information, the rinse model, which releases the entire inventory on contact with water, is often used to simulate waste form releases.

The following sections will describe the four process models incorporated into BLT-MS. BLT-MS has two distinct approaches to modeling waste form release. In the first approach, analytical models are used to represent each of the processes. The analytical approach is conceptually easy to understand, but it does not always account for different interactions between release mechanisms. The second approach represents the waste form numerically using finite differences. In this approach, all release mechanisms are calculated simultaneously. In addition, the finite difference approach provides a natural method for handling ingrowth of progeny when diffusion is important.

In both the analytical and finite-difference release models a distinction is made of the mass available for each release process. In BLT-MS, input defines the amount of mass available for each release mechanism. This permits homogenization of wastes into a single waste form. For example, if in some region of the disposal facility 60% of the activity is in activated metals, 30% in compacted lab trash, and 10% in cement solidified wastes, the code user can specify that 60% of the mass is available for uniform degradation release modeling, 30% of the mass is available for rinse with partitioning, and 10% is available for diffusion controlled release. Transfer of mass does not occur between release mechanisms unless solubility limits are reached or if the container is partially failed. In this case, mass that would be released in the absence of the constraints will be transferred to the rinse with partitioning model to permit faster release once the release constraints are not limiting. This is discussed in more detail in section 2.3.4.1 (partial container failure) and 2.3.6 (solubility limited release).

It is important for the analyst to realize that within the finite element framework, the waste form sources act to inject the contaminants at specific places within the modeled domain, Figure 2.3. Waste form properties are independent of the soil transport properties. This distinction becomes important when simulating rinse release with partitioning and in conceptual model development for waste emplacement in the model. This will be discussed in section 2.4.3 in more detail.

2.3.1 Rinse Release with Partitioning

The conceptual model represented by the rinse release model conforms to one that all of the radioactive contamination is on the surface of the wastes and will be released as soon as water contacts the wastes (e.g., immediately following container failure) subject to equilibrium partitioning and solubility limits. In the absence of partitioning and solubility constraints, an instantaneous release of the entire waste form inventory occurs and the inventory is available for transport.

The more general case occurs when there is partitioning of the mass between the wastes and the contacting porous medium due to sorption. Conceptually, this model considers three media, the waste form, the aqueous solution, and the porous media surrounding the waste form. This is an improvement from the partitioning model found in BLT which did not consider sorption onto the porous media when calculating release. That model would underpredict releases (i.e., equilibrium between the solution and waste form would be lost due to sorption on the porous media).

Initially, the entire inventory is in the waste form and the system is not at equilibrium. After container failure, the mass released from the waste form is calculated to correspond to the amount required such that there is equilibrium between the three components in the system. In theory, this is an instantaneous process. In the implementation in BLT-MS, the mass is released over the time step. The amount of mass released over the time step is obtained by performing a mass balance. Prior to equilibration, the mass in the system is:

$$M_{t,i} = M_{wf,i} + M_{a,i} + M_{p,i} \quad (2.8)$$

where

$M_{t,i}$	=	total mass (g) in the system (i.e., finite element),
$M_{wf,i}$	=	mass on the waste form,
$M_{a,i}$	=	mass in aqueous solution, and
$M_{p,i}$	=	mass sorbed on the porous media.
subscript i	=	represents the i^{th} contaminant

They are given by the following expressions.

$$M_{a,i}(t) = \theta(t) V_e C_i(t) \quad (2.9)$$

where

θ	=	volumetric moisture content in the system,
V_e	=	volume of the porous media and aqueous solution system, (cm ³)
t	=	time (s), and
C_i	=	concentration of the i^{th} contaminant in the aqueous solution (g/cm ³).

$$M_{p,i}(t) = \rho S_{p,i}(t) V_e \quad (2.10)$$

where

ρ	=	bulk density of the porous media, (g/cm ³) and
$S_{p,i}$	=	mass of contaminant i adsorbed on the solid per unit mass of the solid (g/g).

The mass contained in the waste form is the inventory of the waste form at time, t. Expressing the waste form mass in a form similar to the porous media mass yields:

$$M_{wf,i}(t) = \rho_{wf} S_{wf,i}(t) V_{wf} \quad (2.11)$$

where the subscript wf refers to the waste form. Notice, the volumes of the waste form and porous media are assumed to be different. This distinction is important when homogenizing regions of waste and soil into a single computational volume. Computationally, the wastes and the soil occupy the same region of the finite element domain.

The assumption of chemical equilibrium permits a direct relationship between the amount sorbed on the soil (or

waste form) and the solution concentration as expressed by:

$$S_{p,i}(t) = K_{d,i} C_i(t) \quad (2.12)$$

and,

$$S_{wf,i}(t) = K_{p,i} C_i(t) \quad (2.13)$$

where

$K_{d,i}$ = soil-solution distribution coefficient (cm^3/g) for contaminant i, and
 $K_{p,i}$ = waste form-solution partition coefficient (cm^3/g) for contaminant i.

The partition and distribution coefficients are conceptually and physically similar parameters. For clarity in the report, however, distribution coefficient will be used to discuss the soil-solution chemical equilibrium used in the transport equation, and partition coefficient will strictly apply to the waste form-solution equilibrium coefficient. In BLT-MS, each contaminant may have unique values for the partition and distribution coefficients and, therefore, unique release rates.

Assuming that the soil and solution are always in equilibrium, the mass balance becomes:

$$M_{a,i}(t) R_i + M_{wf,i}(t) = M_{a,i}(t+\Delta t) R'_i \quad (2.14)$$

where

R_i = retardation coefficient ($R_i = 1 + \rho K_{d,i}/\theta$) for contaminant i, and
 R'_i = three component (soil, porous media, waste form) retardation coefficient for contaminant i.

$$R'_i = 1 + \frac{\rho K_{d,i}}{\theta} + \frac{\rho_{wf} V_{wf} K_{p,i}}{\theta V_e} \quad (2.15)$$

The three component model accounts for the differences in mass of the waste form and porous media.

Solving Eqn. 2.14 for the mass in solution at time $t + \Delta t$ yields:

$$M_{a,i}(t+\Delta t) = \frac{M_{a,i}(t) R_i + M_{wf,i}(t)}{R'_i} \quad (2.16)$$

To obtain the mass released over the time interval Δt , the difference in the mass contained on the waste form is estimated from:

$$\Delta M_i = M_{wf,i}(t) - \rho_{wf} V_{wf} K_{p,i} C_i(t + \Delta t) \quad (2.17)$$

The estimate for the concentration can be obtained from Eqns. 2.9 and 2.16. To ease the input burden in BLT-MS, the term $\rho_{wf} V_{wf} / V_e$ is approximated as ρV_{ratio} . The density ρ is input as part of the material properties and V_{ratio} is input as part of the waste form properties. Using this assumption and performing a few algebraic manipulations leads to the expression:

$$\Delta M = \frac{R [M_{wf}(t) - \frac{\rho_{wf} V_{ratio}}{\theta} K_p M_a(t)]}{R'} \quad (2.18)$$

BLT-MS requires the mass release per unit time per unit volume, Q_r , as the source to the transport equation. This is:

$$Q_r = \frac{\Delta M_i}{V_e \Delta t} \quad (2.19)$$

where ΔM is determined from Eqn. 2.18.

Examining Eqn. 2.18 the following limiting behavior can be determined. In the case of no partitioning ($K_p = 0$), the entire inventory is released over the first time step. In the other extreme, as the waste form partition coefficient becomes large, the amount sorbed can become negative. That is the waste form will act as a sink to absorb material. Another interesting point about the release equation is that it accounts for sorption on the soil. For example, if $V_{ratio} = 1$ and the partition and distribution coefficients are equal and much greater than unity, then R' is approximately twice the value for R and the mass released at the first time step ($C(0) = 0$) is about $1/2$ of the total inventory. The model in BLT, which did not consider sorption onto the porous media when calculating release, would predict releases proportional to the inverse of the waste form-solution retardation coefficient which would be much less than $1/2$. If the homogenization process has one part waste per ten parts of porous media ($V_{ratio} = 1/10$) larger releases will occur than if the reverse was true. This reflects the amount of mass available for sorption in the porous media and waste form. Use of V_{ratio} permits a convenient method to homogenize the wastes and soils into a single computational element. Equation 2.18 also demonstrates that if the system starts at equilibrium, the release is zero.

The above treatment calculates the release based on the concentrations at the beginning of the time step. As such, it is an explicit numerical procedure and is accurate to order Δt . Over the time step, there may be transport, decay and ingrowth, and releases from other mechanisms (diffusion and uniform degradation). Therefore, the system will be out of equilibrium at the start of the next time step. Typically, the rinse model will predict a large release at the failure time of the container. This is caused by the condition that the solution concentration is often zero prior to failure. Smaller releases are predicted at subsequent time steps.

An alternative approach to model rinse release with partitioning would be to immediately adjust the solution concentrations at the beginning of the time step to force equilibrium. During the time step, equilibrium would be maintained by placing the equilibrium relationship directly into the transport equation and obtaining the modified retardation coefficient, R' . This approach has the advantage of being an implicit approach and is incorporated into the DUST-MS computer code. The fact that the release can be recast into a form that modifies the transport equation by R' is an important consideration. It demonstrates that using a partition coefficient and a distribution coefficient can be viewed as changing the retardation coefficient in the transport equation. The analyst must insure that sorption is not excessively represented. This can be done by appropriate choice of the retardation parameters (ρ , K_d , K_p , V , and V_{ratio}).

2.3.1.1 Time-Dependent Partition Coefficient

Partitioning on the waste form may change in time. In particular, ion-exchange resins may degrade over time. This process is simulated in BLT-MS through the use of an exponentially decaying value for the partition coefficient. The expression may have unique values for each contaminant and is:

$$K_{p,i}(t) = K_{p,i}(0) e^{-\lambda_{p,i}t} + K_{p,i}(\infty) (1 - e^{-\lambda_{p,i}t}) \quad (2.20)$$

where

$$\begin{aligned} K_{p,i}(0) &= \text{initial value for the partition coefficient for contaminant } i, \\ K_{p,i}(\infty) &= \text{value for the partition coefficient as time approaches infinity, and} \\ \lambda_{p,i} &= \text{partition decay coefficient for contaminant } i. \end{aligned}$$

Input for BLT-MS requests $K_{p,i}(0)$, $K_{p,i}(\infty)$, and $\lambda_{p,i}$. This is discussed in detail in section 6.21, waste form input parameters.

Often, it is difficult to obtain reliable parameters for the decay rate constant and the final value for the partition coefficient. If these are unavailable, input the degradation rate as zero and the partition coefficient will be maintained at its initial value at all times.

2.3.2 Diffusion Release

This conceptual model for release assumes that the wastes are uniformly and homogeneously distributed throughout a solidified waste form and that diffusion is the only important process. Under these conditions, analytical solutions for the release rate from the waste forms can be obtained for a variety of geometries. However, exact methods for treating ingrowth of progeny are unavailable. BLT-MS has an approximate method, however, it is recommended to use the finite difference waste form release models, section 2.3.5, model ingrowth.

The BLT-MS code permits selection from three different analytical diffusion release rate models:

- a) plane geometry, release into a semi-infinite medium
- b) plane geometry, zero boundary concentration
- c) cylindrical geometry, zero boundary concentration

The plane geometry models simulate a waste form with finite dimensions in the direction of transport and infinite size in the plane perpendicular to transport. The cylindrical model simulates a cylindrical waste form of fixed height and radius. Other analytical models exist for rectangular and spherical waste forms [Pescatore, 1991] and are implemented into the DUST [Sullivan, 1993] and DUST-MS computer codes.

All three models solve the diffusion equation,

$$\frac{\partial C_i(x,t_f)}{\partial t_f} = D_{w,i} \nabla^2 C_i(x,t_f) - \lambda_i C_i(x,t_f) \quad (2.21)$$

where

$$C_i(x,t_f) = \text{concentration of contaminant } i \text{ within the waste form (g/cm}^3\text{),}$$

$D_{wf,i}$	=	waste form diffusion coefficient for contaminant i (cm^2/s),
λ_i	=	radioactive decay constant for contaminant i (s^{-1}),
x	=	spatial location vector (cm), and
t_f	=	time since container failure (s).

The diffusion time does not start until the container fails. All references to time in this section refer to the time since the diffusion process starts. The BLT-MS code allows selection of a unique diffusion coefficient for each radionuclide.

The initial condition for all three models is:

$$C(x,0) = C_0 \quad (2.22)$$

C_0 is the initial concentration in the pore waters of the waste form. It is estimated from the initial inventory and waste form volume.

2.3.2.1 Finite-Sized Plane Waste Form Releasing into a Semi-Infinite Medium

The first analytical model simulates a plane waste form of half-thickness, h , in the region $0 \leq x \leq h$. The model predicts the release from the waste form into a semi-infinite porous medium. It may be useful to simulate releases from waste forms which are not close enough to other waste forms for their releases to interact and if diffusion is appropriate for transport outside of the waste form. The boundary conditions are, symmetry in the waste form,

$$\frac{\partial C_i(0,t)}{\partial x} = 0 \quad (2.23)$$

and zero concentration as x approaches infinity.

$$C_i(\infty,t) = 0 \quad (2.24)$$

Solution of the diffusion equation for the flux at the edge of the waste form [Crank, 1975] gives:

$$J_i(t) = 0.5 C_0 \sqrt{\frac{D_{wf,i}}{\pi t}} e^{-\lambda_i t} \left[1 - e^{-\frac{h^2}{D_{wf,i} t}} \right] \quad (2.25)$$

The quantity required by the transport equation is the release rate per unit volume. This quantity is obtained by multiplying the flux by the surface area of the waste form, A_{wf} , and dividing by the volume of the computational element, V_e , into which the mass is released.

$$Q_{d,i} = \frac{J_i(t) A_{wf}}{V_e} \quad (2.26)$$

This value of $Q_{d,i}$ is placed into the transport equation as the release from the waste form.

2.3.2.2 Finite-Sized Plane Waste Form with a Zero Concentration Boundary Condition

This model simulates a plane waste form of half-thickness, h , located in the region $-h \leq x \leq h$. At the boundaries, the concentration is assumed to be zero at all times. That is everything that reaches the boundary is swept away instantly. This maximizes the concentration gradient and therefore, the flux (and mass released) is also maximized. This conceptual model predicts the highest release rate possible from a semi-infinite plane waste form. The boundary conditions are:

$$\frac{\partial C_i(0,t)}{\partial x} = 0 \quad (2.27)$$

$$C_i(h,t)=0 \quad (2.28)$$

The solution for the concentration as a function of position and time is obtained using Laplace transforms and can be found in [Crank, 1975; Sullivan, et al., 1988]. The important quantity for source term modeling is the flux from the waste form. In general, the solution involves an infinite series and can be found in [Crank, 1975; Sullivan, et al., 1988]. However, for numerical implementation four cases are considered based on the dimensionless parameter, γ .

$$\gamma_i = \frac{h^2}{D_{wf,i} t} \quad (2.29)$$

If $\gamma < 0.05$

$$J_i(t) = 0.5 C_0 \sqrt{\frac{D_{wf,i}}{\pi t}} e^{-\lambda_i t} \left[1 - e^{-\frac{h^2}{D_{wf,i} t}} \right] \quad (2.30)$$

This is the same solution as for release into a semi-infinite medium. This implies that at early times the release from the concentration at the boundary in the semi-infinite medium model has not increased to a level such that the release is diminished as compared to the case with zero boundary concentration.

If $0.05 < \gamma < 1$

$$J_i(t) = C_0 \sqrt{\frac{D_{wf,i}}{\pi t}} e^{-\lambda_i t} \sum_{n=0}^{\infty} (-1)^n \left[e^{-n^2 \gamma_i} - e^{-(n+1)^2 \gamma_i} \right] \quad (2.31)$$

If $1 < \gamma < 20$

$$J_i(t) = \frac{2 D_{wf,i} C_{0,i}}{h} e^{-\lambda_i t} \sum_{n=0}^{\infty} e^{-\frac{\pi^2 (2n+1)^2 \gamma_i}{4}} \quad (2.32)$$

If $\gamma > 20$

$$J_i(t) = 0 \quad (2.33)$$

The number of terms evaluated in the series is estimated based on the value of γ . It is selected to insure that the terms neglected in the series are at most 10^{-4} of the sum of the previous terms of the series. The solution for $\gamma < 0.05$ is the leading order term in Eqn. 2.31. For $\gamma > 20$ the first term in the series is less than e^{-20} which is approximated as zero. Equations 2.31 and 2.32 are equivalent solutions provided $N = \infty$.

The calculated value for the flux, J_i , is placed into Eqn. 2.26 to obtain the release rate per unit volume required in the transport equation.

2.3.2.3 Finite-Sized Cylindrical Waste Form with a Zero Concentration Boundary Condition

The final analytical model simulates a cylinder with radius, R , and height, H . At the edge of the waste form, the contaminant concentration is zero. As with the finite plane model, this boundary condition causes the maximum concentration gradient to be maintained and leads to the highest release as compared to other possible boundary conditions. The boundary conditions are:

$$\frac{\partial C_i(0,z,t)}{\partial r} = 0 \quad (2.34)$$

$$C_i(R,z,t) = C_i(r,0,t) = C_i(r,H,t) = 0 \quad (2.35)$$

The solution for the cumulative fractional release, CFR, is the product of two infinite series [Nestor, 1980]:

$$CFR_i(t) = 1 - \frac{32 S_{q,i}(t) S_{d,i}(t)}{\pi^2} \quad (2.36)$$

$$S_q(t) = \sum_{n=1}^{\infty} \frac{1}{(2n-1)^2} e^{\frac{-(2n-1)^2 \pi^2 D_{eff} t}{H^2}} \quad (2.37)$$

where:

$$S_c(t) = \sum_{m=1}^{\infty} \frac{1}{\beta_m^2} e^{\frac{-\beta_m^2 D_{eff} t}{R^2}} \quad (2.38)$$

where the β_m are the zeroes of the zeroth order Bessel function.

The American Nuclear Society has published a standard, ANS 16.1, which describes procedures for testing and analyzing the release from solidified low-level radioactive wastes [American Nuclear Society, 1986]. In ANS 16.1, Eqn. 2.36 is the recommended approach for estimating releases from cylindrical waste forms provided the release is greater than 20%. When the release is less than 20% ANS 16.1 recommends using the predicted release based on treating the waste form as a semi-infinite medium. The reason for this is the poor convergence of the semi-infinite series at low CFR values and the minor difference in predicted CFR between the semi-infinite medium model and the finite cylinder model, Eqn. 2.36 when the CFR is less than 0.2. Even though the difference is small, the semi-infinite model always predicts greater release than the series solution. Thus, at the time step when the switch is made, an under prediction of release at that time step will occur.

The semi-infinite waste form model for release is:

$$CFR_i(t) = \frac{2 SA_{wf}}{V_{wf}} \sqrt{\frac{D_{wf,i} t}{\pi}} \quad (2.39)$$

where

$$\begin{aligned} SA_{wf} &= \text{surface area of the waste form and} \\ V_{wf} &= \text{volume of the waste form.} \end{aligned}$$

An improved method for calculating the series solution has been developed [Pescatore, 1991] which permits truncation of the series after only a few terms. In this description the subscript i which refers to the contaminant being modeled is dropped for notational convenience. The improved approximation is:

$$CFR(t) = 1 - \frac{32 S_{q,N}(t) S_{c,M}(t)}{\pi^2} \quad (2.40)$$

where

$$S_{q,N}(t) = \sum_{m=1}^{N-1} \frac{1}{(2n-1)^2} e^{\frac{-(2n-1)^2 \pi^2 D_{wf} t}{H^2}} \quad (2.41)$$

$$+ \frac{N}{(2N-1)^2} e^{\frac{-(2N-1)^2 \pi^2 D_{wf} t}{H^2}}$$

$$- \frac{\sqrt{\pi D_{wf} t}}{2 H} \operatorname{erfc} \left[(2N-1) \pi \frac{\sqrt{D_{wf} t}}{H} \right]$$

and,

$$S_{c,M}(t) = \sum_{m=1}^{m=M-1} \frac{1}{\beta_m^2} e^{-\frac{\beta_m^2 D_{wf} t}{R^2}} \quad (2.42)$$

$$+ \left[\frac{1}{\beta_M f_M} + \frac{1}{2\beta_M^2} \right] e^{-\frac{\beta_M^2 D_{wf} t}{R^2}}$$

$$- \frac{1}{R f_M} \sqrt{\pi D_{wf} t} \operatorname{erfc} \left[\beta_M \frac{\sqrt{D_{wf} t}}{R} \right]$$

where

$$f_M = \pi - \frac{1}{8\pi M^2} \quad (2.43)$$

Through testing it has been determined that setting N and M to ten provides sufficient accuracy.

BLT-MS uses both the semi-infinite model, Eqn. 2.39 and the series solution, Eqn. 2.40 to estimate releases. Estimated releases from both equations are compared, BLT-MS selects the minimum of these two estimates. At early times the series solution over predicts release as it is not fully converged. At later times, the semi-infinite media model predicts higher releases as depletion in the waste form is not simulated.

The equations 2.39 and 2.40 estimate the cumulative fractional release, not the release rate, the quantity needed in the transport equation. The release rate of contaminant i per unit volume due to diffusion over the time step is estimated from the following expression:

$$Q_{d,i} = \frac{CFR_i(t+\Delta t) - CFR_i(t)}{V_e} M_{o,i} e^{-\lambda_i t} \quad (2.44)$$

where $M_{o,i}$ is the original mass in the waste form.

2.3.2.4 Approximate Treatment of Ingrowth in the Analytical Diffusion Models

The analytical diffusion release models described in section 2.3 are all based on the assumption that the production of the radionuclide due to radioactive decay of other species does not occur. When ingrowth occurs, the approximation is

made that the distribution of mass due to ingrowth is identical to the distribution of mass in the waste form generated by diffusion.

This approximation is not true in general due to differing diffusion coefficients of the parent and progeny. However, the approximation does conserve mass. If the parent moves at a slower rate than the progeny, this approximation will under predict release. The cause for this behavior is the parent's diffusion profile will be shifted more towards the outer edge of the waste form as compared to the faster moving progeny. In the limit that the parent is immobile, the production of progeny will occur uniformly throughout the waste form. Therefore, more progeny will be produced closer to the edge of the waste form than would be predicted by the model.

In general, if ingrowth of progeny occurs it is strongly recommended to not use the analytical diffusion models. Instead the finite-difference diffusion models described in section 2.3.5 should be used.

2.3.3 Uniform Degradation Release

The conceptual model for uniform release assumes that the waste form releases the radioactivity at a uniform rate. Typically this release behavior would be caused by degradation reactions occurring at the surface of the waste form (i.e., metal corrosion, glass dissolution, etc.). In the BLT code [Sullivan and Suen, 1989] this model was called the dissolution model and was meant to simulate corrosion of activated metals. Due to the wide variety of waste forms/waste streams that this model may be used to represent and to avoid confusion with the term dissolution which has a specific definition, the name has been generalized to the uniform degradation release model.

In BLT-MS each radionuclide may be assigned a unique uniform release rate. In the absence of ingrowth the release rate per unit volume, $Q_{u,i}$ is estimated from:

$$Q_{u,i} = \frac{u_i M_{0,i}}{V_e} e^{-\lambda_i t} \left[1 - \frac{C_i}{C_{sat,i}} \right] \quad (2.45)$$

where

u_i	=	fractional release rate for contaminant i (s^{-1}),
C_i	=	solution concentration for contaminant i,
$C_{sat,i}$	=	solubility limit for contaminant i, and other quantities have been previously defined.

If ingrowth occurs, the mass available for release, $M_{0,i} e^{-\lambda_i t}$ is generalized to the mass available at that time $M(t)$ based on ingrowth as well as decay. This is discussed further in section 2.3.7

A further difference between BLT and BLT-MS is that in BLT, the model relied upon input of the waste form dissolution velocity. This dissolution velocity was multiplied by the surface area of the waste form and divided by the volume of the waste form to get the fractional release rate, u_i in Eqn. 2.45.

The uniform release model is the only model to explicitly represent solubility constraints. The conceptual model employed in Eqn. 2.45 assumes that as the solubility limit is approached the release rate decreases. The release rate is zero when the solution concentration reaches the solubility limit. The treatment of solubility is discussed further in section 2.3.6

2.3.4 Total Waste-Form Release Rate

BLT-MS permits each waste form to release mass by any of the release mechanisms described in section 2.3.1 (rinse with partitioning), 2.3.2 (diffusion), and 2.3.3 (uniform). In the absence of solubility constraints, the release rate per unit volume to the transport equation is the sum of the three individual release rates given by Eqns. 2.19, 2.26, 2.39, 2.40,

and 2.45. If solubility limits release, the source term to the transport equation is reduced in an attempt to prevent exceedance of the solubility limit. This procedure is discussed in more detail in section 2.3.6.

2.3.4.1 Influence of Localized Failure on Release

If there is localized failure, the intact portion of the container still provides a barrier to release from the waste form-container system. The conceptual model for release from partially failed containers assumes that once a container is breached, there will be a steady flow of water into and out of the container. The flow rate is estimated from the Darcy flux multiplied by the fractional area of container that has failed. Other conceptual models could be envisioned. For example, if the breach occurred at the top, water could begin to fill the container and a bathtub could form until the water level reached the lowest breached area. This could potentially lead to a large pulse of radioactive contaminants. However, accurately predicting the location of failures around the container is beyond the state-of-the-art. The selection of the model for instant flow through the container once a breach has occurred was selected to provide an estimate of the earliest time that releases could occur.

An important aspect of the strategy used to represent localized failure is the treatment of waste form releases. The diffusion model assumes that once the waste form is contacted by water, the release process begins and is given by the analytical models, section 2.3. These models are unaffected by the breached area. Similarly, release from the uniform release model is also calculated independent of the breached ratio. To adjust for the fact that the entire container is not breached, the release rate per unit volume from the diffusion and uniform release models is reduced by the breach ratio, (area of the breach over the total container area). Mass not released is transferred to the rinse release model. This permits the analytical solutions to be retained while still taking credit for partial container failure. Release from the rinse model is treated as release from a mixing cell, all of the mass available for rinse release (including mass transferred from the diffusion and uniform release models) is assumed to enter into a mixing cell. The release from the mixing cell is the product of the Darcy flux, breached ratio, the area available for flow, and the concentration in the mixing cell.

A number of assumptions have been made in developing the waste form release models in the case of partial container failure. Data to support these assumptions (or any other possible set of assumptions) do not exist due to the long time frame over which these processes will occur and the difficulty of experimentally measuring the entire process. Due to the speculative nature of the assumptions the model results are also speculative and care should be used when interpreting the results.

2.3.5 Finite Difference Waste-Form Release Model

BLT-MS provides an alternative approach to simulating release from the waste form as compared to the analytical models presented in section 2.3.3. In this approach all processes, rinse with partitioning, diffusion, and uniform degradation are modeled simultaneously using the method of finite differences. This numerical approach offers the following advantages over the analytical models:

- simultaneous treatment of all release processes,
- direct coupling of diffusion release to the concentration of the contacting solution, and
- a method for modeling ingrowth of radionuclides in the waste form which are released by the diffusion process.

The limitations of the numerical models as compared to the analytical models is the possibility for numerical error and the increased computational requirements. In addition, the finite difference models assume one-dimensional geometry (either planar or cylindrical) as compared to the three-dimensional cylindrical diffusion release model. Experience has shown that calculation of waste form release is a small fraction of the entire BLT-MS calculation. Therefore, the penalty in slower execution time is not large. Testing of the finite difference models and comparison to the analytical models show excellent agreement under most situations.

The finite difference model retains the distinction between mass available for release due to each mechanism (rinse with partitioning, diffusion, and uniform degradation). The finite difference model assumes that the waste form is a porous

medium with a liquid phase which permits movement of aqueous species and a solid phase which releases species due to dissolution of the surface of the waste form. This dissolution will remove the outer layer of the waste form. This alters the diffusion release in two ways. First, "diffusion release" mass in the pore waters of the dissolved region is released. Second, the size of the waste form, and therefore diffusion distance to the boundary, decreases in time. These effects demonstrate the direct coupling between the dissolution and diffusion models which was absent from the analytical models. A discussion of when this coupling is important is provided in [Sullivan and Suen, 1991].

The general equation for predicting release with all three mechanisms is:

$$\theta \frac{\partial C_i}{\partial t} = \nabla \cdot \theta D_{wf, i} \nabla C_i + \nabla \cdot V_{wf} C_i - \lambda_i \theta C_i + \sum_{j=1-N}^{j \neq i} f_{ij} \lambda_j C_j + S_i \quad (2.46)$$

where

θ	=	moisture content within the waste form. For simplicity this is taken as the moisture content within the finite volume element.
C_i	=	concentration of the i^{th} contaminant (g/cm^3),
$D_{wf, i}$	=	waste form diffusion coefficient for the i^{th} contaminant (cm^2/s),
V_{wf}	=	volumetric flow rate per unit area through the waste form (cm/s),
λ_i	=	radioactive decay constant for the i^{th} contaminant ($1/\text{s}$)
f_{ij}	=	fraction of decays of species j that form species i , and
S_i	=	source/sink term within the waste form. This could be used to represent coupling between the immobile and mobile phases in the waste form due to precipitation or sorption ($\text{g}/\text{cm}^3\text{-s}$).

Eqn. 2.46 accounts for ingrowth directly. Theoretically there is one equation for each type of mass (rinse, diffusion, and general degradation). However, the rinse release model simulates a surface process and solution of Eqn. 2.46 is not required. The mass released due to rinse with partitioning is treated using the approach described in section 2.3.1.

Although Eqn. 2.46 is quite general, to solve this equation numerically is difficult when the waste form is dissolving. In this case, the volumes represented by the finite difference mesh may change in time. For example, the outermost volume will decrease as dissolution of the surface occurs. To avoid this problem a change in the position variable is introduced.

$$y = \frac{x}{L(t)} \quad (2.47)$$

where

y	=	dimensionless distance variable
x	=	dimensioned distance variable (cm)
$L(t)$	=	length (radius) of the waste form at time t .

In the transformed variable space, the waste form lies between the region of 0 and 1 at all times, Figure 2.4. However, the distance variable y is now a function of time. Differentiating Eqn. 2.47 with respect to time gives:

$$\frac{dy}{dt} = - \frac{y}{L} \frac{dL}{dt} \quad (2.48)$$

The time derivative of concentration in the transformed plane becomes:

$$\frac{\partial C(y(t), t)}{\partial t} = \frac{\partial C}{\partial t} + \frac{\partial y}{\partial t} \frac{\partial C}{\partial y} \quad (2.49)$$

Waste Form

Figure 2.4 One-dimensional representation of a waste form that undergoes surface degradation at a uniform rate, u . x is the distance variable, y is the normalized distance variable such that at the surface $y=1$ at all times.

The rate of change in waste form length with time is the dissolution velocity, $dL/dt = u(t)$. Using this gives:

$$\frac{\partial C_i(y,t)}{\partial t} = \frac{\partial C_i}{\partial t} - \frac{u y}{L(t)} \frac{\partial C}{\partial y} \quad (2.50)$$

The dissolution velocity is negative since the length of the waste form decreases in time. For consistency with the uniform degradation model, the dissolution velocity is assumed to be solubility limited and is taken to be:

$$u_i(t) = - u_{o,i} L_o \left(1 - \frac{C_{s,i}}{C_{sat}} \right) \quad (2.51)$$

where

- $u_{o,i}$ = fractional degradation rate of the i^{th} contaminant, section 2.3.3 (1/s),
- L_o = original waste form half width (radius) (cm),
- $C_{s,i}$ = solution concentration of the i^{th} in the finite element from the transport equation,
- $C_{sat,i}$ = solubility limit of the i^{th} contaminant.

Using this definition, different radionuclides may have different dissolution rates due to the choice of fractional degradation rate or solubility limit.

Using the transformation in position and the definition of dissolution velocity the mass balance equation for the waste form becomes:

$$\begin{aligned} \theta \frac{\partial C_i}{\partial t} = & \frac{\theta D_{wf,i}}{L(t)^2} \frac{\partial^2 C_i}{\partial y^2} + \frac{V_{wf}}{L(t)} \frac{\partial C_i}{\partial y} + \frac{\theta u_i(t)y}{L(t)} \frac{\partial C_i}{\partial y} \\ & + C_{yi} \left[\frac{-\theta D_{wf}}{yL(t)^2} \frac{\partial C_i}{\partial y} + \frac{V_{wf} C_i}{yL(t)} \right] - \lambda_i \theta C_i + \sum_{j=1-N}^{j=i} f_{ij} \lambda_j C_j + S_i \end{aligned} \quad (2.52)$$

where

$$C_{yi} = \begin{cases} 0 & \text{for plane geometry} \\ 1 & \text{for cylindrical geometry} \end{cases}$$

Eqn. 2.52 forms the basis for the finite difference equations used to solve for the concentration related to diffusive species and immobile dissolving species. In Eqn. 2.52 the parameter θ is the volumetric content of the phase being modeled. For the mobile phase, it is the moisture content. For the immobile phase, it is the fraction of the waste form in the solid phase, $(1 - \eta)$, where η is the porosity of the waste form. In BLT-MS, the velocity of flow through the waste form, V_{wf} is set to zero.

For the immobile phase, Eqn. 2.52 greatly simplifies to the following:

$$(1 - \eta) \frac{\partial C_i}{\partial t} = \frac{(1 - \eta) u_i(t) y}{L(t)} \frac{\partial C_i}{\partial y} - \lambda_i \theta C_i + \sum_{j=1-N}^{j=i} f_{ij} \lambda_j C_j + S_i \quad (2.53)$$

where C_i is the concentration of the immobile species in the waste form. Eqn. 2.53 is used to calculate the immobile species concentrations in the waste form in BLT-MS. If the initial condition is a uniform concentration and the production due to sources and radioactive decay are also uniform, Eqn. 2.53 predicts a uniform concentration of immobile species in the waste form ($dC/dy = 0$ in the waste form). This is identical to the assumptions used to generate the analytical model. To improve the computational efficiency of BLT-MS, solution of Eqn 2.53 could be omitted and the releases due to degradation could be accounted for using the analytical model of section 2.3.3.

The initial conditions used in BLT-MS are homogeneous distribution of the mass within the waste form. This prevents the need to input detailed information on the distribution of contaminant within the waste form. The only information that is required is the waste form inventory, length, and volume. Conceptually, non-uniform initial conditions could be handled by the finite difference approach provided this information was provided.

The boundary condition used to calculate diffusive release from the waste form is the solution concentration in the finite element calculated by the transport equation. This allows direct coupling of the aqueous concentration to waste form release. This coupling is explicit as the aqueous concentration at the beginning of the time step is used and releases do not change this concentration instantly. That is, release is calculated from the finite difference model and the mass release rate per unit volume of the finite element is provided to the transport calculation. The aqueous concentration is calculated as a result of the waste form source as well as transport processes.

The treatment of solubility limited release is provided in section 2.3.6.

2.3.5.1 Qualitative Comparison of Predicted Releases Based on the Finite Difference and Analytical Release Models

The rinse models in the finite difference and analytical models are identical and will give identical release results if solubility limits do not apply.

The diffusion models in the finite difference and analytical models should also give essentially identical predicted release results if the following conditions apply.

- Dissolution does not substantially decrease the size of the waste form during the time required for diffusion release.
- Solubility does not limit release
- Ingrowth of progeny does not occur.

If substantial dissolution of the waste form does occur, the finite difference model will predict higher releases due to the shorter effective diffusion length as well as dissolution of the wastes.

The general degradation models in the finite difference and analytical procedures are slightly different conceptually. The analytical model assumes a fractional release rate independent of geometry. In the finite-difference models the conceptual model assumes a surface process which dissolves the waste form. The total mass release rate over a time step is proportional to the waste form surface area. For a plane waste form, this is constant and the results of the finite-difference model should be identical to the analytical model, section 2.3.3. However, for a cylindrical waste form, as the waste form radius decreases due to surface degradation, the surface area also decreases. At early times, the finite difference model for degradation of a cylindrical waste form predicts higher releases than either the plane finite difference model or the analytical model. This is because the waste form volume dissolved per unit time in a cylinder is initially greater than for a plane waste form. Verification test results for this process and analytical expressions for the releases from cylindrical waste forms for radioactive contaminants that do not experience ingrowth are presented in section 4.3.3.

Ingrowth is modeled in both the analytical and finite-difference degradation models. Since the contaminants available for degradation release are assumed to be immobile within the waste form, their distribution remains uniform at all times. Therefore, the analytical and plane finite difference models should give similar results when ingrowth occurs. The cylindrical geometry degradation model results will differ due to the geometric effect discussed in the previous paragraph.

In the case of solubility limited release, the total release to the transport equation through all mechanisms should be identical. However, the amount released that is attributed to each mechanism may be different due to the accounting procedures used. A full discussion of this process is deferred until section 2.3.6.

2.3.6 Solubility Limited Release

In BLT-MS solubility limited release is treated through attempting to limit the mass release rate per unit volume to the transport equation to a level such that the solubility limit of the radionuclide is not exceeded. BLT-MS uses an explicit procedure to estimate the amount of mass that can be released without exceeding solubility limits. This approach linearizes the equations and does not require solution of the release equations coupled into the matrix equation representing transport. This greatly simplifies the solution procedure.

The following procedure is used to limit releases from the waste form for the analytical release models. In this discussion it is implicit that the procedure applies individually for each contaminant. Therefore, the subscript i , which is used to define the contaminant under consideration, is omitted.

- The mass released due to the diffusion release mechanism is calculated. The aqueous solution concentration, C_{est} , is estimated by dividing the released mass, ΔM_p , by the volume of the water in the finite element (moisture content, θ , multiplied by element volume, V_e) and the porous medium retardation coefficient, R , as follows:

$$C_{est} = C(t) + \frac{\Delta M_d}{\theta V_e R} \quad (2.54)$$

This is the solution concentration that would occur if transport, decay, and ingrowth do not occur over the time step. Inclusion of the retardation factor is important as much of the mass released may sorb on the soil and not contribute to the aqueous solution concentration.

The estimated concentration is compared to a modified solubility limit, C_m , defined as:

$$C_m = C_{sat} + \frac{V_d [C_{sat} - C] \Delta t}{\theta RL} \quad (2.55)$$

Where V_d is the Darcy flow velocity, C is the aqueous solution concentration at the beginning of the time step, Δt is the time step size and L is the length of the finite element in the direction of flow. This is an heuristic attempt to account for transport due to flow over the time step. In general, BLT-MS under predicts releases when solubility limited release occurs because of the explicit solution procedure that is used. If an implicit procedure were used, this problem would not occur and the correction term would not be necessary.

After comparison of the estimated concentration and the modified solubility constraint, if the estimated concentration is less than the constraint, the entire diffusion mass is released. If the estimated concentration exceeds the constraint, the mass released is limited as follows:

$$\Delta M = [C_m - C] \theta V_e R \quad (2.56)$$

In this case ΔM is the mass required to bring the solution concentration to the modified solubility limit.

The analytical diffusion model can not adjust the released mass in a consistent fashion. Therefore, mass predicted to be released due to diffusion but limited by solubility is transferred to the rinse mass. This is equivalent to assuming that the mass is released due to diffusion and precipitates at the surface and is available for release immediately once the aqueous concentration drops below the solubility limit.

The mass released due to general degradation is calculated and the procedure is repeated. However, now, the estimated aqueous solution concentration is the concentration at the start of the time step plus the additional concentration resulting from the mass released due to diffusion and degradation. This estimated concentration is compared to the modified solubility constraint and the release due to degradation is restricted as necessary. Mass not released is transferred to the rinse release process. If the release from the diffusion process is sufficient to reach the modified solubility constraint, release of degradation mass to the transport equation does not occur.

Finally, the mass released due to the rinse with partitioning mechanism is calculated and the procedure is repeated with the estimated aqueous solution concentration based on the concentration at the start of the time step and the release from the diffusion and degradation models. Mass not released because of solubility constraints is available for release during the next time step.

Solubility limited release is treated in a similar fashion in the finite-difference models. However, in the finite difference models release is calculated simultaneously for all three release mechanisms. Therefore, there is a slight difference in the interpretation of the mechanism leading to release. In the finite-difference models, the total release from all three mechanisms is calculated and the estimated aqueous concentration is evaluated as before. If this value is less than the

solubility constraint, the entire mass is released for transport. If it is more than the solubility constraint, the mass released is limited as before. Mass predicted to be released due to dissolution and degradation but not released due to solubility constraints is transferred to the rinse model consistent with the conceptual model of precipitation on the surface. The mass released from each mechanism is estimated based on the fractional contribution of each mechanism. For example, if the models predicted 10% release from diffusion, 30% from degradation processes, and 60% from rinse processes and due to solubility constraints only $\frac{1}{2}$ of the mass was released during the time step, the finite difference models would release $\frac{1}{2}$ of the predicted mass of each mechanism. In contrast, the analytical models would have first released all of the diffusion mass (10%), then all of the degradation mass (30%) and only 10% of the rinse mass.

This difference in interpretation of the mechanism for release is not important in terms of the source to the transport equation. The analytical and finite difference models both provide the same source. In addition, since mass not released is transferred to the rinse model, both types of models (analytical and finite difference) provide the same disposition of mass at the end of the time step. In the above example, at the end of the time step, the finite difference model would end up with all of the mass not released, 50%, (5% from the diffusion process, 15% from the degradation process, and 30% from the rinse process) available for rinse release. As compared to the analytical model which would also have all the mass not released, 50%, available for rinse release.

While the interpretations for solubility limited release do not affect the source to the transport calculation, they do effect mass balances based on release mechanisms performed in BLT-MS. BLT-MS tracks the release by mechanism for the analytical models. Mass transferred from one mechanism to another is carefully followed and the output in the LEACHRL and LEACHMS files described in section 8 is consistent with the original input. For example, if the only mechanism for release is diffusion, the mass released due to diffusion in these files would equal the total mass released. Even if some of the diffusion mass is transferred to the rinse model due to solubility constraints. The code tracks the original source of the mass. In contrast, if the finite difference models are being used, mass transferred to the rinse release mechanism is treated as "rinse" mass. Therefore, when using the finite-difference waste model in solubility limited problems with diffusion and degradation processes, the rinse mass may actually increase in time due to the accounting procedure which transfers mass to the rinse release model.

2.3.7 Treatment of Chain Decay in the Waste-Form

Decay of radionuclides to produce other radionuclides can be an important process for uranium and thorium containing wastes. Progeny of these nuclides may be more mobile and provide higher doses per unit intake. BLT-MS accounts for production of progeny in the waste form prior to release and during transport. Definition of the decay chains is controlled by user supplied input. BLT-MS permits multiple decay chains and branching of decay chains. Guidance on how to simulate these processes within the BLT-MS framework is provided in section 6.

The treatment of chain decay is complicated by the multiple release models permitted in BLT-MS. Within a single waste form each radionuclide can have unique release mechanisms. For example, consider a three member decay chain. Species 1 could have all of the mass designated to be released via diffusion. While for species 2 it could be assumed that mass release is a uniform degradation process and species 3 could be assumed to release via rinse with partitioning. To complicate matters, each species may designate a fraction of the initial inventory to each of the release mechanisms. There is no obvious method for determining the release mechanism for the decay product, i.e., should the release mechanism remain that of the parent or of the progeny. This is an artificial result of defining multiple release mechanisms for a waste form. However, cases could be envisioned where the parent is released via diffusion while the progeny could be incorporated into the solid phase of the waste form and released by dissolution. Generally, data on the release from a waste form of different radionuclides in a decay chain do not exist. For this reason, it is strongly recommended that when using BLT-MS to simulate decay chains, that all members of the chain have the same fraction of mass available for release to each mechanism. Unusual results may occur when altering the release mechanisms on a radionuclide specific basis for members of a decay chain.

In BLT-MS the following assumptions are used when different release mechanisms are specified for the members of a decay chain:

- Prior to container breach, the mass that decays to the progeny are apportioned consistent with the input choices of release mechanism. For example, if the release mechanisms assigned to species 1 are 30% diffusion release and 70% rinse release while for species 2 100% uniform degradation release is specified, all of the mass that decays to species 2 will be assigned for release via the degradation model.
- After container breach, the release mechanism for the decayed mass remains the same as the parent. Using the above example after container failure, all of the mass that decays from the diffusion release portion is assigned to diffusion release for species 2 and similarly the decayed rinse mass is assigned to be released via the rinse mechanism for species 2. None of the decayed mass is assigned to the degradation release mechanism. This approximation was selected to avoid complications when solubility limited release occurs and to simplify the treatment of the finite difference equations. In the finite difference approach, with this assumption, mass that decays is transferred directly into the next member of the chains finite difference equation. Transferring mass among release mechanisms is possible, but difficult to achieve numerically in the finite difference equations.

The actual process for estimating ingrowth is accomplished by using an explicit estimate of decay. Prior to breach and at all times for the analytical models, the decay mass produced over a time step, Δt , for the j^{th} member of a chain is estimated from:

$$\Delta M_j = \sum_{i=1-N}^{i+j} f_{ij} M_i(t) [1 - e^{-\lambda_i \Delta t}] \frac{ATM(i)}{ATM(j)} \quad (2.57)$$

where

f_{ij} = fraction of decays of species i that produce species j ,
 $M_i(t)$ = mass available at time t , and
 ATM = atomic mass.

The ratio of atomic masses correction term is needed because the mass of the parents and progeny per atom are not identical. Eqn. 2.57 is repeated for each release mechanism and the mass is apportioned to the release mechanisms of the progeny according to the procedure described above.

After breach, for the finite difference release model, the decay is treated directly in the model equations as defined in the summation expression found Eqns. 2.52 and 2.53.

The coupling between different species due to radioactive decay is treated explicitly. That is, the mass or concentration value used to estimate ingrowth is that at the beginning of the time step. This approach removes the need to simultaneously solve each transport equation to determine the appropriate values to be used for ingrowth.

2.3.8 Selection of Waste Form Release Parameters

Due to the wide range of waste forms used in low-level waste disposal there is extremely little information on releases that is waste form specific. Even when there is information, it tends to focus on the short-lived radionuclides that have the highest activity in the wastes but not the highest impact in terms of potential dose to the public as evaluated through performance assessments. Typically, long-lived, mobile radionuclides are responsible for the majority of the estimated dose.

In estimating waste form release parameters it is recommended to use the rinse model without partitioning when contaminant specific, waste form specific data are unavailable. This model provides the highest release rate (instantaneous release of the entire inventory at the time of container failure) and therefore, highest doses through the ground water pathway in most instances. If ingrowth is of concern, the high release rate may cause releases from the facility to occur prior to substantial ingrowth and this may under predict release of progeny.

For many solidified waste forms it can be shown that diffusion is the rate controlling release process. If this is the case, and if waste-form specific contaminant specific data are unavailable, modeling of diffusion release can be accomplished with a waste form diffusion coefficient of 10^{-6} cm²/s. This value is the maximum acceptable value for a waste form diffusion coefficient [Lohaus, 1991]. A compilation of diffusion coefficients for solidified waste forms is presented in [Sullivan and Suen, 1989].

For metallic waste forms (activated metals) and glass waste forms surface degradation processes often control release. Estimates for metallic corrosion rates can be obtained by examining the soil corrosion data [Romanoff, 1957; Gerhold et al., 1981]. A discussion of these data and their applicability to modeling waste form release is in [Sullivan and Suen, 1989]. Similar, glass dissolution rates may be estimated from values reported in the literature. Often, due to the uncertainties in these processes, waste form release rates due to degradation processes are estimated based on values at the high end of those reported in the literature.

In all cases when there are large uncertainties in the release rate parameters, it is recommended that multiple analyses be performed sampling from the range of expected release rate parameters.

The waste form properties are independent of the transport properties and care must be taken to insure that properties are not accounted for twice. For example, if BLT-MS is used to model contaminated soils, it is inappropriate to use partitioning with waste form release and a distribution coefficient in the soil. If the soil is in a container, the rinse model should be used. After release, the contaminant will sorb to the soil based on the distribution coefficient used in the transport section of the code. In general, extreme care must be used when selecting to use a non-zero value for the waste form partitioning coefficient. Negative releases (i.e., sorption onto the waste form) can occur and the potential for accounting for sorption twice (in waste form release and during transport) is large. The waste form partitioning model has been the most widely misused of all BLT release models.

2.4 Migration (Transport)

The major pathway for release of most radionuclides disposed in a low-level waste disposal facility is movement with the groundwater. Movement of subsurface contaminants is influenced by the processes of groundwater flow, dispersion, diffusion, radioactive production and decay, geochemistry (solubility and sorption) and sources and sinks (waste form releases). The relative importance of these processes is site- and contaminant-specific.

In BLT-MS, after the completion of the waste form release calculations, the movement of the radionuclides through the subsurface system is calculated using a two-dimensional finite element approximation to simulate transport. The solution procedure is based on the computer code FEMWASTE-1 [Yeh, 1982] and it is a standard finite-element procedure.

The governing transport equation that is solved in BLT-MS is derived from a mass balance over the solid and liquid phases. The solid phase is treated using the assumption that it is immobile and the aqueous concentration is in chemical equilibrium with the solid phase concentration. The constitutive relationship between the mass adsorbed on the solid phase and that in the liquid phase is known as the sorption isotherm. BLT-MS uses a linear sorption isotherm. Water flow and moisture contents within the modeled domain are supplied through one of two procedures: separate input files created by FEMWATER [Yeh, 1987] or possibly other computer codes, or as part of the BLT-MS input file. The governing equation simulates the distribution and movement of contaminants due to advection, dispersion, diffusion, radioactive production and decay, sorption, first order liquid and solid degradation, and external sources and sinks (i.e., waste forms as well as other sources).

After obtaining the waste form mass release rates per unit volume for each container and each contaminant, BLT-MS takes this information and solves for the movement of each contaminant individually.

2.4.1 Transport Equation with Chain Decay

The governing transport equation is:

$$\theta R_i \frac{\partial C_i}{\partial t} = \nabla \cdot \theta D \nabla C_i + \nabla \cdot V_d C_i - \lambda_i \theta R_i C_i + \sum_{j=1}^{N-1} f_{ij} \lambda_j R_j C_j + S_i \quad (2.58)$$

$$- \chi_i \theta C_i - \mu_i \rho K_{di} C_i$$

where:

$$\theta D_{kl} = a_t |V_d| \delta_{kl} + (a_l - a_t) \frac{V_k V_l}{|V_d|} + D_m \theta \delta_{kl} \quad (2.59)$$

and

C_i	=	concentration of the i^{th} contaminant in the aqueous phase (g/cm ³),
t	=	time (s)
θ	=	volumetric moisture content,
R_i	=	retardation coefficient for contaminant i ,
R_i	=	$1 + \rho K_{di} / \theta$
ρ	=	bulk density of the soil (g/cm ³),
K_{di}	=	distribution coefficient for i^{th} contaminant in the porous media
θD_{kl}	=	component of the dispersion-diffusion tensor (cm ² /s),
a_t	=	transverse dispersion coefficient (cm),
V_d	=	Darcy flux through the porous medium (cm/s),
δ_{kl}	=	Kronecker delta, = 0 if k does not equal l and 1 when $k = l$
k and l	=	principal directions of the finite element domain,
a_l	=	longitudinal dispersion coefficient (cm),
D_m	=	molecular diffusion coefficient corrected for tortuosity through the porous medium (cm ² /s),
λ_i	=	radioactive decay coefficient of contaminant i (s ⁻¹),
f_{ij}	=	fraction of decays of contaminant i that form contaminant j ,
N	=	number of contaminants in the simulation,
χ_i	=	first order liquid phase degradation rate constant (s ⁻¹)
μ_i	=	first order solid phase degradation rate constant (s ⁻¹)
S_i	=	external source injection rate per unit volume (g/cm ³ -s).

Although not explicitly addressed in the above equation, many of the above parameters can also vary spatially due to local differences in the physical and chemical properties of the porous media. Typically when using BLT-MS to represent variations in transport properties, regions are defined with a unique set of material properties. For example, the cover system could be designated as material 1, the engineered concrete structure as material 2, the waste containing region as material 3, and the undisturbed soil surrounding the facility as material 4. Each of these material regions could be assigned unique transport properties. In BLT-MS, the diffusion coefficient, dispersion coefficients, bulk density, and porosity are allowed to vary for each material. The distribution coefficient and the liquid and solid degradation coefficients may vary with each contaminant and material.

In principal, the diffusion coefficients and dispersion coefficients could also vary with the contaminant being modeled. This is not considered in BLT-MS in order to reduce the input requirements. Typically, diffusion is not a dominant process in subsurface transport and therefore, using a single molecular diffusion coefficient representative of all contaminants in a material should not have a large effect on predicted outcomes. The effective diffusion coefficient (molecular diffusion coefficient divided by retardation coefficient) is material and contaminant specific. The dispersivity term is a mathematical

construct which has been shown to be useful in describing transport of contaminants in subsurface systems. Typically contaminant specific dispersion coefficients do not exist. Further discussion of dispersion coefficients is presented in section 2.4.4.

Eqn. 2.58 contains a generalized source term, S_i . This term represents all external sources to the transport equation. BLT-MS considers three distinct types of sources, waste form sources, volumetric sources, and well (point) sources. The values for the waste form source are calculated in accordance with the expressions provided in section 2.3. Their implementation into the transport equation is discussed in section 2.4.3. Volumetric and well sources are specified through tabular input of the source strength versus time as described in section 6.18 and 6.19. Volumetric sources are distributed over the volume of the finite element at which they are injected. Well sources are injected at a specific point in the modeled domain.

2.4.2 Initial and Boundary Conditions

BLT-MS permits the user to define the initial condition of each contaminant at each spatial location in the modeled domain. Typically, the initial concentration is zero everywhere.

For each contaminant, BLT-MS permits a selection from three boundary conditions:

Specified concentration:

$$C_i(x_b, z_b, t) = f_i(t) \quad (2.60)$$

Specified Total Flux:

$$n \cdot (V_d C_i(x_b, z_b, t) - \theta D \nabla C_i(x_b, z_b, t)) = g_i(t) \quad (2.61)$$

Specified Dispersive Flux:

$$-n \cdot \theta D \nabla C_i(x_b, z_b, t) = h_i(t) \quad (2.62)$$

Where n is the outward directed unit normal vector to the surface and the subscript b on the spatial coordinates identifies the location as being part of the boundary. In Eqn. 2.60 - 2.62 all boundary conditions are represented as a function of time. In addition, each contaminant can have its own unique set of boundary conditions. The values for the boundary condition functions, f_i , g_i , and h_i , are supplied through input as described in sections 6.17, and 6.18. Different boundary conditions can be used over different regions in the modeled domain. For example, for a contaminant, one boundary could have a specified total flux, while another boundary could have a specified concentration.

Selection of the boundary condition is an important aspect of defining the conceptual model of the system. The choice of boundary conditions will affect the model results. For example, consider a problem with vertically downward flow, selecting a zero concentration at the bottom boundary would lead to the maximum flux out of the system. However, it will not accurately calculate the concentrations at (or near) the boundary. Similarly, specifying a zero flux boundary condition will maximize the concentration at the boundary, but will not accurately represent the flux.

2.4.3 Treatment of Waste Form Sources

It is important for the analyst to recognize that within the finite-element framework, the waste form acts to provide a source to specific locations within the finite element domain, Figure 2.3. BLT-MS uses a substantially different approach to allocating the waste form source available for transport as compared to BLT.

In BLT, waste form sources were treated as volumetric sources and the mass released was delivered to the four nodal points within the finite element uniformly. For example, assuming the mass release rate per unit volume was one, the four corners would each receive 1/4 of the mass. While this is a consistent finite element approach, it is felt that this approach may underestimate peak concentrations that could occur.

In BLT-MS it is postulated that the waste form source should enter the two downstream nodes in the element. Using the preceding example and for simplicity assuming flow is downward and parallel to the z-axis, with the BLT-MS approach the concentrations in the two downstream nodes (i.e., the two bottom nodes) would be $\frac{1}{2}$ and the concentrations in the upstream nodes (i.e., two top nodes) would be zero. This may lead to higher predicted peak concentrations and earlier releases.

Calculation of the distribution of the source in BLT-MS depends on the flow direction. For the degenerate case of no flow, the source is split equally between the bottom two nodes of the finite element. When flow occurs, the allocation of the source depends on the geometry of the finite element and the magnitude of flow in both the X and Z directions. Figure 2.5 provides a graphical display of the selection of downstream nodes for a finite element with local node numbers 1, 2, 3, and 4 in the lower left, lower right, upper right, and upper left corners, respectively. The downstream nodes are selected based on the quadrants defined in Fig. 2.5 and the direction of flow. As drawn in Figure 2.5, nodes 2 and 3 are the downstream nodes.

Figure 2.5 General procedure to select upstream nodes based on the Darcy flux vector.

The amount released to each node is a function of the relative magnitude of velocities in the X and Z direction. For example, if flow is vertically downward, $V_x = 0$, the release is split evenly between nodes 1 and 2 in Fig. 2.5. As the horizontal velocity increases, the Darcy flux vector begins to point more towards node 2 and the waste form release is weighted in favor of node 2. For example, if the magnitude of V_x is $\frac{1}{2}$ of V_z , 75% of the waste form release rate would be given to node 2 and 25% to node 1. As the flow in the x-direction increases until the magnitude of velocity in each direction is equal, the weighting becomes more pronounced towards node 2. When the magnitude of the X and Z components of the velocity are equal, i.e., the flow lies parallel to one of the lines that defines the boundaries of the four quadrants, the entire source is placed in the one node. In our example, this would be node 2. As the X component of the velocity increases to a value greater than the Z component of velocity, the downstream nodes shift to become nodes 2 and 3. As long as V_z is negative, node 2 will receive greater weighting than node 3.

2.4.4 Selection of Transport Parameters

Proper selection of the transport parameters is critical to obtaining defensible estimates of the release and transport

of contaminants in the subsurface system. Whenever possible, site-specific, material specific values should be obtained.

The moisture content and Darcy flux required in Eqn. 2.58 are obtained through tabular input or other computer code analysis. A full discussion of how to obtain flow rates using the FEMWATER [Yeh, 1987] code is found in the data input guide for BLT [Sullivan and Suen, 1989]. Obtaining flow rates in unsaturated systems is a challenging task and beyond the scope of discussion here. A number of excellent reviews are available [Meyers et al., 1996; U.S. Nuclear Regulatory Commission, 1990]. These parameters are often critical to transport and care should be exercised to insure that the Darcy flux used to simulate flow adequately represent the system.

In general, diffusion coefficients are contaminant specific and porous media specific. However, they typically do not play a large role in transport in subsurface systems as transport in most systems is dominated by advective transport. Typical values for diffusion coefficients (including the effects of tortuosity) in soil are of the magnitude 10^{-6} cm²/s. If diffusion is the dominant transport process (low flow systems) more effort should be placed in accurately determining the diffusion coefficient under site specific conditions.

Dispersion is a term that refers to the observed spreading of contaminants in an advective flow field. Dispersion results from the fact that in a porous medium individual contaminants move at a different rate than the seepage velocity, which represents an average flow rate. The cause for the variation around the average flow rate is the different transport paths experienced by the individual particles as they flow through the pores and around the soil particles. Theoretically, if the exact flow paths were known for each particle, a model could be devised in which inclusion of the dispersion term is not needed. However, from a practical standpoint, these flow paths will not be known on a field scale and inclusion of the dispersion term provides a useful mathematical construct to examine contaminant transport.

Field measurements of dispersivity involve injection of a source and measuring the concentration at a downstream well. Using these data, the dispersivity values can be estimated. There are few measurements of field scale dispersivity. The measurements that do exist [Waldrop, 1985] generally indicate that the dispersivity increases with distance. Longitudinal dispersivities range from 0.1% to 10% of the distance between the source and measurement location. Transverse dispersivities are less than longitudinal dispersivities by a factor of 0.05 to 0.2. It is often recommended [Yeh, 1982; Looney et al., 1987] to use a longitudinal dispersivity value of 0.1 times the field scale and a transverse dispersivity of 0.1 of the longitudinal dispersivity. While this approach is useful as a guide to selecting dispersivity values, the data do not support selection of any particular value [Gelhar et al., 1992]. Dispersion is a site-specific process and requires site-specific parameters for accurate estimation.

Due to the uncertainties involved in estimating dispersivity values it is recommended that they should be varied within the range of expected values to determine the influence on release. In general, higher values of dispersivity will tend to spread the contamination out and lead to lower peak concentrations, while lower values of dispersivity provides less spreading and generally higher peak concentrations. For short-half life radionuclides dispersion may provide a mechanism to reach the monitoring point prior to decay.

The distribution coefficient is a measure of the amount sorbed on to the porous media in equilibrium with the aqueous solution concentration. It is often a critical parameter in estimating transport. A number of compilations of values for distribution coefficients in soil systems exist [Baes and Sharp, 1983; Looney et al., 1987; Thibault et al., 1990]. For most radionuclides, the compilations typically show a several order of magnitude range in distribution coefficient. This highlights the site-specific nature of this parameter and need for site-specific values. Again, due to the uncertainties involved in estimating this parameter, it is recommended to perform several analyses with K_d varied among the range of expected values to determine the importance of K_d on transport.

2.5 Limitations in the BLT-MS Computer Code

BLT-MS is capable of simulating a wide range of container, waste form, and material behaviors that will impact on subsurface transport of radionuclides disposed in a low-level waste facility. However, a number of assumptions have been made in the development of BLT-MS. Under certain conditions these assumptions may lead to limitations in the

applicability of BLT-MS. The potential limitations are:

- BLT-MS approximates only two spatial dimensions in rectangular co-ordinates.
- BLT-MS is structured as a deterministic computer code. The range of uncertainties in many transport parameters may require multiple simulations using BLT-MS. However, BLT-MS does not have a formal procedure for sampling among the input parameters. This task is left to the code user.
- The localized corrosion model is developed for pitting corrosion of carbon steels. Data for other materials are non-existent.
- Time-dependent changes in transport parameters are not modeled. For example, solubility and sorption properties are likely to change as the disposal facility degrades (degradation of concrete barriers, corrosion of metallic containers, etc.).
- Time-dependent changes in waste form release properties are not modeled with the exception of the partition coefficient. In addition to changes in chemical conditions which may effect release, physical changes to the waste form may occur (plugging of pores in concrete due to precipitation, surface layer formation on glasses and metals, swelling of resins, incorporation of radionuclides into the solid phase of the waste forms, etc) that may also effect release.
- The transport equation does not limit concentrations based on solubility. This may cause a problem for species produced due to radioactive decay during transport. For example, consider a two member decay chain at secular equilibrium with the solubility of the first member of the chain several orders of magnitude greater than that of the second member. Further, assume that the difference in decay constants is smaller than the difference in solubility limits. In this case, if the concentration of the first member is near its solubility limit, the predicted concentration of the second species will be above its solubility limit.
- Darcy flux and moisture content values are not calculated within BLT-MS. They must be supplied by input. Time dependent velocities can be accommodated through input files containing these data.
- The waste form leaching models consider surface rinse with partitioning, diffusion, and surface degradation. If other processes occur, such as swelling of bitumen wastes, or fracturing of glass or cement waste forms due to handling, other models may be necessary.

3 BLT-MS SOLUTION PROCEDURE

The first step towards using BLT-MS as a method for analyzing release and transport from a low-level waste disposal system is to define a conceptual model of the system and its behavior. This conceptual model should include all of the physical and chemical processes that are expected to significantly influence radionuclide release and transport. Based on this conceptual model, appropriate data on inventory, waste forms, containers, and transport properties are collected. The geometry of the different regions (engineered barriers, cover systems, waste containing region, soil layers, location of the water table, etc.) would also be defined.

In developing a conceptual model, assumptions are made to reduce the system into a form amenable for numerical simulation. A simple conceptual model would assume that the water flow is the natural infiltration rate, all containers fail instantly, all radionuclides are released from the waste forms instantly, and advective transport is limited by sorption and radioactive decay. More complexity could be added to the conceptual model to take credit for the engineered barriers, waste containers, and waste forms as needed. The general procedure to analyze releases from a low-level waste disposal facility is presented in Figure 3.1.

Figure 3.1 Flow chart of the procedure to examine releases from a subsurface disposal facility using BLT-MS.

Typically, four major processes are assumed to control the release and transport of radioactive contaminants in the groundwater pathway. They are:

- water flow,
- container performance,
- waste form performance, and
- transport.

The coupling between these four models in BLT-MS is schematically represented in Figure 3.2 and described below to provide the background for understanding the calculational procedure used in BLT-MS.

Figure 3.2 Coupling between major processes simulated in BLT-MS.

Water flow is a function of the local hydrology, disposal system design, and precipitation. Frequently, water flow is assumed constant for long periods of time with step changes in flow rate to simulate degradation of the cover system and engineered barriers. Transient events such as large storms or seasonal variations are generally not considered in safety assessment analysis. The justification for this is the long time frame of the analysis (hundreds or thousands of years), and the belief that over this time frame average flow rate values are acceptable for estimating transport.

In BLT-MS water flow is not calculated explicitly, it is defined through input. This implies that container

performance and leaching do not influence bulk water flow. In general, these effects are expected to be small. However, if subsidence occurs due to container collapse (or engineered barrier collapse) the flow rate may change drastically and will be a function of container performance.

Water flow rates and moisture content can be defined in the BLT-MS input file, or they can be defined in an auxiliary input file. Use of the auxiliary input file has the advantage of permitting time-dependent flow rates to be used during the simulation. The use of time-dependent flow rates can be used to represent engineered barrier failure or subsidence phenomena. Ancillary models would be necessary to predict barrier degradation and how it impacts on flow rates.

Container degradation modeling is contaminant independent and involves prediction of local corrosion effects (pitting) or general degradation (time to failure). The general degradation rate is independent of water flow as modeled in BLT-MS. The local corrosion rate can depend on the moisture content. It is assumed to be independent of waste form leaching and transport processes.

Modeling waste form release includes coupling with the water flow, container degradation, and transport models. The initial release and the release rate depend on the degree of container failure as a function of time as supplied by the container degradation models. The rinse release model with partitioning depends on the aqueous solution concentration surrounding the waste form which is a function of flow rate and other transport properties. The finite-difference waste form diffusion release model also depends on the aqueous solution concentration. If release is solubility limited, releases will depend heavily on transport processes (i.e., the faster the material moves away from the waste form, the faster the release rate is to maintain solubility). To simplify the numerical solution procedure, coupling between aqueous solution concentrations and waste form release is done explicitly (i.e., aqueous concentrations at the beginning of the time step are used when modeling release). This allows decoupling of the waste form release models from the transport models over a time step. This permits calculation of all waste form release rates prior to performing the transport calculation.

Modeling the migration of radionuclides requires the release rate per unit volume from the waste form leaching models and the water velocity and moisture content from input.

The BLT-MS calculational procedure is presented in Figure 3.3. The framework outlined in Figure 3.3 has the following procedures within each time step:

- update the water flow rates and moisture contents based on input, if necessary.
- calculate container performance.
- calculate radioactive production and decay in each waste form.
- if container failure has occurred, calculate waste form release rates for each contaminant in each container.
- calculate the transport of each contaminant over the time step.

Figure 3.3 Flow chart of BLT-MS solution procedure

4 VERIFICATION PROBLEMS

It is important to verify that BLT-MS can solve the types of problems for which it is intended. Verification is critical to building confidence in the reliability of the computer model. Verification is usually accomplished through comparison with other codes or known analytical solutions. Both approaches are used here.

Successful code verification does not imply that the model can or will be successfully applied to any particular problem. It is the job of the code user to demonstrate that the models incorporated into BLT-MS capture the major physical and chemical processes that influence release from the disposal facility, that the data selected to represent the system accurately reflect the expected values, and the code is properly used (i.e., time step selection, element size, application of the initial and boundary conditions, proper translation of the physical model into a form amenable to solution by computer, etc.).

Even when properly applied, BLT-MS, in all likelihood, will not be able to reproduce the actual release rates that will eventually occur with a high degree of accuracy. The causes for the discrepancies are the long time frame (hundreds or thousands of years) in most simulations, the complex, heterogeneous nature of the natural and engineered physical setting, the variability in wastes and container, and lack of understanding of the physical and chemical processes that control release and transport. These limitations apply to all models. BLT-MS provides an excellent method for evaluating the interaction between several processes that are believed to control release from a disposal site.

BLT-MS is an extension of the BLT code [Sullivan and Suen, 1989] and, as such, the waste form leaching and container degradation models have undergone extensive verification studies previously [Sullivan and Suen, 1989, 1991]. Verification test cases were performed to demonstrate that in the absence of chain decay the BLT-MS model could reproduce the results generated by BLT. The container degradation, waste form leaching, and transport models were all tested independently. For presentation in this report, verification problems focused on the improvements to the original BLT code which permit solution of multiple species in a single simulation. Two major classes of problem were investigated: multi-species transport with chain decay and release of contaminants from the waste form when ingrowth occurs due to radioactive decay. The results of these studies are presented in the following sections.

4.1 One-Dimensional Transport of a Single Three-Member Decay Chain

To demonstrate that BLT-MS can accurately simulate transport, a one-dimensional test problem for a three-member decay chain was simulated. This problem contained a boundary source for the three members of the chain. At the left boundary, $x = 0$, the incoming flux is the Darcy flux multiplied by the concentration of the radionuclide of interest. For the first member of the chain, the initial concentration is unity and this changes in time due to exponential decay. The concentration of the second and third members of the chain are calculated using Bateman's equation [Bateman, 1910] with the assumption that their initial concentration is zero. The time dependence of the boundary condition was simulated through tabular input of the boundary condition flux values at specified times, Table 4.1. Linear interpolation was used for times not in the table. For convenience, the concentration at the boundary that corresponds to the flux in Table 4.1, is also presented in Table 4.1. The initial conditions were zero concentration at all locations for all radionuclides being simulated. The distance simulated in this problem was 70 meters. This distance is large enough such that during the problem simulation time, 273 years, essentially no material reached the right boundary. An analytical solution for this problem on a semi-infinite domain exists [Coats and Smith, 1964]. For comparison purposes, the contaminant and material specific transport parameters for this test problem were chosen to match with those reported by Huyakorn [Huyakorn et al., 1989]. These parameters are reported in Table 4.2.

The decay chain in this problem assumes that species one always decays to species two which always decays to species three. Branching of the decay chain is not considered. The values of the half-lives in Table 4.2 for the three contaminants are similar to those of Am-241, Pu-241, and Pu-240. These three contaminants do not form a decay chain (e.g., Pu-241 decays to Am-241 which decays to Np-237). The half-lives were chosen to reflect a variety of decay rates over the time scale of interest (hundreds of years). The test problem selected the half-life of the first member of the chain to be

short enough to insure that decay would occur and long enough such that it would not all decay. The contaminants are referred to as species 1, 2, and 3 to emphasize that this problem does not represent a real decay chain.

Table 4.1 Incoming Flux and Concentration at the Boundary for the Single Decay Chain Problem

Flux versus time at the boundary (values used for the boundary conditions in the numerical simulations). Flux values are in (g/cm²/yr). Flux values are negative indicating material is flowing into the region bounded by $x = 0$.

Contaminant	Time(yrs)			
	0	91	200	300
1	-7.29 10 ³	-6.30 10 ³	-5.29 10 ³	-4.51 10 ³
2	0.0	-2.22 10 ²	-1.90 10 ²	-1.62 10 ²
3	0.0	-7.51 10 ²	-1.8 10 ³	-2.57 10 ³

Concentrations versus time at the boundary. Concentration values are in g/cm³.

Contaminant	Time (yrs)			
	0	91	200	300
1	1.0	.861	0.725	0.619
2	0	0.0305	0.026	0.022
3	0	0.103	0.247	0.353

Table 4.2 Transport Properties Used in the Three-member Decay Chain Transport Problem

Contaminant	Radionuclide Dependent Properties	
	T ½ (years)	Distribution Coefficient (K _d)
1	433	400
2	15	400
3	6540	400

Transport Properties for all Contaminants

Moisture Content	0.1
Darcy Flux	2.31 10 ⁻⁴ cm/s
Bulk Density	2.34 g/cm ³
Dispersion Coefficient	259 cm
Molecular Diffusion Coefficient	0 cm ² /s

The finite element solution was obtained on a uniform grid consisting of two elements 100 cm high in the z-direction and 70 elements 100 cm long in the X-direction. Flow was uniform in the X-direction and all transport properties were held constant over the modeled domain. The time step was one year for the entire simulation.

The distribution of the three contaminants as a function of distance at 273 years is presented in Figure 4.1. Comparison of the predicted concentrations with results obtained using VAM2D [Huyakorn et al., 1989] shows excellent agreement [Table 4.3]. Differences between the two simulations are generally less than a few percent in the regions where the concentration is within two orders of magnitude of the maximum incoming concentration (unity). Comparisons at other times during the simulation showed similar differences in predicted results. The largest differences occurred for contaminant three. This may be due to the different treatment of radioactive decay. The VAM2D simulations used a central time difference procedure whereas, BLT-MS used a fully implicit backward difference solution procedure. VAM2D results were compared directly to the analytical solution and the results were judged to accurately represent transport [Huyakorn et al., 1989].

Figure 4.1 Comparison of BLT-MS and VAM2D Predicted Concentrations at 273 Years for a Three Member Decay Chain

Comparison of the analytical values for the boundary concentration to the results predicted by the two codes indicates that in general BLT-MS provides slightly better estimates. The cause for this most likely lies in the different numerical treatment of the boundary conditions used in the two codes. It has not been demonstrated that the BLT-MS methodology is superior to VAM2D for anything other than this test problem. The analytical value for the concentration at the boundary at 273 years for contaminant one is 0.646 which is between the values projected by the two codes (0.66 for VAM2D and 0.638 for BLT-MS). For contaminant two, the analytical boundary value is 0.0232 which again lies between the VAM2D (0.0237) and the BLT-MS (0.0229) predictions. For contaminant three, the analytical value is 0.326, which is slightly greater than the BLT-MS estimate, 0.320, and the VAM2D estimate, 0.305.

Table 4.3 Comparison of VAM2D and BLT-MS Results at 273 Years for the One-dimensional Single Decay Chain Problem

Species 1	Distance (m)					
	<u>0</u>	<u>10</u>	<u>20</u>	<u>30</u>	<u>40</u>	<u>50</u>
BLT-MS	0.639	0.560	0.347	0.124	0.0229	0.0021
VAM2D	0.660	0.558	0.341	0.129	0.0220	N/A
Difference	-0.021	0.002	0.006	-0.005	0.0009	
% Difference	-3.2	0.4	1.8	-3.9	4.1	
Species 2	Distance (m)					
	<u>0</u>	<u>10</u>	<u>20</u>	<u>30</u>	<u>40</u>	<u>50</u>
BLT-MS	0.0229	0.020	0.0124	0.00446	0.000827	.7E-5
VAM2D	0.0237	0.020	0.0122	0.00465	0.000799	/A
Difference	-0.00080.0	0.0002	-0.00019	0.000028		
% Difference	-3.4	0.0	1.6	-4.1	3.5	
Species 3	Distance (m)					
	<u>0</u>	<u>10</u>	<u>20</u>	<u>30</u>	<u>40</u>	<u>50</u>
BLT-MS	0.32	0.281	0.175	0.0633	0.0119	0.0011
VAM2D	0.305	0.259	0.160	0.062	0.0114	N/A
Difference	0.015	0.022	0.015	0.0013	0.0005	
% Difference	4.9	8.4	9.4	2.1	4.4	

4.2 One-dimensional Transport with Two Decay Chains

To demonstrate the ability of BLT-MS to simulate multiple decay chains with branching, the preceding test problem was modified. The change in the problem involves the definition of the decay chain. In this simulation, species one decays to species two one-half the time and it decays to species three one-half of the time. Species two always decays to species three. The change in decay chain causes a change in the boundary conditions for the second and third species. The new boundary conditions are presented in Table 4.4. In the multiple decay chain model, all transport parameters are identical to the problem described in section 4.1 and Table 4.2

The change in the decay scheme reduces the source for species two by a factor of one-half. This is reflected in the boundary flux specified in Table 4.4. Therefore, predicted concentrations for species two should be one-half the value of the previous test case. The situation is more complex for species three. One-half of the decay from species one goes directly to species three while the other half goes to species two before decaying to species three. The decay directly to species three would indicate that the predicted concentrations should be higher than in the previous case when all of species one decayed to species two prior to becoming species three. Due to the short-half life of species two (15 years) this effect is not large.

If the half-life of species two were much larger (hundreds or thousands of years), the effect of branching on species three would be much more pronounced.

Table 4.4 Incoming Flux and Concentration at the Boundary for the Two Decay Chain Problem

Flux versus time at the boundary (values used for the boundary conditions in the numerical simulations). Flux values are in (g/cm²/yr). Flux values are negative indicating material is flowing into the region bounded by $x = 0$.

Contaminant	Time(yrs)			
	0	91	200	300
1	-7.29 10 ³	-6.30 10 ³	-5.29 10 ³	-4.51 10 ³
2	0.0	-1.11 10 ²	-9.50 10 ¹	-8.1 10 ¹
3	0.0	-8.60 10 ²	-1.89 10 ³	-2.65 10 ³

Concentrations versus time at the boundary. Concentration values are in g/cm³.

Contaminant	Time (yrs)			
	0	91	200	300
1	1.0	0.861	0.725	0.619
2	0	0.016	0.013	0.011
3	0	0.118	0.260	0.364

The results from this simulation are presented in Table 4.5 and compared to the previous results from BLT-MS. The results are as expected. Species one predicted concentrations remain unchanged, species two concentrations have decreased by ½, and species three concentrations have increased by a few percent. A graphical display of the results generated by VAM2D is presented in [Huyakorn et al., 1989]. Comparison of the BLT-MS predicted concentrations to those in the graph showed agreement similar to that found for the problem described in section 4.1 (i.e., differences in predicted values less than 10%). A detailed estimation of the differences could not be made because of the difficulties in obtaining two significant figures from the graph.

Table 4.5 Comparison of BLT-MS Results at 273 Years for Chain Decay and Chain Decay with Branching

In the branched chain example, species one decays to species two one-half of the time and to species three the other half. Species two decays to species three all the time.

Species 1	Distance (m)					
	0	10	20	30	40	50
Single chain	0.639	0.560	0.347	0.124	0.023	0.0021
Branched chain	0.639	0.560	0.347	0.124	0.023	0.0021
Species 2	Distance (m)					
	0	10	20	30	40	50
Single chain	0.0229	0.020	0.0124	0.00446	0.000827	7.7E-5
Branched chain	0.01148	0.010	0.00622	0.00223	0.000414	3.8E-5
Species 3	Distance (m)					
	0	10	20	30	40	50
Single chain	0.32	0.281	0.175	0.063	0.0119	0.0011
Branched chain	0.331	0.290	0.181	0.065	0.0123	0.0016

4.3 Ingrowth of Progeny Prior to Release from the Waste Form

For radionuclides that are members of a decay chain, their inventory will change in time prior to release from the waste form. A test problem was devised to demonstrate that BLT-MS could accurately simulate ingrowth in the waste form. In the test problem, there are two containers with identical waste forms. The first container fails at emplacement, (time = 0) and the second fails after 99 years. In BLT-MS for the analytical release models, the mass assigned for release due to one mechanism is independent of the other mechanisms (i.e., mass apportioned to diffusion must be released via diffusion).

4.3.1 Rinse Model

The rinse model releases all of its available inventory during the first time step after container breach. Therefore, it provides an excellent method of testing the BLT-MS calculation of ingrowth in the waste form because the analytical inventory prior to release can be calculated using the Bateman equations. In this test problem, the three contaminants from the previous example were used. The initial inventory of species one was selected to be unity while the initial inventory of species two and three was zero. Therefore, any inventory of species two and three is a result of radioactive decay and ingrowth. The half lives are given in Table 4.2.

The results of this test are presented in Table 4.6. For the container that failed at time 0, species one released the entire inventory as expected. At 99 years, the time of failure for the second container, the predicted results matched the analytical results to three significant figures.

Table 4.6 BLT-MS Predicted Rinse Release Compared to Analytical Rinse Release (Analyt)

Container Failure Time (yrs)	Species 1		Species 2		Species 3	
	BLT-MS	Analyt	BLT-MS	Analyt	BLT-MS	Analyt
0	1.0	1.0	0	0	0	0
99	0.852	0.852	0.0309	0.309	0.116	0.116

4.3.2 Diffusion Model

BLT-MS contains two classes of waste form leaching diffusion release models. The first class contains analytical solutions for diffusion from a finite-sized cylinder or plane with a uniform initial concentration and zero concentration at the boundary between the outside edge of the waste form and the contacting solution. When diffusion can be shown to be the dominant release mechanism, these models can be an excellent approximation to release from solidified waste forms. The second class contains a one-dimensional finite difference representation of diffusion through a solidified medium. This procedure is more general and permits solution feedback effects (non-zero concentrations at the boundary, e.g., solubility limited), and non-uniform production due to decay to be addressed in the framework of diffusion controlled release. These models are discussed in detail in section 2.3.2 and 2.3.5.

When ingrowth occurs, the assumptions used to generate the analytical solution are no longer met. The production of progeny depends on the distribution of the precursor radionuclide. Even if the parent radionuclide begins with a uniform distribution in the waste form, due to the diffusion process, in time, the parent will have a spatially dependent distribution which implies a spatially dependent production rate of the progeny. To overcome the lack of an analytical solution for the case of a spatially varying source, the approximation is made that the spatial distribution of the source due to decay is identical to the spatial variation in concentration of the progeny in the waste form. In this case, the effect is to shift the entire concentration versus location curve in the waste form up to account for ingrowth. This approximation allows the analytical solution for diffusion release to be retained by simply adjusting the "initial concentration". This approximation does not have a physical basis although it will conserve mass. In most cases, this approximation will tend to under predict releases from the waste form of the progeny species. If diffusion controlled release from the waste form is important, the use of the analytical diffusion models is not recommended when ingrowth occurs.

In contrast, the finite-difference leaching model accounts for the spatial variation in production rate as the problem evolves. Ingrowth is calculated within each finite difference volume used to represent the waste form. Therefore, if the parent and progeny have different diffusion rates this is automatically calculated as part of the solution procedure.

Several test problems were simulated to test the diffusion-controlled release leaching model when ingrowth occurs. The test problems considered three species. The initial inventory of species one was unity while the initial inventory of the second and third species was zero. In the first test problem, the diffusion coefficient of each species was 10^{-8} cm²/s. The waste form was assumed to be represented by a plane with a half-width of 25 cm. Two containers were considered, the first failed upon emplacement, the second failed after 99 years. The half-lives of the contaminants are those used previously and can be found in Table 4.2.

Table 4.7 contains the cumulative release and mass available for release after 273 years for the three species. For the first species the results of the two models are essentially identical. This indicates that the finite-difference model can accurately reproduce the analytical solution when ingrowth is not a concern. For the second species the available mass in the two models is almost identical. This is due to the short-half life of the second species as compared to the first. It is in equilibrium with the parent at this time. This result indicates that the finite-difference model is accurately accounting for ingrowth. The amount of species two released is substantially higher for the finite-difference model as compared to the approximate analytical model. Similarly for species three, the amount released is higher for the finite-difference model. For

both species two and three, the difference between the two models is greatest for the container that failed at $t = 0$. This is expected because as the diffusion time increases, the approximation used in the analytical model to correct for ingrowth loses accuracy.

Table 4.7 Comparison of Finite-Difference (FD) and Approximate Analytical Model (AAM) Predictions for Cumulative Fractional Release (Rel) from a Plane Waste Form with Each Species Having Identical Diffusion Coefficients

Mass in the waste form available for release is presented under the columns labeled Avl.

Model	Species 1		Species 2		Species 3		Container Failure time
	Avl	Rel	Avl	Rel	Avl	Rel	
FD	0.376	0.363	0.0135	9.37E-3	0.1892	0.0442	0
AAM	0.375	0.365	0.0136	1.74E-3	0.2051	0.0345	0
FD	0.430	0.259	0.0154	9.28E-3	0.216	0.0630	99
AAM	0.429	0.261	0.0156	4.64E-3	0.224	0.0594	99

Assuming negligible decay of the third species (half-life 6540 years) over the 273-year time frame that was simulated an approximate mass balance can be obtained by summing up the mass available for each species and the mass released for each species. It should sum to approximately one. The mass balance error for all four cases is less than 1%.

A similar test problem was simulated for a cylindrical waste form with a 25 cm. radius. The analytical diffusion model in cylindrical geometry also accounts for the finite height of the waste form. In this problem the height was set to a large value (>5000 cm) to insure that release occurred primarily in the radial direction. This allowed direct comparison with the finite-difference model which only simulates the radial direction. Other than the change in geometry, all other parameters were unchanged from the problem described above in this section.

Table 4.8 presents the cumulative release and mass available after 273 years for three species from a cylindrical waste form. The releases of the first species are much higher in this case. This is due to the geometry, more of the mass lies closer to the outside boundary in a cylinder of 25 cm radius as compared to a plane of 25 cm half-width. Thus, the average diffusion length is shorter and the release is higher. Again agreement between the analytical diffusion model and the finite-difference model is excellent for the first species. For the second and third species, the results were similar to those found for plane geometry. The finite-difference model predicts higher releases of each species with the difference between the two models more pronounced as the diffusion time (time since breach) increases. Again, mass balance errors were less than 1%.

Table 4.8 Comparison of Finite-difference (FD) and Approximate Analytical Model (AAM) Predictions for Cumulative Fractional Release (Rel) from a Cylindrical Waste Form with Each Species Having Identical Diffusion Coefficients

Mass in the waste form available for release is presented under the columns labeled Avl.

Model	Species 1		Species 2		Species 3		Container Failure time
	Avl	Rel	Avl	Rel	Avl	Rel	
FD	0.204	0.607	7.3E-3	0.0147	0.103	0.063	0
AAM	0.195	0.619	7.4E-3	0.0029	0.143	0.039	0
FD	0.276	0.451	9.9E-3	0.0163	0.138	0.105	99
AAM	0.266	0.462	1.0E-2	0.008	0.188	0.096	99

4.3.3 Uniform Degradation Model

There are two major classes of solution procedure for the uniform degradation model. The analytical uniform degradation model, which in the absence of ingrowth and decay, projects a uniform time independent release rate until the entire inventory is released. For example, if the fractional degradation rate was 0.01 per year, 1% of the inventory would be released for 100 consecutive years after breach. This release is adjusted for decay and ingrowth as discussed in section 2.3.7.

The second class of degradation model is the finite-difference models, discussed in section 2.3.5. The finite-difference models can simulate either plane or cylindrical geometry. In either case, the fractional degradation rate is multiplied by a characteristic length (width for plane geometry, radius for cylindrical geometry) to obtain a dissolution velocity. The release rate is the concentration in the waste form available for uniform degradation release multiplied by the dissolution velocity multiplied by the surface area to volume ratio of the waste form. For plane geometry, this reduces to an expression identical to the analytical model. For cylindrical geometry, the effects of curvature cause a time-dependent release rate. That is, the amount released is proportional to the surface area which is a function of the time-dependent radius. As the radius decreases due to dissolution, the surface area decreases and so does the release rate.

To test the dissolution models in BLT-MS the test problem described in the previous section was modified slightly. The problem again considers three species with the initial condition that species one has a unit inventory while species two and three are initially absent. The fractional degradation rate was set to 0.001 for all three species. Two container failure times, 0 and 99 years, were simulated. For the finite-difference models, the half-width was set to 25 cm for plane geometry and the radius was set to 25 cm for cylindrical geometry.

The results of this test problem are presented in Table 4.9. As expected, the analytical model and the plane-geometry finite difference model gave identical results for all three species. The cylindrical release model exhibits higher releases as expected. As before an approximate mass balance can be obtained by summing up the mass available for each species and the mass released for each species. In all three cases, the mass balance error was less than 1%.

Table 4.9 Comparison of Plane Finite-difference (PFD), Cylindrical Finite Difference (CFD) and Analytical Model (AM) Predictions for Cumulative Fractional Release (Rel) from a Waste Form with Each Species Having Identical Fractional Release Rates

Mass in the waste form available for release is presented under the columns labeled Avl.

Model	Species 1		Species 2		Species 3		Container Failure time
	Avl	Rel	Avl	Rel	Avl	Rel	
PFD	0.470	0.221	0.0168	7.48E-3	0.24	0.0448	0
AM	0.469	0.221	0.0165	7.38E-3	0.239	0.0445	0
CFD	0.342	0.386	0.0123	0.0129	0.224	0.073	0
PFD	0.534	0.129	0.0191	4.84E-3	0.271	0.0395	99
AM	0.533	0.129	0.0187	4.75E-3	0.272	0.0396	99
CFD	0.441	0.238	0.0158	8.88E-3	0.1745	0.0711	100

To verify the accuracy of the models an analytical expression for the cumulative fractional release is obtained for the first member of the chain.

$$Q = \int_0^t u L_0 M_0 e^{(-\lambda t)} \frac{A(t)}{V_0} \quad (4.1)$$

Where u is the fractional degradation rate, L_0 is the characteristic length (width for plane geometry, radius for cylindrical geometry), M_0 is the initial inventory in the waste form, λ is the decay constant, V_0 is the volume of the waste form at emplacement, and $A(t)$ is the surface area of the waste form. For plane geometry, $L_0 A(t)/V_0$ is unity and the expression reduces to:

$$Q_p = \frac{u M_0}{\lambda} [1 - e^{(-\lambda t)}] \quad (4.2)$$

For the container that fails at emplacement, evaluation of the above expression at 273 years yields a value of 0.22 as predicted by the BLT-MS analytical model and plane finite-difference model. For the container that fails at 0.99 years, M_0 is reduced to 0.85 (to account for decay prior to breach and t is 174 years. In this case, the analytical release is 0.13 which agrees with the BLT-MS model predictions. The above relationship could be generalized by replacing $M_0 e^{(-\lambda t)}$ by the expression for the mass as a function of time as determined from the Bateman equations.

For cylindrical geometry, L_0 is the initial radius r_0 , V_0 is the initial volume of the waste form, $\pi r_0^2 h$, and $A(t)$ is the area which can be expressed as:

$$A(t) = 2 \pi h r_o (1 - ut) \quad (4.3)$$

Using these expressions,

$$L_o A(t)/V_o = 2(1 - ut) \quad (4.4)$$

Placing this into the integral for Q(t) yields:

$$Q_c = \frac{2 u M_o}{\lambda} \left[\left(1 - \frac{u}{\lambda}\right) (1 - e^{(-\lambda t)}) + u t e^{(-\lambda t)} \right] \quad (4.5)$$

Evaluation of this expression at 273 years yields a cumulative fractional release of 0.38, consistent with the prediction of the cylindrical finite-difference model.

5 BLTMSIN: A PRE-PROCESSOR FOR CREATING INPUT FILES FOR BLT-MS

BLTMSIN is a FORTRAN program designed to assist the BLT-MS code user in creating input for BLT-MS. It is capable of creating a new input file, or modifying an existing file. Use of BLTMSIN offers two major advantages over creating BLT-MS input without the aid of the preprocessor. First, BLTMSIN relieves the code user of knowing the exact format and structure of the input file, as discussed in detail in section 6. While most numeric input in BLT-MS is list-directed and therefore, not limited to any particular region of an input line, the input is still structured. That is, input for parameter A appears before input for parameter B and so on. The second major advantage in using the BLTMSIN code is that it provides an annotated input file for BLT-MS. This greatly facilitates direct modifications of the input when changing a few variables.

A BLT-MS input file is structured into 23 data sets. Each data set contains a group of variables that are used to describe certain processes that are simulated in BLT-MS. For example one data set will contain all of the variables that describe container performance while another data set will define initial conditions, and so on. BLTMSIN is structured with a one to one correspondence to the data sets in a BLT-MS input file.

BLTMSIN is an interactive code that works by supplying a series of menu's that direct the user through the steps necessary to create BLT-MS input. Upon starting BLTMSIN, the code user is asked if a new input file is to be created or an existing file is to be modified. After this selection and if necessary, reading an input file, the main menu is displayed, table 5.1. The main menu is structured to correspond to the input structure described in section 6. Each main menu item controls access to one of the data sets of section 6. From menus, the code user can modify any variable in the input. This flexibility makes it nearly impossible to guarantee that valid BLT-MS input will be created. Although many checks have been placed within the code to prevent obvious problems, it is possible to create an input file that is not valid. For this reason, when reading in an existing file, BLTMSIN does not perform checks on the validity of the input file.

Table 5.1 Main Menu in BLTMSIN Program

(1)	Problem Identification (Data Set 1)
(2)	Integer Velocity and Steady state Parameters (Data Set 2)
(3)	Container and Waste Parameters (Data Set 3)
(4)	Integer Integration Parameters (Data Set 4)
(5)	Integer Time Control Parameters (Data Set 5)
(6)	Grid and Element Parameters (Data Set 6)
(7)	Parameters for Boundary Conditions (Data Set 7)
(8)	Parameters for Sources (Data Set 8)
(9)	Chemical Component Information (Data Set 9)
(10)	Time Control Parameters (Data Set 10)
(11)	Parameters for Nonlinear Solve (Data Set 11)
(12)	Element & Node Coordinate Data (Data Set 12)
(13)	Porous Media Properties (Data Set 13)
(14)	Material Type Correction (Data Set 14)
(15)	Initial/Pre-Initial Conditions (Data Set 15)
(16)	Cauchy/Neumann Boundary Conditions (Data Set 16)
(17)	Dirichlet Boundary Conditions (Data Set 17)
(18)	External Volumetric Sources (Data Set 18)
(19)	External Point (Well) Sources (Data Set 19)
(20)	Waste Container Parameters (Data Set 20)
(21)	Waste Form And Leaching Info (Data Set 21)
(22)	Printer and Auxiliary Control (Data Set 22)
(23)	Hydrological Data (Data Set 23)
(24)	Exit/Make Deck

For example, the number of containers defined in data set 3 could be set to 10 while the container locations, which are specified in data set 20, could be left undefined. If this occurs, the input file made by BLTMSIN would not work when used by BLT-MS. BLT-MS would print an error message with information pertaining to the cause for failure. In addition, as discussed in section 8, when using BLT-MS the file INPTECHO.DAT is created. INPTECHO.DAT acts to print out the input as it is read by the code before any processing occurs. Between INPTECHO.DAT, the BLT-MS primary output file, and the error message the cause for failure can be determined. At this point, the input file is read back into BLTMSIN and the error corrected.

After selecting an item from the main menu, a sub-menu appears. For data sets that require input of large amounts of information, this sub-menu will contain a list of choices to define which variable to modify. Upon selecting the variable to define, BLTMSIN prints the current values for the parameters and asks if they are:

- acceptable, in which case the program returns to the menu one level above the current menu.
- if modifications are desired, in which case several options are permitted depending on the parameter being defined. For single-valued real and integer parameters, BLTMSIN will list the current value of the variable (this is called the default value in BLTMSIN) and await for input to change the value. If the user hits the enter key, the 'default' value is retained for numeric input. For character input, a blank will be entered into the variable in this case. After a value is input it becomes the new 'default' value. For arrays, often a sequence of values can be defined through input of a few parameters. Instructions on how to define sequences of values are provided in the parameter definition sections. Again when defining new values if the user hits the enter key, the current value is retained.
- if a description of the parameters is desired a detailed text definition is supplied.

BLTMSIN is structured to read certain types of input (real, integer, or alpha-numeric character) based on the parameter defined. Improper input may cause the program to fail. Many checks are supplied in the code to prevent this from occurring. However, the checks are not foolproof. For example entering a character string when numeric input is required under certain cases will cause termination of the program. If an integer is input into a real variable, the code will translate the integer to a real number.

6 BLT-MS INPUT GUIDE

BLT-MS is an extension of the BLT code, it handles up to 10 different contaminants in a single run and can simulate multiple decay chains. In many respects, the input variables of BLT-MS are similar to those found in BLT. The reader is referred to the BLT input guides, NUREG/CR-5387, "Low-Level Waste Shallow Land Disposal Source Term Model: Data Input Guides" for additional guidance [Sullivan and Suen, 1989].

While there are many similarities between the BLT and BLT-MS input formats, there are also substantial differences. The BLT-MS code uses an annotated input file that allows the user to write comment lines and define the input variables that follow. In this sense, it is similar to the DUST code [Sullivan, 1993]. In addition, many of the variables are read into BLT-MS using free-format (list-directed) input. This removes the restriction of aligning variables within certain columns as required by BLT. However, values of zero can no longer be input by leaving certain columns blank. A value must be specified for each value required for input. List directed input also permits placing comments at the end of the line after all of the numeric information has been completed.

BLT-MS input is divided into 23 data sets, Table 6.1. Each data set is a unique grouping of input variables which perform a specific function within BLT-MS. In the BLT-MS input, each data set starts with a comment line (up to eighty characters) that identifies the data set. Each data set ends with a blank line. In the examples, this is denoted by the word BLANK'. Between the data set title card and the blank line a series of comment lines and data lines are found, the number depending upon the data set and the amount of information requested. The structure of a typical data set is found in Table 6.2.

The remainder of this section proceeds through all 23 data sets providing definition of each variable in BLT-MS and the FORTRAN read statements and the logic used when deciding which input to read. An example is provided for each data set. Each example is printed in **bold face**. The example input can be found in its entirety on the file CHAIN7.DAT included with the code package and reproduced at the end of this chapter as Table 6.3. In practice, depending on the options selected, actual input may not require numeric input for each variable. If an example is provided for an option that is not used by CHAIN7.DAT, this will be clearly marked and the example will be printed in *italics*. The first nine data sets contain integer parameters used to define the problem and select options.

When using BLT-MS, the code asks for the name of the input file for this problem. This file is designated as unit 5. BLT-MS creates a file called INPTECHO.DAT. This file echos the input as it is read. It is extremely useful in determining the cause of an error in the input. In BLT-MS INPTECHO.DAT is designated as unit 4. These unit designations can be seen in the FORTRAN programming found in BLT-MS and presented in this section.

6.1 DATA SET 1: Title and Problem Definition

This data set reads in the problem identification number and the title of the problem. This data set contains one of the few formatted reads used for input. The integer NPROB must end in column 5.

Definitions:

NPROB = Problem identifier. If NPROB is greater than 0, the problem is run. If NPROB is less than or equal to 0, the program is stopped.

TITLE = Alpha-numeric description of the test problem.

Format:

```
100    read(5,9) set1
       write(4,9) set1
```



```

9    format(80a1)
      READ (5,10) NPROB,TITLE
      write(4,10) NPROB,TITLE
10   format(15,70A1)
      read(5,9)blank
      write(4,9)blank

```

Example:

```

C *** DATA SET 1: PROBLEM IDENTIFICATION AND DESCRIPTION-- BLTMS-DATA
1  Prob2: Three species decay chain. Containers
BLANK '

```

Table 6.1 BLT-MS Data Sets

<u>Data Set</u>	<u>Title</u>	<u>Types of Values Defined</u>
1	Problem Identification	Title and problem identifier
2	Integer Velocity and Steady state Parameters	Selection of source for Darcy flux
3	Container and Waste Parameters	Number of contaminants, containers and waste types
4	Integer Integration Parameters	Numerical solution control factors
5	Integer Time Control Parameters	Number of time steps
6	Grid and Element Parameters	Number of nodal points and finite elements
7	Parameters for Boundary Conditions (BC)	Number of BC nodes, profiles, table length
8	Parameters for Sources	Number of element and point sources, profiles, table length
9	Chemical Component Information	Contaminant name, half-life, solubility limit
10	Time Control Parameters	Time step size, maximum simulation time
11	Parameters for Nonlinear Solve	Not used in BLT-MS
12	Element & Node Coordinate Data	X and Z locations, element definitions, automatic mesh generation if selected
13	Porous Media Properties	Diffusion, dispersion, coefficients, porosity, and isotope dependent properties such as distribution coefficient
14	Material Type Correction	Redefine material index
15	Initial/Pre-Initial Conditions	Initial concentrations for all contaminants
16	Cauchy/Neumann Boundary Conditions	Flux at the specified boundaries
17	Dirichlet Boundary Conditions	Concentration at the specified boundaries
18	External Volumetric Sources	Element source strength versus time and their location
19	External Point (Well) Sources	Point source strength versus time and their location
20	Waste Container Parameters	Container performance parameters, container locations
21	Waste Form And Leaching Info	Waste form performance parameters, inventory
22	Printer and Auxiliary Control	Output control for the main output file and the trace files
23	Hydrological Data	Velocity at each nodal point, and moisture content in each finite element.

Table 6.2 Sample Structure of a BLT-MS Data Set

1ST line Alpha-numeric Data Set identifier
 2nd line Alpha-numeric label describing data
 3rd - Nth line Numeric data (list directed so data is ordered, but not restricted to any column)
 Final line 'Blank'. All data sets end with an alpha-numeric line. Any alpha-numeric identifier could be used, however, it is typically left blank.

For example,

```
C ***** DATA SET 3: INTEGER PARAMETERS FOR CONTAINERS AND WASTE
      NISO      NCON      NCTYPE      NWTYPE      IDIFF      IACT
      3          6          2          1          3          0
'Blank'
```

6.2 DATA SET 2: Velocity and Steady-State Input Options

This data set reads in two parameters that control the source for input of water flow Darcy flux and determine whether a steady-state or transient calculation will be performed.

Definitions:

- KVI = Velocity Input Control
 - ≤ 0, Card input for Darcy flux and moisture content. Pressure head data is not required.
 - = 1, Steady state flux and pressure input via a file created by FEMWATER and stored on logical unit 1.
 - = 2, Transient flux and pressure head input via a file created by FEMWATER and stored on logical unit 1.
- KSS = Steady-State controls
 - = 0, Steady state solution calculated. A steady-state solution may be desired to obtain the initial conditions for a transient calculation, or to obtain the final state of the system.
 - = 1, Steady state solution is not calculated.

If KVI is greater than zero, the spatial locations of all node coordinates and the finite element definition are also read in through the FEMWATER files. This is discussed in detail in section 6.12.

Format:

```
C ***** DATA SET 2: BASIC INTEGERS
C-----
      read(5,9) set2
      write(4,9)set2
      read(5,9) label
      write(4,9)label
      READ (5,*) KVI,KSS
      write(4,10) KVI,KSS
      read(5,9) blank
      write(4,9)blank
C-----
```

```

C ***** DATA SET 2: INTEGER PARAMETERS FOR VELOCITY INPUT AND STEADY STATE
      KVI  KSS
      -1   1
      BLANK'

```

Comments:

In this example, KVI is set to require input for velocity and moisture content as part of this input deck. A steady state solution is not desired (this is the normal situation). Note that the data is read using a list directed read statement. Also note that in defining the label card, variable names were written. Any valid alpha-numeric text is acceptable.

6.3 DATA SET 3: Integer Parameters for Waste Form and Contaminants

Integer parameters to define the number of isotopes, plus parameters used to define the container and waste form properties are specified in this data set.

Definitions:

- NISO = Number of isotopes in the simulation ($1 \leq \text{NISO} \leq 10$).
- NCON = Number of containers with waste forms ($0 \leq \text{NCON} \leq 100$).
- NCTYPE = Number of different container types. Each container type has unique corrosion rate properties (i.e., corrosion rate and pitting rate parameters). ($\text{NCTYPE} \leq 20$)
- NWTYPE = Number of different waste form types. Each waste form type has unique release rate properties (i.e., diffusion coefficient, etc.). ($\text{NWTYPE} \leq 20$)
- IDIFF = Used in selecting the waste-form diffusion controlled release model. In all cases, the models assume a uniform concentration within the waste form at the start of leaching. Diffusion is assumed to be spatially symmetric and therefore, the gradient at $X = 0$ (or $r = 0$ for cylindrical waste forms) is zero. Five models are available as described below.
 - = 0, Plane geometry, semi-infinite medium model. The waste form is treated as a plane with half-length POREL(I) and diffusion occurs into a semi-infinite medium. The boundary condition is that the concentration approaches zero as X approaches infinity.
 - = 1, Plane geometry, finite medium model. The waste form is treated as a plane with half-length POREL. In this model, transport processes outside of the waste form are assumed to be rapid enough to maintain the concentration at the edge of the waste form as zero. This leads to higher release rates than selecting IDIFF = 0, and is the recommended model for plane geometry.
 - = 2, Cylindrical geometry, finite medium model. The waste form is treated as a cylinder of radius POREL and height HT (HT is calculated based on the input value of the volume of the waste form, VOLWF). This model assumes that the concentration at the boundary of the waste form is zero. This model is consistent with the models recommended in ANS 16.1 to calculate diffusion coefficients based on experimental leaching data.
 - = 3, Plane geometry finite-difference model. The waste form is simulated using a one-dimensional finite difference model with half-length POREL (data set 22). This model is most useful when simulating ingrowth of radionuclides during transport within the waste-form. The analytical

models (IDIFF = 0,1, or 2) can not accurately simulate ingrowth.

- = 4, Cylindrical geometry finite-difference model. The waste form is simulated using a one-dimensional finite-difference model with radius, POREL. This model is most useful when simulating ingrowth of radionuclides during transport within the waste-form. The analytical models (IDIFF = 0,1, or 2) can not accurately simulate ingrowth.

- IACT
- = Activity flag.
 - = 0, Waste form inventory, initial conditions and boundary conditions are input with units of grams.
 - = 1, Waste form inventory, initial conditions, and boundary conditions are input with units of Curies.

Format:

```
read(5,9) set3
write(4,9) set3
read(5,9) label
write(4,9) label
read(5,*) niso,ncon,nctype,nwtype,idiff,iact
write(4,10) niso,ncon,nctype,nwtype,idiff,iact
read(5,9) blank
write(4,9) blank
```

Example:

```
C ***** DATA SET 3: INTEGER PARAMETERS FOR CONTAINERS AND WASTE
      NISO   NCON   NCTYPE   NWTYPE   IDIFF   IACT
      3      6      2        1        2        0
BLANK'
```

6.4 DATA SET 4: Integer Numerical Integration Parameters

This data set contains information on integer parameters that control the selection of numerical solution techniques.

- ILUMP = Mass lumping control; 0 = No lumping, 1 = lumping. Lumping leads to a more diagonally dominant system which tends to be more stable but less accurate. 1 is the recommended value.
- IMID = Mid-point time difference integration flag.
0 = No, 1 = Yes. Recommended value is 0.
- IWET = Weighting function control. 0 = Galerkin weighting, 1 = Upstream weighting. Upstream weighting is appropriate for advection dominated transport and is generally recommended. Upstream weighting leads to numerical dispersion, however this is usually unimportant for advection driven transport. Galerkin weighting is appropriate for diffusion dominated transport.
- IOPTIM = Optimization factor for Galerkin or Upstream weighting. 0 = optimization factor is set to 1 or -1. 1 = optimization factor is calculated. Recommended value is 1.
- IVML = Flux-solving matrix lumping. 0 = No, 1 = Yes, Recommended value is 1.

Format:

```

read(5,9) set4
write(4,9) set4
read(5,9) label
write(4,9) label
read(5,*) ILUMP,IMID,iwet,IOPTIM,ivml
write(4,10) ILUMP,imid,iwet,IOPTIM,ivml
read(5,9) blank
write(4,9) blank

```

Example:

```

C ***** DATA SET 4: INTEGRATION INTEGER PARAMETERS
      ILUMP   IMID   IWET   IOPTIM   IVML
      1       0     1     1         0
BLANK '

```

6.5 DATA SET 5: Integer Time Step Parameters

This data set contains integers used to control the number of time steps in the simulation and the number of times where a change in the time step is requested.

Definitions:

NTI = Maximum number of time steps in the problem.

NDTCHG = Number of times at which the time step is reset to its original value. It is often useful to have a variable time step size which is allowed to increase until a change in the system performance occurs. At this time, the time step can be reset to its original value. For example, large time steps may be used prior to container failure and at this time, the time step can be reset to the original time step.

Format:

```

read(5,9) set5
write(4,9) set5
read(5,9) label
write(4,9) label
read(5,*) nti, ndtchg
write(4,10) nti, ndtchg
read(5,9) blank
write(4,9) blank

```

Example:

```

C ***** DATA SET 5: INTEGER SOLUTION CONTROL PARAMETERS
      NTI   NDTCHG
      273   1
BLANK '

```

6.6 DATA SET 6: Integer Geometry and Material Parameters

This data set contains integer parameters that define the finite element grid and the number of different materials. Each material has unique transport parameters.

Definitions:

- NNP = Number of nodal points.
- NEL = Number of finite elements.
- NMAT = Number of material regions with unique physical and chemical properties that influence transport.
- NCM = Number of elements that need material property reassignment. In many situations, only a small number of elements differ in transport properties from the majority of elements. Therefore, it is often easier to initialize the whole field with one material type, and then reassign this small number of elements NCM. Initially, all elements are defined as having material type 1. To select another type of material requires material property reassignment, data set 14, or reassignment directly in the geometry definitions section, data set 12.
- KMSH = Automatic mesh generation flag. If the nodal locations and finite element grid are not defined from an auxiliary input file created by FEMWATER (i.e., KVI < 0, data set 2), the nodal locations and finite element grid definition can be defined automatically. In this case, the required input becomes the (X,Z) coordinates of the four corners of the region being defined and the number of elements in each direction within the region. A more detailed explanation is provided in section 6.12.
- = 0; Read grid data from cards in data set 12.
- = 1; Use automatic mesh generation input in data set 12.

Format:

```
read(5,9) set6
write(4,9) set6
read(5,9) label
write(4,9) label
read(5,*) nnp,nel,nmat,ncm,kmsch
write(4,10) nnp,nel,nmat,ncm,kmsch
read(5,9) blank
write(4,9) blank
```

Example:

```
C ***** DATA SET 6: GRID AND ELEMENT PARAMETERS
      NNP      NEL      NMAT      NCM      KMSH
      213      140      1        0        0
BLANK'
```

6.7 DATA SET 7: Integer Boundary Condition Parameters

Data set 7 consists of three sets of integer parameters. Each set contains one line of input for each contaminant being modeled. The sets define the number of boundary nodal points, number of time-dependent boundary profiles, number of element sides where a specified flux boundary condition is specified and the number of data points in each profile for the three different boundary conditions: Dirichlet (specified concentration); Cauchy (specified flux), and Neumann (specified diffusive/dispersive flux).

The first set specifies parameters for the Dirichlet boundary conditions. In each set, there are two text lines for defining the boundary conditions. The first is typically used to define the type of boundary condition (i.e., Dirichlet, Cauchy, or Neumann), while the second is used to define the specific parameters. After these two lines there is one line of input for each contaminant. Note that the use of free-format read statements requires the input of a value for each parameter. Blanks are not treated as being zero, as is the case with a formatted read statement.

Definitions for Dirichlet boundary conditions:

NDNP(iso) = Number of boundary nodes for contaminant iso with specified concentration (Dirichlet nodes).

NDPR(iso) = Number of Dirichlet profiles (time vs. concentration) for contaminant iso.

NDDP(iso) = Number of data points in each profile for contaminant iso.

Format:

```
      read(5,9) set7a
      write(4,9)set7a
      read(5,9) label
      write(4,9)label
do 7771 iso = 1, niso
      read(5,*) ndnp(iso),ndpr(iso),nddp(iso)
      write(4,10)ndnp(iso),ndpr(iso),nddp(iso)
7771  continue
      read(5,9) blank
      write(4,9)blank
```

Example:

C *** DATA SET 7A: DIRICHLET INTEGER PARAMETERS FOR BOUNDARY CONDITIONS**

NDNP (I)	NDPR (I)	NDDP (I)
0	0	0
0	0	0
0	0	0

BLANK '

Comment:

Values are needed even though the number of Dirichlet points for each contaminant is zero. Three sets of values are needed in this problem because the number of isotopes being simulated is 3 (NISO in data set 3).

Definitions for Cauchy boundary conditions:

NCNP(iso) = Number of boundary nodes for contaminant iso with specified total flux.(Cauchy nodes).

NCES(iso) = Number of Cauchy element sides for contaminant iso.
 NCPR(iso) = Number of Cauchy profiles (time vs. Flux) for contaminant iso.
 NCDP(iso) = Number of data points in each profile for contaminant iso.

Format:

```

      read(5,9) set7b
      write(4,9)set7b
      read(5,9) label
      write(4,9)label
do 7772 iso = 1, niso
      read(5,*) ncnpr(iso),nces(iso),ncpr(iso),ncdp(iso)
      write(4,10)ncnp(iso),nces(iso),ncpr(iso),ncdp(iso)
7772  continue
      read(5,9) blank
      write(4,9)blank

```

Example:

```

C ***** DATA SET 7B: CAUCHY INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NCNP (I)      NCES (I)      NCPR (I)      NCDP (I)
      3             2             1             4
      3             2             1             4
      3             2             1             4
BLANK '

```

Definitions of Neumann Boundary conditions:

NNNP(iso) = Number of boundary nodes for contaminant iso with specified dispersive flux (Neumann nodes).
 NNES(iso) = Number of Neumann element sides for contaminant iso.
 NNPR(iso) = Number of Neumann profiles (time vs. dispersive Flux) for contaminant iso.
 NNDP(iso) = Number of data points in each profile for contaminant iso.

Format:

```

      read(5,9) set7c
      write(4,9)set7c
      read(5,9) label
      write(4,9)label
do 7773 iso = 1, niso
      read(5,*) nnnpr(iso),nnes(iso),nnpr(iso),nndp(iso)
      write(4,10)nnnp(iso),nnes(iso),nnpr(iso),nndp(iso)
7773  continue
      read(5,9) blank
      write(4,9)blank

```

Example:

```

C ***** DATA SET 7C: NEUMANN INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NNNP (I)      NNES (I)      NNPR (I)      NNDP (I)

```


3	2	1	4
3	2	1	4
3	2	1	4

BLANK'

Comments:

Table 6.3 has an example of how this data set looks in its entirety.

6.8 DATA SET 8: Integer External Source Parameters

Data set 8 contains the integer parameters that define the number of external volumetric sources and point (well) sources for each isotope.

Definitions:

NSEL(iso) = Number of volumetric source elements for contaminant iso.
 NSPR(iso) = Number of source strength versus time profiles for contaminant iso.
 NSDP(iso) = Number of data points in the source strength profile for contaminant iso.
 NWNP(iso) = Number of well point sources for contaminant iso.
 NWPR(iso) = Number of well source strength versus time profiles for contaminant iso.
 NWDP(iso) = Number of data points in the well source strength profile for contaminant iso.

Format:

```

      read(5,9) set8
      write(4,9)set8
      read(5,9) label
      write(4,9)label
do 888 iso = 1, niso
      read(5,*) nsel(iso),nspr(iso),nsdp(iso)
      write(4,10)nsel(iso),nspr(iso),nsdp(iso)
888 continue
      read(5,9) blank
      write(4,9)blank
      read(5,9) label
      write(4,9)label
do 999 iso = 1, niso
      read(5,*) nwnp(iso),nwpr(iso),nwdp(iso)
      write(4,10)nwnp(iso),nwpr(iso),nwdp(iso)
999  continue
      read(5,9) blank
      write(4,9)blank
  
```

C ***** DATA SET 8: INTEGER PARAMETERS FOR SOURCES

NSEL(I)	NSPR(I)	NSDP(I)	volume/element sources
0	0	0	AM241
0	0	0	PU241
0	0	0	PU240

BLANK'

NWNP(I)	NWPR(I)	NWDP(I)	well/point source
0	0	0	

0	0	0
0	0	0

BLANK'

Comment:

Notice that after the three required values are input for the volumetric sources, text to define the isotope can be added to the line. Each contaminant can have unique source/sink locations. Therefore, data is needed for each contaminant.

6.9 DATA SET 9: Contaminant and Decay Chain Definition Parameters

This data set contains information pertaining to each contaminant species and defines the decay chains (if any).

Definitions:

RADNUC(iso) = Alpha-numeric contaminant descriptor for contaminant iso, e.g., Tc99. Maximum of five characters.

ATM(iso) = Atomic mass of contaminant iso. Used to convert mass input in Curies to grams.

DECAYC(iso) = Half-life of the contaminant in years. If this value is input as 0, it is assumed that the element is stable and does not undergo radioactive decay. This value is converted to the decay constant in (s^{-1}) internally within BLT-MS.

CSAT(iso) = Solubility limit for contaminant iso (g/cm^3). This value can not be input with mass units of Curies.

ICHAIN = Number of decay chains. If ICHAIN = 0, decay chains are not simulated.

LCHAIN(ICH) = Length (number of contaminants) of the ICHth decay chain ($1 \leq ICH \leq ICHAIN$).

IDECAY(I,ICH) = Integer identifier of the Ith member of the ICHth chain. The contaminants are numbered by the order of input of their parameters. In the example below, Am-241 is isotope 1, Pu-241 is isotope 2, and Pu-240 is isotope 3.

FBRANCH(I,ICH) = Branching fraction for decay of contaminant I to the next contaminant in the decay chain (determined from IDECAY(I+1,ICH)). This number must be between 0 and 1.

Format:

```

      read(5,9) set9
      write(4,9)set9
      read(5,9) label
      write(4,9)label
do 33 iso = 1, niso
  read(5,*) radnuc(iso),atm(iso), decayc(iso), csat(iso)
  write(4,23) radnuc(iso),atm(iso), decayc(iso), csat(iso)
33 continue
      read(5,9) blank
      write(4,9)blank

```

C

C*****THE FOLLOWING SECTION READS DECAY CHAIN DATA

```

        read(5,9) set9
        write(4,9)set9
        read(5,9) label
        write(4,9)label
    READ(5,*) ICHAIN
        write(4,10) ichain
        read(5,9) blank
        write(4,9)blank
    IF(ICHAIR .GE. 1) THEN
C
C Read pointers for each decay chain
    ICH = 1
    DO WHILE (ICH .LE. ICHAIN)
        read(5,9) set9
        write(4,9)set9
        READ(5,*) LCHAIN(ICH)
            write(4,10) lchain(ich)
            read(5,9) blank
            write(4,9)blank
        read(5,9) set9
        write(4,9)set9
        CALL INPTI(IDECAV(1,ICH),MAXISO,LCHAIN(ICH))
            write(4,10) (idecay(i,ich),I=1,lchain(ich))
            read(5,9) blank
            write(4,9)blank
        read(5,9) set9
        write(4,9)set9
        CALL INPTR2(FBRANCH(1,ICH),MAXISO,LCHAIN(ICH)-1)
            write(4,21) (fbranch(i,ich),I=1,lchain(ich)-1)
            read(5,9) blank
            write(4,9)blank
        ICH = ICH + 1
    ENDDO

```

Example:

```

C ***** DATA SET 9: CONTAMINANT MATERIAL INFORMATION
      Contam(I)   ATM(I)      T ½ (I)  CSAT(I)
      Am241       241.00      4.33D2   1.000
      Pu241       241.00      15.000    1.000
      Pu240       240.00      6.54D3    1.000
BLANK'
      DECAY CHAIN INFORMATION:
      NUMBER OF CHAINS
      1
BLANK'
      LENGTH OF CHAIN
      3
BLANK'
      COMPONENTS OF THE CHAIN (Numerical order Am241 = 1; Pu241=2; PU240=3
      1      2      3
BLANK'
      BRANCHING FRACTIONS OF THE CHAIN (need length of chain - 1 values)

```

1.0 1.0
BLANK'

Comments:

This procedure reads in all of the data for each isotope before determining if decay chains are to be modeled. The section beginning with 'Length of chain' and finishing with the BLANK' after branching fractions' is required only if chains are specified. Therefore, if the number of chains, ICHAIN, is 0, the blank' after this value is the last input required in this data set. If ICHAIN is greater than zero, the series of cards defining the length, member, and branching fractions of the chain are required for each decay chain. In the preceding example, Am241 is isotope 1, Pu241 is isotope 2, and Pu240 is isotope 3. This chain has Am241 (1) decay to Pu241 (2) which decays to Pu240 (3). There are three members in this chain, therefore, only two branching fractions are needed. The first specifies the fraction of species 1 going to species 2, while the second specifies the fraction of species 2 going to species 3. These branching fractions are used only to calculate ingrowth. Decay of species 3 is modeled consistent with its half-life as input above. However, the decayed species 3 are not transferred to another species in this simulation.

Subroutine INPTI, used to read the components of the chain, uses a free-format read statement to obtain the integer data requested. The call statement has three variables. The first, IDECAY, is the variable to which the input is assigned. The second, MAXISO, is the maximum number of isotopes and is used for dimensioning arrays within INPTI. The third, LCHAIN (length of the chain), is the number of variables that will be read through input.

Subroutine INPTR2, used to read the branching fractions, uses a free-format read statement to obtain the real data requested. The call statement has three variables. The first, FBRANCH, is the variable to which the input is assigned, the second, MAXISO, is the maximum number of isotopes and is used for dimensioning arrays within INPTI and the third, LCHAIN-1, is the number of variables that will be read through input.

6.10 DATA SET 10: Time Step Parameters (Real Values)

This data set contains all of the real values that control the time step size and the time-integration scheme. In BLT-MS values of time are input with units of years. This differs from BLT, which requires input in units of seconds. BLT-MS converts from years to seconds internally.

Definitions:

DELT	=	Initial time step size (years)
CHNG	=	Fractional change in time step size (dimensionless)
DELMAX	=	Maximum time step size (years)
TMAX	=	Maximum problem simulation time (years)
W	=	Time integration parameter for the transport equation. Recommended value is 1.
	=	1, fully implicit backward difference
	=	0.5, Crank-Nicholson central difference
	=	0.0, fully explicit forward difference
WV	=	Time integration parameter for the velocity terms. Recommended value is 1.
	=	1, fully implicit backward difference
	=	0.5, Crank-Nicholson central difference
	=	0.0, fully explicit forward difference

Format:

C Input all time values in units of years!
read(5,9) set10
write(4,9) set10

```

      read(5,9) label
      write(4,9)label
      READ (5,*) DELT,CHNG,DELMAX,TMAX,w,wv
      write(4,21) DELT,CHNG,DELMAX,TMAX,w,wv
      read(5,9) blank
      write(4,9)blank
IF(NDTCHG.GT.0) THEN
      read(5,9) label
      write(4,9)label
      read(5,*) (tdtch(I),I=1,ndtchg)
      write(4,21)(tdtch(I),I=1,ndtchg)
      read(5,9) blank
      write(4,9)blank
ELSE
      NDTCHG = 1
      TDTCH(1) = TMAX + 1.0
ENDIF

```

Example:

```

C ***** DATA SET 10: TIME INTEGRATION CONTROL PARAMETERS
      DELT(yrs) CHNG      DELMAX(yr) TMAX(yrs)      W      WV
      1.000000  0.0D0      1.00      300.0      1.0D0      1.0D00
BLANK'
Set 10a: DELTA T CHANGES at year(s):
      3.15E02
BLANK'

```

Comments:

If the number of times at which DELTA T' is to be reset, NDTCHG, is zero, SET 10a above is not needed. In this example NDTCHG = 1.

6.11 DATA SET 11: Not Used in BLT-MS

This data set is not used in BLT-MS. It is included as part of the code in order to have a consistent structure between BLT-MS and BLT-EC. Even though the data set is not used, three input cards are required as follows.

Format:

```

      read(5,9) set11
      write(4,9)set11
      read(5,9) label
      write(4,9)label
      read(5,9) blank
      write(4,9)blank

```

Example:

```

C ***** DATA SET 11: REAL PARAMETERS FOR NONLINEAR SOLVE
      DUMMY SET: NOT USED IN BLTMS
BLANK'

```

6.12 DATA SET 12: Geometry Definitions (Real Values)

This data set contains the information to define the finite element grid. There are three options for grid definition: a) read grid data from an input file (generally created by FEMWATER), b) read grid data for the X and Z coordinates individually, or c) use automatic uniform grid generation for regions within the domain. In this example, option b was selected. An example for options a and c will also be provided. Selection of option a, b, and c is obtained based on the values of KVI and KMSH as follows:

<u>KVI (Data set 2)</u>	<u>KMSH(Data set 6)</u>	<u>Option</u>
> 0	N. A.	a
≤ 0	0	b
≤ 0	1	c

Definitions:

Option a, b and c variable:

WIDFAC = Width of the facility (cm). Used to calculate concentrations. Often the total inventory of the facility is known. Since BLT-MS only models two-dimensions, a value for the third dimension is needed to properly estimate concentrations. For example, consider a trench which is 100 m long, 25 m wide, and 10 m deep with an initial inventory of 100 Ci. Typically, BLT-MS would model a slice of the facility that is 25 m wide by 10 m deep. If the value for WIDFAC is set to 10,000 cm, then the inventory can be input as 100 Ci and the concentrations will be calculated correctly.

Option b variables:

In this option, the X and Z locations, element definitions, and number of elements in each direction are defined. The element definition specifies which nodal points correspond to which element. The following variables are used only when defining nodal point coordinates through option b. In this case, X and Z coordinates are read in through subroutine READR. READR requires six variables per line and uses a free-format read. The end of READR is signaled through input of zero for the first variable on the line.

X-Coordinates:

NI = Node number of the first node in the sequence.
 NSEQ = NSEQ + 1 nodes will be generated automatically.
 NAD = Increment of the node number for each of the NSEQ + 1 nodes.
 XNI = X coordinate of Node NI (cm.)
 XAD = Increment of the X coordinate for each node in this series.
 XRD = Fractional increase of the increment over its preceding increment.

The values for the X locations are calculated from:

$$X(NI) = XNI,$$

$$X(NI + N*NAD) = XNI + XAD*(1 + XRD)^{(N)}$$

where N ranges from 1 to NSEQ.

The end of this input set is identified by defining NI = 0.

Z-Coordinates

NI = Node number of the first node in the sequence.
NSEQ = NSEQ + 1 nodes will be generated automatically.
NAD = Increment of the node number for each of the NSEQ + 1 nodes.
ZNI = Z coordinate of Node NI (cm.)
ZAD = Increment of the Z coordinate for each node in this series.
ZRD = Fractional increase of the increment over its preceding increment.

The values for the Z locations are calculated from:

$$Z(NI) = ZNI$$
$$Z(NI + N*NAD) = ZNI + ZAD*(1 + ZRD)^{(N)}$$

where N ranges from 1 to NSEQ.

The end of this data set is identified by defining NI = 0.

Element Definition

MI = Global element number

IE(MI,1) = Global node number of the first node of element MI. Assuming the elements are numbered starting from the lower left hand corner of the modeled domain, the lower left hand corner node is the first node in the element. Local indexing proceeds in the counter-clockwise direction around the element.

IE(MI,2) = Global node number of the second node of element MI (lower right)

IE(MI,3) = Global node number of the second node of element MI (upper right)

IE(MI,4) = Global node number of the second node of element MI (upper left)

IE(MI,5) = Material type index for element MI.

Geometry Definition

MODL = Number of elements in the z-direction

NLAY = Number of elements in the x-direction

Numbering of elements and nodes proceeds along the direction with the least finite-elements. This is done for computational efficiency. Storage requirements depend on the maximum difference in node numbers within an element. For example, Figure 6.1 consider a grid that is five elements high, MODL=5, and ten wide, NLAY=10. Numbering starts at the lower left corner and proceeds up the five elements. Thus, element one is the lower left corner and element five is the upper left corner. Node 1 is at the lower left corner and node 6 is at the upper right corner. Thus, element 1 contains nodes 1, 7, 8, and 2. If numbering of elements had proceeded in the other direction, element one would have contained nodes 1, 2, 12, and 11.

Figure 6.1 Example finite element grid that is 5 elements high by 10 elements wide. Element numbers are listed inside the grid, node numbers are listed outside the grid.

Option c variables:

The following variables are used only when defining nodal point coordinates through option c, automatic mesh generation.

NELX	=	Total number of elements in the X-direction.
NELZ	=	Total number of elements in the Z-direction.
NREG	=	Number of regions with ordered pairs for the coordinates.
IMIN	=	Node number for the minimum X-direction node in the region.
JMIN	=	Node number for the minimum Z-direction node in the region.
IMAX	=	Node number for the maximum X-direction node in the region.
JMAX	=	Node number for the maximum Z-direction node in the region.

In this input structure the X and Z-direction nodes are numbered independently. For this problem there are 71 (NELX + 1) nodes in the X-direction and 3 nodes (NELZ + 1) in the Z-direction. Coordinate pairs are ordered from the lower left hand corner, counter clockwise. That is, the (X,Z) coordinates of the (IMIN, JMIN) node, (IMAX, JMIN) node, (IMAX, JMAX) node, and (IMIN, JMAX) node.

Format:

C if kvi > 0 read grid data from file created by FEMWATER
c if kmsh=0, then read ni,nseq,nad ,x, z, etc from input data
c if kmsh.gt.0 then generate the grid automatically.

c-----
read(5,9) set12A
write(4,9)set12A
read(5,9) label
write(4,9)label


```

        READ(5,*) WIDFAC
        WRITE(4,9) WIDFAC
        read(5,9) blank
        write(4,9)blank
    IF(KVI.LE.0) go to 200
        read(5,9) label
        write(4,9)label
        read(5,9) blank
        write(4,9)blank
C
c      if kmsh=0, then read ni,nseq,nad ,x, z, etc from input data
c      if kmsh.gt.0 then generate the grid with R. Mackinnons subs
c-----
        IF(KVI.GT. 0) THEN
        print *,'ENTER NAME OF THE INPUT FILE CREATED BY FEMWATER: '
        READ 98, INFILE1
        OPEN(UNIT=1,FILE=INFILE1,STATUS='OLD',ACCESS='SEQUENTIAL')

C ----- READ NODAL AND ELEMENT DATA FROM LOGICAL UNIT 1 IF KVI.GT.0
C
c*****
        READ(1,1111) (TITLEM(I),I=1,20)
        write(4,1111)(TITLEM(I),I=1,20)
1111 FORMAT(20A4)
        READ(1,2222) NPROBM,NNP,NEL,NBNP,NBES,NTIM,NRSNP
2222 FORMAT(16I5)
        nprobm = nprobm
        ntim = ntim
        nrsnp = nrsnp
        READ(1,2222) ((IE(M,I),M=1,NEL),I=1,4),(MBES(M),M=1,NBES),
1          ((ISB(I,M),I=1,4),M=1,NBES),(NPB(N),N=1,NBNP)
        READ(1,3333) (X(N),N=1,NNP),(Z(N),N=1,NNP),(DLB(M),M=1,NBES),
1          (DCOSXB(M),M=1,NBES),(DCOSZB(M),M=1,NBES)
3333 FORMAT(5E14.7)
        ENDIF
7777 continue
c-----
C      SET ALL MATERIAL PROPERTIES TO TYPE 1 AND REDEFINE AS NECESSARY
C      IN DATA SET 12B( old set 8)
c-----
        DO 197 M=1,NEL
        IE(M,5)=1
197 CONTINUE
C End of input from auxiliary file
        GO TO 310
200 CONTINUE
        read(5,9) label
        write(4,9)label
        if(kmsh.gt.0) then
C Use automatic mesh generation
        call mnode(x,z,ie,maxel,maxnp)
        else
C Read node and element data for X and Z

```

```

nset12x = 121
CALL READR(x,MAXNP,NNP,nset12x)
    read(5,9) blank
    write(4,9)blank
    read(5,9) label
    write(4,9)label
nset12z = 122
CALL READR(Z,MAXNP,NNP,nset12z)
    read(5,9) blank
    write(4,9)blank
C-----
C***** DATA SET 12B Element Indices
C ***** DATA SET 12B: ELEMENT INDICES AND MATERIAL TYPES VIA CARD IF
C ***** KVI LE 0; and kmsh le 0
C-----
    read(5,9) set12b
    write(4,9)set12b
C
    MJ = 0
    read(5,9) label
    write(4,9)label
230 READ (5,*) MI,(IE(MI,I),I=1,5)
    read(5,9) blank
    write(4,9)blank
    read(5,9) label
    write(4,9)label
    read (5,*) MODL,NLAY
    read(5,9) blank
    write(4,9)blank

```

Example found in CHAIN7.DAT (Option 2 read coordinate data)

```

C ***** DATA SET 12: NODAL POINT COORDINATE read if KVI le 0; kmsh ge 0
    WIDTH OF THE WASTE CONTAINING REGION MODELED (CM)
    100.0
BLANK'

```

ni	nseq	nad	fni	fad	frd
1	2	1	0.0	00.0	0.0
4	2	1	100.0	00.0	0.0
7	2	1	200.0	00.0	0.0
10	2	1	300.0	00.0	0.0
13	2	1	400.0	00.0	0.0
16	2	1	500.0	00.0	0.0
19	2	1	600.0	00.0	0.0
22	2	1	700.0	00.0	0.0
25	2	1	800.0	00.0	0.0
28	2	1	900.0	00.0	0.0
31	2	1	1000.0	00.0	0.0
34	2	1	1100.0	0.00	0.0
37	2	1	1200.0	0.00	0.0
40	2	1	1300.0	0.00	0.0
43	2	1	1400.0	0.00	0.0
46	2	1	1500.0	0.00	0.0

49	2	1	1600.0	0.00	0.0
52	2	1	1700.0	0.00	0.0
55	2	1	1800.0	0.00	0.0
58	2	1	1900.0	0.00	0.0
61	2	1	2000.0	0.00	0.0
64	2	1	2100.0	0.00	0.0
67	2	1	2200.0	0.00	0.0
70	2	1	2300.0	0.00	0.0
73	2	1	2400.0	0.00	0.0
76	2	1	2500.0	0.00	0.0
79	2	1	2600.0	0.00	0.0
82	2	1	2700.0	0.00	0.0
85	2	1	2800.0	0.00	0.0
88	2	1	2900.0	0.00	0.0
91	2	1	3000.0	0.00	0.0
94	2	1	3100.0	0.00	0.0
97	2	1	3200.0	0.00	0.0
100	2	1	3300.0	0.00	0.0
103	2	1	3400.0	0.00	0.0
106	2	1	3500.0	0.00	0.0
109	2	1	3600.0	0.00	0.0
112	2	1	3700.0	0.00	0.0
115	2	1	3800.0	0.00	0.0
118	2	1	3900.0	0.00	0.0
121	2	1	4000.0	0.00	0.0
124	2	1	4100.0	0.00	0.0
127	2	1	4200.0	0.00	0.0
130	2	1	4300.0	0.00	0.0
133	2	1	4400.0	0.00	0.0
136	2	1	4500.0	0.00	0.0
139	2	1	4600.0	0.00	0.0
142	2	1	4700.0	0.00	0.0
145	2	1	4800.0	0.00	0.0
148	2	1	4900.0	0.00	0.0
151	2	1	5000.0	0.00	0.0
154	2	1	5100.0	0.00	0.0
157	2	1	5200.0	0.00	0.0
160	2	1	5300.0	0.00	0.0
163	2	1	5400.0	0.00	0.0
166	2	1	5500.0	0.00	0.0
169	2	1	5600.0	0.00	0.0
172	2	1	5700.0	0.00	0.0
175	2	1	5800.0	0.00	0.0
178	2	1	5900.0	0.00	0.0
181	2	1	6000.0	0.00	0.0
184	2	1	6100.0	0.00	0.0
187	2	1	6200.0	0.00	0.0
190	2	1	6300.0	0.00	0.0
193	2	1	6400.0	0.00	0.0
196	2	1	6500.0	0.00	0.0
199	2	1	6600.0	0.00	0.0
202	2	1	6700.0	0.00	0.0
205	2	1	6800.0	0.00	0.0

```

208      2      1      6900.0      0.00      0.0
211      2      1      7000.0      0.00      0.0
0        0      0      0        0        0.0
Set12A:  z-coordinates
ni nseq  nad  fni  fad  frd
1      70    3      0.0    00.0    0.0
2      70    3     100.0    00.0    0.0
3      70    3     200.0    00.0    0.0
0        0    0        0        0        0.0
BLANK'
DATA SET12b: ELEMENT INDICES AND MATERIAL TYPES VIA CARDS IF KVI.LE. 0
mi ie(mi,i), I=1,5;-
1      1      4      5      2      1
BLANK'
modl nlay
2      70
BLANK'

```

Comments:

In this problem, we have 213 nodal points with 140 elements in two layers of 70 elements each. Therefore, we use 71 lines to describe the X nodal coordinate points and 3 lines for the Z nodal coordinate points. The nodal coordinates are read in subroutine READR. The end of the data set is specified by having NI = 0. Note, values are specified for each input requested on this line. This is required because of the free-format read statement (in BLT, input of a blank line would be treated as having all zero values).

In the element definition section, only one set of values was needed to completely define the system. The reason for this is the modeled domain is that of a single material. If multiple materials are present, the sequence of lines beginning with the label line *mi ie(mi,i), I= 1-5;-* and ending with the blank line following the integer values for MODL and NLAY must be repeated for each region.

If the number of nodal coordinates in either the X or Z directions does not equal the number of nodal points, NNP, an error message is printed and the program is stopped. Similarly, if the variable IE is not defined for each element, NELM, an error message is printed and the program is stopped.

Example Case c, automatic grid generation.

```

This example completely replaces the input required for option B if KMSH = 1.
C ***** DATA SET 12: NODAL POINT COORDINATE read if KVI le 0; kmsh ge 0
WIDTH OF THE WASTE CONTAINING REGION MODELED (CM)
100.0
BLANK'
kmsh = 1 perform automatic grid generation
Nelx Nelz Nreg
70      2      1
For each of the NREG regions read nodal identifiers and coordinates
Imin Jmin Imax Jmax
1      1      71      3
Enter four coordinate pairs start at lower left hand and go counter clockwise
0.0d0 0.0d0 7.0d03 0.0d0 7.0d03 2.0d02 0.0d0 2.0d02
blank'

```

Comments:

Automatic grid generation assigns all materials as type 1. These can be redefined using material type-reassignment, DATA SET 14.

Example Case A Data read from auxiliary file

```
C ***** DATA SET 12: NODAL POINT COORDINATE read if KVI le 0; kmsh ge 0
  WIDTH OF THE WASTE CONTAINING REGION MODELED (CM)
    100.0
  BLANK'
  Grid generation read from FEMWATER tape. Input file name interactively
  BLANK'
```

Comments:

Grid generation through use of an auxiliary file assigns all materials as type 1. These can be redefined using material type-reassignment, DATA SET 14.

6.13 DATA SET 13: Material Properties (Real Values)

This data set contains information on the material properties. Some properties are contaminant specific. Therefore, the material properties have been divided into two categories contaminant non-specific (i.e., density, etc.) and contaminant specific (i.e., distribution coefficient). The order of the data input is different from BLT for this reason.

Definitions for contaminant non-specific parameters:

prop(1,i)	=	molecular diffusion coefficient (cm ² /s) of material i.
prop(2,i)	=	bulk density of the soil (g/cm ³) of material i.
prop(3,i)	=	longitudinal dispersivity (cm) of material i.
prop(4,i)	=	transverse dispersivity (cm) of material i.
prop(5,i)	=	porosity of material i.

Definitions of contaminant specific properties:

prop1(1,k,i)	=	distribution coefficient (cm ³ /g) of material k and contaminant i.
prop(2,k,i)	=	liquid degradation constant (1/s) of material k and contaminant i.
prop(3,k,i)	=	solid phase degradation constant (1/s) of material k and contaminant i.

Format:

```
      read(5,9) set13A
      write(4,9) set13A
      read(5,9) label
      write(4,9) label
      read(5,9) label
      write(4,9) label
DO 110 I=1,NMAT
  read (5,*) pr1,pr2,pr3,pr4,pr5
  prop(1,i) = pr1
  prop(2,i) = pr2
  prop(3,i) = pr3
  prop(4,i) = pr4
  prop(5,i) = pr5
C-----
```

```

        write(4,21) (PROP(J,I),J=1,nmppm)
110 continue
        read(5,9) blank
        write(4,9)blank
C-----
C ***** DATA SET 13B: MATERIAL PROPERTIES    part of old set 6
C-----
        read(5,9) set13B
        write(4,9)set13B
        read(5,9) label
        write(4,9)label
        read(5,9) label
        write(4,9)label
        do 112 I= 1, nmat
        do 111 iso=1,niso
        READ (5,*) (prop1(J,I,iso),J=1,nmppm1)
        write(4,21) (prop1(J,I,iso),J=1,nmppm1)
111 continue
        read(5,9) blank
        write(4,9)blank
112 continue

```

Example:

```

        DATA SET 13: Material Properties
        Properties dependent on material type
mol-dif-co  density    long-disp  trans-dsp  porosity  Material
0.000E+00   2.340E+00  2.590E+02  2.590E+01  2.000E-01    1

        Properties dependent on material and contaminant
        Kd          Liq Degr   Sol Degr          Material, Contaminant
        4.0D2       0.0D0      0.0D0             k=1,i=1
        4.0D2       0.0D0      0.0D0             i=2
        4.0D2       0.0D0      0.0D0             i=3

```

Comments:

If there is more than one material, the contaminant non-specific data is input for each material first. The contaminant specific material properties are input for each isotope of material 1 first. Then, for each isotope of material 2, and so on. In the above example, the information defining the material type, at the end of the first line, and defining material type and contaminant at the end of the other data lines is not required by the code. It is put there to clarify what properties are being defined. The liquid and solid degradation rate constants have units of s^{-1} .

6.14 DATA SET 14: Material Type Definitions

This data set reads the material type correction. Recall that for automatic mesh generation, or mesh generation from an auxiliary file, all material types are set to 1. The number of material changes, NCM, is input previously in data set 6.

Definitions used in subroutine READR if NCM > 0:

```

NI          =   Element number of the first node in this sequence.
NSEQ        =   NSEQ + 1 elements will be reassigned in this sequence.

```

NAD = Increment of the element number for this sequence.
 NITYP = Material type index for element MI.
 NTYPAD = Increment for the material type index for each of the elements in this sequence, normally = 0.

Material types are calculated from the equation:

$$MI(MI + N*NAD,5) = NITYP + N*NTYPAD$$

where N ranges from 0 to NSEQ.

Format:

```

      read(5,9) set14
      write(4,9) set14
      read(5,9) label
      write(4,9) label
      write(4,10) NCM
      IF(NCM.GT.0) then
        nset14 = 14
        CALL READN(IE(1,5),MAXEL,NCM,nset14)
      ENDIF
      read(5,9) blank
      write(4,9) blank
  
```

Example:

DATA SET 14: Material type reassignment
Data set not used in this simulation, NCM = 0.
BLANK'

Comments:

If NCM is non-zero, the routine READN is used to read the input for material changes. READN requires each line to have five integer values for the parameters described in the definition section above. Completion of the READN routine is signified by setting the first value, NI, to 0. The free-format read statement in READN requires values to be input for each parameter, i.e., zero's must be input as zero and not blanks.

6.15 DATA SET 15: Initial Conditions

Initial conditions are read in for each contaminant in the simulation. Each set of initial conditions begins with an alpha-numeric label card which is generally used to identify the contaminant. The units for the initial conditions depend upon the activity flag, IACT. If IACT = 0, input should be in gm/cm³. If IACT = 1, input should be in Ci/cm³.

Definitions (Variables read in subroutine READR1):

NI = Node number of the first node in this sequence.
 NNODE = NNODE + 1 nodes will be reassigned in this sequence.
 NAD = Increment of the node number for this sequence.
 RNI = Concentration for the first node in this sequence.
 RAD = Increment for the concentration for each of the elements in this sequence, normally = 0.
 RRD = Fractional increase in the concentration to be added, normally 0.

The concentration, RP, of contaminant, ISO, is calculated from the equation:

$RP(NI) = RNI$
 $RP(NI + NAD*(N - 1), ISO) = RNI + RAD*(1 + RRD)^N$

where N ranges from 1 to NSEQ.

Format:

```

      read(5,9) set15
      write(4,9) set15
      read(5,9) label
      write(4,9) label
do iso = 1, niso
      read(5,9) label
      write(4,9) label
nset15 = 15
CALL readr1(RP,MAXNP,NNP,iso,nset15)
enddo
      read(5,9) blank
      write(4,9) blank

```

Example:

DATA SET 15: Input for initial or Pre-initial Conditions						
	NI	NNODE	NAD	RNI	RAD	RRD
AM241						
	1	212	1	0.0	0.0	0.0
	0	0	0	0	0	0
PU241						
	1	212	1	0.0	0.0	0.0
	0	0	0	0	0	0
PU240						
	1	212	1	0.0	0.0	0.0
	0	0	0	0	0	0
blank'						

Comments:

In this example, all 213 nodes were given an initial concentration of 0.0 for each species. Note, if the user attempts to specify concentrations for more, or less, than the number of nodal points, NNP, an error message is printed and the code is stopped. A zero value for NI is required to indicate the end of the input for the contaminant.

6.16 DATA SET 16: Cauchy and Neumann Boundary Conditions

In this data set, information defining Cauchy boundary conditions (specified total flux) and Neumann (specified dispersive flux) is input. In general, boundary conditions are input for specific locations on the boundary as a function of time, for each contaminant. Time dependence of the boundary conditions is achieved through an input table with ordered pairs for the time and value at that time. Linear interpolation is used to estimate the boundary value at times not found in the tables. If a boundary condition is not specified for any boundary location, BLT-MS uses a default boundary condition of zero total flux (i.e., Cauchy condition).

The number of Cauchy (Neumann) data points, element sides, profiles, and data points in each profile were defined in Data Set 7B (7C). If Cauchy (Neumann) nodes are not used for any isotope, the required input is three alpha-numeric

cards. The first card identifies the Data Set, the second card would typically state that Cauchy (Neumann) nodes are not used (however, any alpha-numeric message can be used) and the third card would be blank'.

When Cauchy (Neumann) boundary conditions are requested, the input routine collects all information for a single contaminant prior to moving on to the next contaminant. The information is divided into four subsets. The first set requires the time and value of the specified flux for each profile. The second set requires the definition of the nodal points at which the Cauchy boundary conditions are applied. The third set requires the definition of which Cauchy (Neumann) profile applies to which Cauchy (Neumann) node. The fourth set defines the boundary element side which has a Cauchy (Neumann) boundary. Each of these subsets is separated by a blank card.

If Cauchy (Neumann) nodes are specified for some but not all contaminants, two alpha-numeric lines are required (a label line and a blank line) for contaminants without Cauchy (Neumann) nodes.

The units for the specified flux are mass/cm²/yr. If the mass flag, IACT, is 0, the unit of mass is grams. If IACT = 1, the unit of mass is Ci. When the input is in Ci, the mass is converted to grams internally in the code. The code also internally converts the units of time from years to seconds.

6.16.1 SET 16 A: Cauchy Boundary Conditions

Definitions:

Cauchy Boundary Flux Tables:

TQCBF(j,i,iso)	=	Time of j th data point in the i th profile for contaminant, iso (years).
QCBF(j,i,iso)	=	Specified flux value of the j th data point in the i th profile for contaminant, iso (mass/cm ² /year).

Cauchy Nodal Locations:

NPCB(i,iso)	=	Global nodal number of the i th Cauchy node for contaminant iso.
-------------	---	---

Cauchy Profile Assignment:

Assignment of Cauchy nodes to a specific profile is done using subroutine READNI. This subroutine reads the following five values repeatedly until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

NI	=	Compressed Cauchy nodal number of the first node in the sequence.
NSEQ	=	NSEQ + 1 Cauchy node profile definitions will be generated.
NAD	=	Increment of NI for each of the NSEQ + 1 nodes.
NITYP	=	Type of Cauchy-flux profile assigned to node NI.
NTYPAD	=	Increment of NITYP for each of the NSEQ + 1 nodes.

Cauchy profile type, ICTYP(I,ISO) is calculated from the equation:

$$ICTYP(NI + N*NAD,ISO) = NITYP + N * NTYPAD$$

where N ranges from 0 to NSEQ.

Cauchy boundary-element sides assignment:

Assignment of Cauchy boundary-element sides is achieved using the following input variables.

MI	=	Compressed Cauchy element side number for the first element-side in the sequence.
NSEQ	=	NSEQ + 1 element-sides will be generated.
M	=	Global element number to which the MI th Cauchy element side belongs.
ISI	=	Compressed Cauchy nodal number of the first node on the element-side, MI.
IS2	=	Compressed Cauchy nodal number of the second node on the element-side, MI.
MIAD	=	Increment for MI for each of the NSEQ + 1 element-sides.
MAD	=	Increment for M for each of the NSEQ + 1 element-sides.
IS1AD	=	Increment for IS1 for each of the NSEQ + 1 element-sides.
IS2AD	=	Increment for IS2 for each of the NSEQ + 1 element-sides.

The input calculates three variables, 1) MCES(I,ISO), the global element number to which the Ith Cauchy element side belongs; 2) ISC(1,I,ISO), the compressed Cauchy nodal number of the first node of the Ith Cauchy element side and 3) ISC(2,I,ISO), the compressed Cauchy nodal number of the second node of the Ith Cauchy element side.

The following equations are used:

$$MCES(MI+N*MIAD,ISO) = M + N*MAD$$

$$ISC(1,MI+N*MIAD,ISO) = IS1 + N*IS1AD$$

$$ISC(2,MI + N*MIAD,ISO) = IS2 + N*IS2AD$$

Format:

```

      read(5,9) set16a
      write(4,9)set16a
C ncnpsum = sum of all Cauchy nodes
  if(ncnpsum.eq.0) then
    read(5,9) label
    write(4,9)label
    read(5,9) blank
    write(4,9)blank
    else
C
  do 925 iso = 1,niso
  if(nces(iso).eq.0 .or. ncnp(iso) .eq. 0) go to 925
    read(5,9) label
    write(4,9)label
  write(8,8000)
  write(8,7001) radnuc(iso),iso
C-----
  DO 810 I=1,NCPR(iso)
    read(5,9) label
    write(4,9)label
  READ (5,*) (TQCBF(J,I,iso),QCBF(J,I,iso),J=1,NCDP(iso))
  write(4,26) (TQCBF(J,I,iso),QCBF(J,I,iso),J=1,NCDP(iso))
    read(5,9) blank
    write(4,9)blank
  write (8,9100) I
  write(8,9110) (TQCBF(J,I,iso),QCBF(J,I,iso),J=1,NCDP(iso))
810 CONTINUE

```

C ----- READ CAUCHY NODES AND TYPE OF CAUCHY FLUX PROFILE

C

```

      read(5,9) label
      write(4,9)label
      READ (5,*) (NPCB(I,iso),I=1,NCNP(iso))
      write(4,10) (NPCB(I,iso),I=1,NCNP(iso))
      read(5,9) blank
      write(4,9)blank

```

C

```

      read(5,9) label
      write(4,9)label
      nset16c = 161
      CALL READN1(ICTYP,MXCNP,NCNP(iso),iso,nset16c)
      read(5,9) blank
      write(4,9)blank

```

c-----

C

C ----- READ CAUCHY BOUNDARY ELEMENT SIDES

C

```

      read(5,9) label
      write(4,9)label
      MPI= 0
      830 READ (5,*)      MI,NSEQ,M,IS1,IS2,MIAD,MAD,IS1AD,IS2AD
      if(mi.ne.0)write(4,10) 1      MI,NSEQ,M,IS1,IS2,MIAD,MAD,IS1AD,IS2AD
      IF(MI.EQ.0) GO TO 840
      MJ=MI+NSEQ
      DO 835 MP=MI,MJ
      I=MI+(MP-MI)*MIAD
      MCES(I,iso)=M+(MP-MI)*MAD
      ISC(1,I,iso)=IS1+(MP-MI)*IS1AD
      ISC(2,I,iso)=IS2+(MP-MI)*IS2AD
      MPI=MPI+1
      835 CONTINUE
      GO TO 830
      840 IF(MPI.EQ.NCES(iso)) GO TO 850
      write(8,8300)
      STOP

```

C

```

      850      read(5,9) blank
      write(4,9)blank

```

Example:

SET 16: Cauchy Boundary Conditions

AM-241 boundary conditions: units of time and rates is years

Tqcbf	Qcbf	Tqcbf	Qcbf	Tqcbf	Qcbf	Tqcbf	Qcbf
-0.000e3	91.11	-0.000E3	200.0	-0.000e3	277.0	-0.000e3	

blank'

Set 16a: Cauchy Nodes- left side layer- NPCB

1	2	3

blank'

Ni	Nseq	Nad	Nityp	Ntypad:	Set 16b: Type Cauchy Node
1	2	1	1	0	

```

0      0      0      0      0
blank'
  Mi  Nseq  M   Is1  Is2  Miad  Mad  Islad  Is2ad:  ELEMENT SIDE
    1   1    1   1   2    1    1    1    1
    0   0    0   0   0    0    0    0    0
blank'
  Pu-241 boundary conditions:  units of time and rates is years
  Tqcbf Qcbf      Tqcbf Qcbf
    0.0 -0.0e-0  91.11 -0.0e-0  200.0 -0.0e-6  277.0 -0.0e-6
blank'
Set 16a: Cauchy Nodes- left side layer- NPCB
  1      2      3
blank'
  Ni Nseq  Nad Nityp Ntypad: Set 16b: Type Cauchy Node
    1  2    1    1    0
    0  0    0    0    0
blank'
  Mi Nseq  M   Is1  Is2  Miad      Mad  Islad  Is2ad:  ELEMENT SIDE
    1  1    1   1   2    1      1    1    1
    0  0    0   0   0    0      0    0    0
blank'
  Pu-240 boundary conditions:  units of time and rates is years
  Tqcbf Qcbf      Tqcbf Qcbf
    0.0 -0.0e0  91.11 -0.0e-0  200.0 -0.000e-0  277.0 -0.0e-0
blank'
Set 16a: Cauchy Nodes- left side layer- NPCB
  1      2      3
blank'
  Ni Nseq  Nad Nityp Ntypad: Set 16b: Type Cauchy Node
    1  2    1    1    0
    0  0    0    0    0
blank'
  Mi Nseq  M   Is1  Is2  Miad      Mad  Islad  Is2ad:  ELEMENT SIDE
    1  1    1   1   2    1      1    1    1
    0  0    0   0   0    0      0    0    0
blank'

```

Comments:

The preceding example sets Cauchy boundary conditions at nodes 1 - 3 for each isotope. Input is completed for each contaminant before proceeding to the next contaminant. Information on Cauchy Nodes is required only for the contaminants that have Cauchy boundary conditions as specified in data set 7.

6.16.2 SET 16 B: Neumann Boundary Conditions

Definitions

Neumann Boundary Flux Table:

$TQNB(j,i,iso)$ = Time of j^{th} data point in the i^{th} profile for isotope,iso (years).

QNBf(j,i,iso) = Specified dispersive flux value of the jth data point in the ith profile for isotope, iso (mass/cm²/year).

Neumann Nodal Locations:

NPNB(i,iso) = Global nodal number of the ith Neumann node for contaminant iso.

Neumann Profile Assignment:

Assignment of Neumann nodes to a specific profile is accomplished using subroutine READNI. This subroutine reads the following five values repeatedly until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

NI	=	Compressed Neumann number of the first node in the sequence.
NSEQ	=	NSEQ + 1 Neumann node profile definitions will be generated.
NAD	=	Increment of NI for each of the NSEQ + 1 nodes.
NITYP	=	Type of Neumann-flux profile assigned to node NI.
NTYPAD	=	Increment of NITYP for each of the NSEQ + 1 nodes.

Neumann profile type, INTYP(I,ISO) is calculated from the equation:

$$\text{INTYP}(\text{NI} + \text{N} * \text{NAD}, \text{ISO}) = \text{NITYP} + \text{N} * \text{NTYPAD}$$

where N ranges from 0 to NSEQ.

Neumann boundary-element side assignment:

Assignment of Neumann boundary-element sides is achieved using the following input variables.

MI	=	Compressed Neumann element side number for the first element-side in the sequence.
NSEQ	=	NSEQ + 1 element-sides will be generated.
M	=	Global element number to which the M th Neumann element side belongs.
ISI	=	Compressed Neumann nodal number of the first node on the element-side, MI.
IS2	=	Compressed Neumann nodal number of the second node on the element-side, MI.
MIAD	=	Increment for MI for each of the NSEQ + 1 element-sides.
MAD	=	Increment for M for each of the NSEQ + 1 element-sides.
IS1AD	=	Increment for ISI for each of the NSEQ + 1 element-sides.
IS2AD	=	Increment for IS2 for each of the NSEQ + 1 element-sides.

The input calculates three variables, 1) MNES(I,ISO), the global element number to which the Ith Neumann element side belongs; 2) ISN(1,I,ISO), the compressed Neumann nodal number of the first node of the Ith Neumann element side and 3) ISN(2,I,ISO), the compressed Neumann nodal number of the second node of the Ith Neumann element side.

The following equations are used:

$$\text{MNES}(\text{MI} + \text{N} * \text{MIAD}, \text{ISO}) = \text{M} + \text{N} * \text{MAD}$$

$$\text{ISN}(1, \text{MI} + \text{N} * \text{MIAD}, \text{ISO}) = \text{ISI} + \text{N} * \text{IS1AD}$$

$$\text{ISN}(2, \text{MI} + \text{N} * \text{MIAD}, \text{ISO}) = \text{IS2} + \text{N} * \text{IS2AD}$$

Format:

```

        read(5,9) set16b
        write(4,9)set16b
C nnnpsum is the sum of all Neumann nodes for all isotopes
        if(nnnpsum.eq.0) then
            read(5,9) label
            write(4,9)label
            read(5,9) blank
            write(4,9)blank
        else
            do 996 iso = 1, niso
            if(nnnp(iso).eq.0 .or. nnes(iso) .eq. 0) go to 996
                read(5,9) label
                write(4,9)label
            write(8,9000)
            write(8,7001) radnuc(iso),iso
            DO 910 I=1,NNPR(iso)
                read(5,9) label
                write(4,9)label
            READ (5,*) (TQNB(I,I,iso),QNB(I,I,iso),J=1,NNDP(iso))
            write(4,26) (TQNB(I,I,iso),QNB(I,I,iso),J=1,NNDP(iso))
                read(5,9) blank
                write(4,9)blank
910 CONTINUE
C ----- READ NEUMANN NODES AND TYPE OF NEUMANN FLUX PROFILE TO
C
        read(5,9) label
        write(4,9)label
        READ (5,*) (NPNB(I,iso),I=1,NNNP(iso))
        write(4,10) (NPNB(I,iso),I=1,NNNP(iso))
        read(5,9) blank
        write(4,9)blank
        read(5,9) label
        write(4,9)label
        nset16 = 162
        CALL READN1(INTYP,MXNNP,NNNP(iso),iso,nset16)
        read(5,9) blank
        write(4,9)blank
C ----- READ NEUMANN BOUNDARY ELEMENT SIDES
        read(5,9) label
        write(4,9)label
        MPI=0
930 READ (5,*) MI,NSEQ,M,IS1,IS2,MIAD,MAD,IS1AD,IS2AD
        if(mi.ne.0)write(4,10) 1 MI,NSEQ,M,IS1,IS2,MIAD,MAD,IS1AD,IS2AD
        IF(MI.EQ.0) GO TO 940
        MJ=MI+NSEQ
        DO 935 MP=MI,MJ
            I=MI+(MP-MI)*MIAD
            MNES(I,iso)=M+(MP-MI)*MAD
            ISN(1,I,iso)=IS1+(MP-MI)*IS1AD
            ISN(2,I,iso)=IS2+(MP-MI)*IS2AD
            MPI=MPI+1
935 CONTINUE
        GO TO 930

```

```

940 IF(MPIEQ.NNES(iso)) GO TO 945
      write(8,9300)
      STOP

```

C

```

945      read(5,9) blank
          write(4,9)blank

```

Example:

```

      Set 16b: Neumann Boundary Conditions
      Am-241 boundary conditions :units of time and rates is years
Am-241:  Tqnbfb  Qnbfb  Tqnbfb  Qnbfb
          0.0    0.0    91.1    0.0    200.0    0.0    300.0    0.0
blank'
Am-241:  Set 16a: Neuman Nodes- right side layer- NPNB
          211    212    213
blank'
      Ni  Nseq  Nad  Nityp  Ntypad:  set 16 b: Type Neumann modes
          1      2      1      1      0
          0      0      0      0      0
blank'
      Mi  Nseq      M  Is1  Is2  Miad  Mad  Islad  Is2ad : AM241
          1      1  139      1      2      1      1      1      1
          0      0      0      0      0      0      0      0      0
blank'
      Pu-241 boundary conditions :units of time and rates is years
Pu-241:  Tqnbfb  Qnbfb  Tqnbfb  Qnbfb
          0.0    0.00    91.1    0.00    200.0    0.00    300.0    0.0
blank'
Pu-241:  Set 16a: Neuman Nodes- right side layer- NPNB
          211    212    213
blank'
      Ni  Nseq  Nad  Nityp  Ntypad:  set 16 b: Type Neumann modes
          1      2      1      1      0
          0      0      0      0      0
blank'
Pu-241      Mi  Nseq      M  Is1  Is2  Miad  Mad  Islad  Is2ad :
          1      1  139      1      2      1      1      1      1
          0      0      0      0      0      0      0      0      0
blank'
      PU-240 boundary conditions.
      Tqnbfb  Qnbfb  : units of time and rates is years
          0.0  0.0-0    91.1    0.0-0    200.0    0.0-0    300.0    0.0-0
blank'
Pu-240: right side layer-
          211    212    213
blank'
      Ni  Nseq  Nad  Nityp  Ntypad:  set 16 b: Type Neumann nodes
          1      2      1      1      0
          0      0      0      0      0
blank'
      Mi  Nseq  M  Is1  Is2  Miad  Mad  Islad  Is2ad : Neumann element
          1      1  139      1      2      1      1      1      1

```

0 0 0 0 0 0 0 0 0
blank'

Comments:

In this example, Neumann nodes are defined for each contaminant at the right boundary, Nodes 211, 212 and 213. In the Neumann node and element side definition input, input is completed by having a value of zero for NI and MI, respectively. Information on Neumann nodes is required only for the contaminants that have Neumann nodes as specified in data set 7. The format and structure for the Neumann and Cauchy input sections is identical.

6.17 DATA SET 17: Dirichlet Boundary Conditions

Dirichlet (specified Concentration) boundary conditions are defined in this data set. In general, boundary conditions are input for specific locations on the boundary as a function of time, for each contaminant. Time dependence of the boundary conditions is achieved through an input table with ordered pairs for the time and the value at that time. Linear interpolation is used to estimate the boundary value at times not found in the tables. The unit of time is years and the unit of mass is grams or Curies depending on the value of IACT (0 = grams, 1 = Curies).

The input routine is structured to obtain all the values needed to completely define the isotope for one contaminant before moving on to the other contaminants.

Definitions:

Dirichlet Boundary Concentration Table:

TCDBF(j,i,iso) = Time of jth data point in the ith profile for contaminant, iso (years).
CDBF(j,i,iso) = Specified concentration value of the jth data point in the ith profile for contaminant, iso (mass/cm³).

Dirichlet Boundary Locations:

NPDB(i,iso) = Global nodal number of the ith Dirichlet node for contaminant iso.

Dirichlet Profile Assignment:

Assignment of Dirichlet nodes to a specific profile is done using subroutine READNI. This subroutine reads the following five values repeatedly until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

NI = Compressed Dirichlet number of the first node in the sequence.
NSEQ = NSEQ + 1 Dirichlet node profile definitions will be generated.
NAD = Increment of NI for each of the NSEQ + 1 nodes.
NITYP = Type of Dirichlet concentration profile assigned to node NI.
NTYPAD = Increment of NITYP for each of the NSEQ + 1 nodes.

Dirichlet profile type, IDTYP(I,ISO) is calculated from the equation:

$$IDTYP(NI + N * NAD, ISO) = NITYP + N * NTYPAD$$

where N ranges from 0 to NSEQ.

Format:

```

        read(5,9) set17
        write(4,9)set17
C
        if(ndnpsum.eq.0) then
            read(5,9) label
            write(4,9)label
            read(5,9) blank
            write(4,9)blank
            else
C
        do 725 iso = 1, niso
        IF(NDNP(iso).EQ.0) GO TO 725
        write(8,7000)
        write(8,7001) radnuc(iso),iso
7001 format(///,' Radionuclide ', a5,' isotope', i5,/)
            read(5,9) label
            write(4,9)label
        DO 710 I=1,NDPR(iso)
            read(5,9) label
            write(4,9)label
        READ (5,*) (TCDBF(J,I,iso),CDBF(J,I,iso),J=1,NDDP(iso))
        write(4,26) (TCDBF(J,I,iso),CDBF(J,I,iso),J=1,NDDP(iso))
            read(5,9) blank
            write(4,9)blank
        write(8,7100) I
        write(8,9110) (TCDBF(J,I,iso),CDBF(J,I,iso),J=1,NDDP(iso))
710 CONTINUE
C convert input from years to seconds.
        do I = 1,ndpr(iso)
        do j=1,nddp(iso)
        tcdbf(j,i,iso) = tcdbf(j,i,iso)*timeyr
        end do
        end do
C
C ----- READ DIRICHLET NODES AND TYPE OF CONCENTRATION PROFILE
C
        read(5,9) label
        write(4,9)label
        READ (5,*) (NPDB(I,iso),I=1,NDNP(iso))
        write(4,10) (NPDB(I,iso),I=1,NDNP(iso))
            read(5,9) blank
            write(4,9)blank
            read(5,9) label
            write(4,9)label
        nset14 = 14
        CALL READN1(IDTYP,MXDNP,NDNP(iso),iso,nset14)
            read(5,9) blank
            write(4,9)blank
```

Example:

SET 17: DIRICHLET BOUNDARY CONDITIONS
NOT USED IN THIS PROBLEM
BLANK'

Comment:

In this problem, the number of Dirichlet nodal points for each isotope is zero. Therefore, the boundary condition input is not required. The three lines listed are all that is needed. Information on Dirichlet nodes is required only for the contaminants that have Dirichlet nodes as specified in data set 7.

6.18 DATA SET 18: External Volumetric Sources

Normally, when using BLT-MS, the sources for each element are calculated from the releases from the waste forms, and external sources are not used. In this case, the number of volumetric sources is zero. When external volumetric sources are modeled, this is achieved through tabular input of source strength versus time for each profile (different source type) requested in Data Set 8. In addition, the location of each source must be specified and the source types must be allocated to each element containing a source. Sources are defined on a contaminant specific basis. For example, contaminant 1 may have external sources, while other contaminants in the simulation do not. The input of time units is in years and mass units are in grams or Curies depending on the value of IACT (0 = grams, 1 = Curies).

Definition:

LES(I,ISO)	=	Global element number containing the I th source for contaminant, iso.
TSOSF(J,I,ISO)	=	Time of the J th data point in the I th source strength versus time table for contaminant, iso. (years)
SOSF(J,I,ISO)	=	Value of the J th data point in the I th source strength versus time table for contaminant, iso. If SOSF > 0, units are mass/cm ³ /yr. If SOSF < 0, the source represents the volume removed per unit volume and time and the units are 1/yr. If IACT = 0, mass units are grams, otherwise, mass units are Curies. BLT-MS internally converts mass units to grams and time units to seconds.

Assignment of volumetric source elements to a specific profile is done using subroutine READNI. This subroutine reads the following five values repeatedly until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

NI	=	Compressed volumetric source number of the first element in the sequence.
NSEQ	=	NSEQ + 1 volumetric source profile definitions will be generated.
NAD	=	Increment of NI for each of the NSEQ + 1 nodes.
NITYP	=	Type of volumetric source concentration profile assigned to node NI.
NTYPAD	=	Increment of NITYP for each of the NSEQ + 1 nodes.

Volumetric source profile type, ISTYP(I,ISO) is calculated from the equation:

$$\text{ISTYP}(\text{NI} + \text{N} * \text{NAD}, \text{ISO}) = \text{NITYP} + \text{N} * \text{NTYPAD}$$

where N ranges from 0 to NSEQ.

Format:

```
read(5,9) set18
write(4,9) set18
read(5,9) label
```

```

        write(4,9)label
    if(nselsum.eq.0) then
        read(5,9) blank
        write(4,9)blank
    else
C-----
        do 3344 iso = 1, niso
        IF(NSEL(iso).EQ.0) GO TO 3344
C
C ----- READ SOURCE TYPE ASSIGNED TO EACH ELEMENT
C
        read(5,9) label
        write(4,9)label
        READ (5,* ) (LES(I,iso),I=1,NSEL(iso))
        write(4,10) (LES(I,iso),I=1,NSEL(iso))
        read(5,9) blank
        write(4,9)blank
C-----
        write(8,5300)
        read(5,9) label
        write(4,9)label
        DO 520 I=1,NSPR(iso)
        READ (5,*) (TSOSF(J,I,iso),SOSF(J,I,iso),J=1,NSDP(iso))
        write(4,25) (TSOSF(J,I,iso),SOSF(J,I,iso),J=1,NSDP(iso))
        read(5,9) blank
        write(4,9)blank
        write(8,5500) I
        write (8,9110) (TSOSF(J,I,iso),SOSF(J,I,iso),J=1,NSDP(iso))
520 CONTINUE
C
C READ SOURCE TYPE ASSIGNED TO EACH SOURCE ELEMENT
C
        read(5,9) label
        write(4,9)label
        nset18 = 18
        CALL readn1(ISTYP,MXSEL,NSEL(iso),iso,nset18)
        if(iso.ne.niso) then
            read(5,9) blank
            write(4,9)blank
        endif
1111 continue
3344 continue
C
        read(5,9) blank
        write(4,9)blank
    endif
! end of nselsum check

```

Example:

```

SET 18: EXTERNAL ELEMENT SOURCE/SINK
NOT USED IN THIS PROBLEM
BLANK'

```

Comment:

Input is required only for the contaminants that have volumetric sources as specified in Data Set 8.

6.19 DATA SET 19: External Point (Well) Sources

Normally, when using BLT-MS, the sources for each element are calculated from the releases from the waste forms and external sources are not used. In this case, the number of point (well) sources is zero. When external point sources are modeled, this is achieved through tabular input of source strength versus time for each profile (different source type) requested in Data Set 8. In addition, the location of each source must be specified and the source types must be allocated to each nodal point containing a source. Sources are defined on a contaminant specific basis. For example, contaminant 1 may have external sources, while other contaminants in the simulation do not.

Definition:

NPW(I,ISO)	=	Global node number containing the I th source for contaminant, iso.
TWSSF(J,I,ISO)	=	Time of the J th data point in the I th source strength versus time table for contaminant, iso. (years)
WSSF(J,I,ISO)	=	Value of the J th data point in the I th source strength versus time table for contaminant, iso. If WSSF > 0, units are mass/cm/yr. If WSSF < 0, the source represents the volume removed per unit time per unit width and the units are cm ³ /cm/yr. If IACT = 0, mass units are grams, otherwise, mass units are Curies. BLT-MS internally converts mass units to grams and time units to seconds.

Assignment of point source nodes to a specific profile is done using subroutine READNI. This subroutine reads the following five values repeatedly until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

NI	=	Compressed point source number of the first node in the sequence.
NSEQ	=	NSEQ + 1 point source profile definitions will be generated.
NAD	=	Increment of NI for each of the NSEQ + 1 nodes.
NITYP	=	Type of point source concentration profile assigned to node NI.
NTYPAD	=	Increment of NITYP for each of the NSEQ + 1 nodes.

Point source profile type, IWTYP(I,ISO) is calculated from the equation:

$$IWTYP(NI + N*NAD,ISO) = NITYP + N * NTYPAD$$

where N ranges from 0 to NSEQ.

Format:

```
read(5,9) set19
write(4,9) set19
read(5,9) label
write(4,9) label
if(nwnpsum.eq.0) then
  read(5,9) blank
  write(4,9) blank
else
```

```

C-----
      do 3355 iso = 1, niso
      IF(NWNP(iso).EQ.0) GO TO 3355
C ----- READ WELL SOURCE/SINK NODES AND TYPE OF PROFILES ASSIGNED TO
C ----- EACH OF NWNP NODES.
C
      read(5,9) label
      write(4,9)label
      READ (5,*) (NPW(I,iso),I=1,NWNP(iso))
      write(4,10) (NPW(I,iso),I=1,NWNP(iso))
      read(5,9) blank
      write(4,9)blank
C
C ----- READ AND WRITE WELL SOURCE/SINK PROFILES
C
      write(8,5700)
      read(5,9) label
      write(4,9)label
      DO 580 I=1,NWPR(iso)
      READ (5,*) (TWSSF(J,I,iso),WSSF(J,I,iso),J=1,NWDP(iso))
      read(5,9) blank
      write(4,9)blank
      write(4,25) (TWSSF(J,I,iso),WSSF(J,I,iso),J=1,NWDP(iso))
580 CONTINUE
      read(5,9) label
      write(4,9)label
      nset19 = 19
      CALL readn1(IWTYP,MXWNP,NWNP(iso),iso,nset19)
      if(iso.ne.niso) then
      read(5,9) blank
      write(4,9)blank
      endif
3355 continue
      read(5,9) blank
      write(4,9)blank
      endif      ! end of nwnpsum check

```

Example:

```

      SET 19:  WELL POINT SOURCE/SINK
NOT USED IN THIS PROBLEM
BLANK'

```

6.20 DATA SET 20: Container Degradation Parameters

Container degradation parameters include all of the values necessary to define localized and general corrosion rates and the location of the containers in the finite element grid. The time to failure for general corrosion is estimated from the general corrosion rate and the thickness of the container. Note, the thickness does not necessarily have to be the actual thickness of the container, it can be made smaller to account for mechanical failure due to the pressure of the overburden. The calculation for estimating local corrosion assumes that pitting is the corrosion phenomena. The equation for the pit depth is $h = kt^m A^m$, where h is the maximum pit depth, k , n , and m are the empirical parameters, PITN, PITK, and ASCALE.

A is the surface area of the container, AREA, normalized to the area of the National Bureau of Standards test samples and t is the time in years. More detailed descriptions of these parameters follows in the definition section.

Definitions:

- THICK(J) = Thickness of the Jth container (cm.). 55 gallon drums are typically 0.127 - 0.152 cm thick.
- PITN(J) = Pitting parameter n for the Jth container (dimensionless). If PITN(J) = 0, a value for PITN is estimated by the code based on input parameters for clay content (CLAY), soil aeration (IAER), and the moisture content. Measured values for PITN range from 0 - 1.
- PITK(J) = Pitting parameter k for the Jth container (cm/yrⁿ). If PITK is input as zero, a value is estimated based on the soil pH. Measured values for PITK range from 0.03 - 0.15. If soil pH is input as zero, PITK is set to 0.0737, the average for all soils.
- AREA(J) = Area of the Jth waste container (cm²). The area of a 55 gallon drum is 21,000 cm². The value is used to calculate the maximum pit depth and the area breached by pitting.
- ASCALE(J) = Area scaling exponent (dimensionless) for container J. Values have been measured by Logan [Logan, 1939] for wrought iron pipes buried in 47 different soils. Values ranged from 0.08 to 0.32 with a mean value of 0.15 and a standard deviation of 0.04. If ASCALE is input as zero, a default value of 0.2 is used.
- PITS(J) = Number of penetrating pits in the container (dimensionless) for container J. The total area breached is linearly proportional to the number of pits that penetrate the container, PITS(J). Measurement of the total number of pits on Fe samples ranged from 14 - 80 pits/cm² [Isaacs, 1988]. Of these only a small fraction will grow large enough to penetrate the container. Based on the carbon steel pitting data obtained by Marsh [Marsh, et al., 1985], an estimate of 0.05 penetrating pits/cm² has been made. For a 55 gallon drum, this implies approximately 1000 penetrating pits. The default value used by BLT-MS is 1000.
- GRATE(J) = The general corrosion rate (cm/s) of container J. Values measured in the NBS study reported by Romanoff [Romanoff, 1957] for the corrosion rate of carbon steel ranged from 2.7E-11 - 6E-10 cm/s. For a wall thickness of 0.127 cm, these corrosion rates correspond to penetration in 6.7 - 150 years. If the input values of GRATE(J) is zero, then a default value of 3E-10 cm/s is used.
- CLAY(J) = Clay fraction of the soil (0 .LE. CLAY(J) .LE. 1) around container J. If PITN is input as zero, PITN is calculated as a function of clay and moisture content as well as the degree of aeration (IAER).
- SPH(J) = Soil pH. If PITK is input as zero, PITK is calculated as a function of pH. If SPH(J) is input as zero, a default value of 7.0 is used.
- IAER(J) = Aeration index for the soil around container J. 1 = good, 2 = fair, 3 = poor, and 4 = very poor. Used in calculating PITN. If PITN and IAER are input as zero, PITN is set equal to 0.26, 0.39, 0.44, 0.59 for IAER = 1, 2, 3, 4 respectively. Most soils considered for low-level waste disposal will have good or fair aeration.
- NELCON(J) = Global element number for the Jth container.
- ICTYPE(J) = Waste container type for each element that has a container.

Assignment of container types to a specific container is done using subroutine READN. This subroutine reads the following five values repeatedly until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

NI = Compressed element number of the first element in the sequence.
 NSEQ = NSEQ + 1 container type definitions will be generated.
 NAD = Increment of NI for each of the NSEQ + 1 nodes.
 NITYP = Type of container type assigned to node NI.
 NTYPAD = Increment of NITYP for each of the NSEQ + 1 nodes.

Container profile type, ICTYP(I) is calculated from the equation:

$$ICTYP(NI + N*NAD) = NITYP + N * NTYPAD$$

where N ranges from 0 to NSEQ.

Format:

```

      if(ncon.eq.0) then      ! ncon test A
C
C ***** IF DATA SET 20 IS NOT BEING USED
      read(5,9) set20
      write(4,9)set20
      read(5,9) label
      write(4,9)label
      read(5,9) blank
      write(4,9)blank
C ***** IF DATA SET 21 IS NOT BEING USED
      read(5,9) set21a
      write(4,9)set21a
      read(5,9) label
      write(4,9)label
      read(5,9) blank
      WRITE(4,9) BLANK
      endif
C
C ***** end of ncon test A *****
C
C ----- READ AND WRITE CONTAINER/PACKAGE SOURCE DATA -----
C
C IF(NCON.NE.0)THEN      !ncon test B
C
      read(5,9) set20
      write(4,9)set20
      9 format(80a1)
      11 format(8i10)
C
C READ FROM INPUT FILE THE PARAMETERS OF EACH CONTAINER TYPE
C
      DO 505 J=1,NCTYPE
        read(5,9) label

```

```

        write(4,9)label
READ(5,*) THICK(J),PITN(J),PITK(J),AREA(J),ASCALE(J),PITS(J)
write(4,26)THICK(J),PITN(J),PITK(J),AREA(J),ASCALE(J),PITS(J)
        read(5,9) blank
        write(4,9)blank
        read(5,9) label
        write(4,9)label
read(5,*) GRATE(J),CLAY(J),SPH(J),IAER(J)
write(4,26)GRATE(J),CLAY(J),SPH(J),IAER(J)
        read(5,9) blank
        write(4,9)blank
505  CONTINUE
C  READ AND WRITE GLOBAL ELEMENT NO. AND THE CONT. TYPE
C
        read(5,9) label
        write(4,9)label
READ(5,*) (NELCON(I),I=1,NCON)
write(4,10)(NELCON(I),I=1,NCON)
        read(5,9) blank
        write(4,9)blank
        read(5,9) label
        write(4,9)label
nset20 = 20
CALL READN(ICTYPE,MXCON,NCON,nset20)
        read(5,9) blank
        write(4,9)blank

```

Example:

```

      SET 20:  WASTE CONTAINER PARAMETERS
THICK    PITN    PITK    AREA    ASCALE    PITS  CONTAINER 1
1.000D0  0.01D0  0.007D0  2.1D4    0.2D0    5.0D3
'BLANK'
      GRATE      CLAY      SPH      IAER
      0.317D-09  0.15D0    6.0D0    2
'BLANK'
THICK    PITN    PITK    AREA    ASCALE    PITS  CONTAINER 2
1.000D0  0.01D0  0.007D0  2.1D4    0.2D0    5.0D3
'BLANK'
      GRATE      CLAY      SPH      IAER
      0.317D+09  0.15D0    6.0D0    2
'BLANK'
      NELCON(1) (2)  (3) (4)  (5)  (6)  (7)  (8)  (9)
      21      22  41  42  61  62
'BLANK'
      MI      MSEQ      MAD      MITYPE      MTYPAD
      1      3      1      1      0
      5      1      1      2      0
      0      0      0      0      0
'BLANK'

```

Comment:

The preceding example has six containers, specified in data set 3. The first four are type 1 containers, that is, their failure rate parameters are defined by the first set of parameters. The fifth and sixth containers are type two containers. To avoid pitting causing container failure, PITN and PITK are set to very low values for both container types. To simulate instantaneous failure, the failure rate of container type 2 is set very high (3.17E8 cm/s). Container type 1 fails by general corrosion at 100 years (thickness = 1 cm, corrosion rate = 3.17E-10 cm/s, time of failure is thickness divided by corrosion rate).

6.21 DATA SET 21: Waste Form Leaching Parameters

Release rates from the waste forms are contaminant dependent. This data set collects the information that defines the waste form and their contaminant dependent release rate characteristics. BLT-MS allows three different release mechanisms to control release. Surface rinse subject to partitioning, diffusion controlled release, and dissolution controlled release.

The input required for the dissolution controlled release model has been altered slightly from the original model in BLT. In BLT, the user was required to input the dissolution rate, U (cm/s), surface area of the waste form, SA (cm²) and the volume of the waste form, VWF (cm³). The amount of mass released was proportional to $U*SA/VWF$ (1/s). In BLT-MS, the input for the dissolution model is a single value which represents the fractional dissolution rate of the waste form (1/yr). This value is equivalent to $U*SA/VWF$ in BLT. The mass release rate calculated using this model is the fractional dissolution rate multiplied by the mass available for dissolution release. For example, if the fractional release rate is 0.01 yr⁻¹, 1% of the initial inventory is released per year with release complete after 100 years. The release is corrected for radioactive decay and ingrowth.

The rinse release model has been expanded from the model found in the original version of BLT to include partitioning on the waste form. Although physically similar, for the purpose of clarity in this report, the term distribution coefficient will be used to refer to sorption on the soil and the term partition coefficient will be used to refer to sorption on the waste form. Use of a non-zero partition coefficient is not recommended unless careful consideration is given to the value of the waste form partition coefficient and soil distribution coefficient. This issue is presented in more detail in the discussion of the rinse model with partitioning, section 2.3.1. First, a non-zero partition coefficient may lead to negative releases, i.e., sorption onto the waste form. Second, due to the conceptualization that waste forms exist within a finite element, sorption is calculated in two places; on the waste form and on the soil within the finite element due to the distribution coefficient. Appropriate choice of the proper value of each sorption coefficient will depend upon the volume amount of waste form and soil represented within the finite element volume. This is handled through the input of the variable, VRATIO, which represents the ratio of the volume of the waste form to the volume of the finite element. If VRATIO is much less than one, most of the mass is released and sorbed on the soil. In the limit of VRATIO equal to zero, all of the mass is released from the waste form instantaneously as if the waste form partition coefficient was equal to zero. If VRATIO equals one, and the waste form partition coefficient equals the soil distribution coefficient, approximately 1/2 of the mass is released at the first opportunity. This mass sorbs on the soil subject to equilibrium partitioning in solution and is not immediately available for transport. As VRATIO increases to values much greater than one, release from the waste form decreases.

The intent of the partitioning model was to examine releases from sorbing media, such as ion-exchange resins, and other waste forms that are likely to exhibit significant sorption. To allow these sorption properties to change over time (due to degradation of the resins, for example), a three parameter exponential model is used for the partition coefficient. The model discussed in section 2.3.1.1 and is:

$$P(t) = P_0 \exp(-ut) + P_{inf}(1.0 - \exp(-ut))$$

where $P(t)$ = partition coefficient (cm³/g)
 P_0 = partition coefficient at $t = 0$
 P_{inf} = partition coefficient at $t = \text{infinity}$
 u = degradation rate constant (1/yr).

Data set 21 is subdivided into three sections. The first section reads in the isotope dependent release rate parameters for each waste form type and the parameters that define waste form geometry. The second set reads in the initial inventory of each contaminant in each waste form. The third set defines the waste type (i.e., which release rate parameters are used for each waste form).

Definitions:

SFRACT(J,ISO) =	Fraction of the mass in the J th waste form that is available for surface wash-off in the rinse release model for contaminant iso. Useful for surface contaminated waste forms such as lab trash ($0 \leq \text{SFRACT}(J) \leq 1$).
PFRACT(J,ISO) =	Fraction of the mass in the J th waste form that is available for diffusion controlled release for contaminant iso. Useful for cement solidified waste forms ($0 \leq \text{PFRACT}(J) \leq 1$).
BFRACT(J,ISO) =	Fraction of the mass in the J th waste form that is available for release due to dissolution of the waste form for contaminant iso. Useful for waste forms such as activated metals or when modeling a constant release rate in time. ($0 \leq \text{BFRACT} \leq 1$).
DEFF(J,ISO) =	J th waste form effective diffusion coefficient for contaminant iso cm ² /s. Used only if PFRACT(J,ISO) > 0.
DISOL(J,ISO) =	J th waste form fractional release rate (1/yr) for contaminant iso. Used only if BFRACT(J,ISO) > 0.
PARTKO(J,ISO) =	J th waste form partition coefficient for contaminant iso cm ³ /g at time t = 0. Used only if SFRACT > 0.
PARTKI(J,ISO) =	J th waste form partition coefficient for contaminant iso cm ³ /g at time t = ∞.
PARTD(J,ISO) =	J th waste form partition coefficient degradation rate constant for contaminant iso (1/yr). PARTD(J,ISO) must be greater than or equal to 0.
POREL(J) =	Radius or half-length of waste form J (cm). Used in calculating diffusion and dissolution controlled release (PFRACT > 0).
VOLWF(J) =	Volume of waste form J (cm ³). Used in calculating the height of cylindrical waste forms and initial concentrations within the waste form.
VRATIO(J) =	Ratio of the volume of waste form J to the finite element in which it is located. ($0 \leq \text{VRATIO}(J)$). Used in the rinse with partitioning model.
WTINIT(J,ISO) =	Initial inventory of contaminant iso in waste form J. If IACT = 0, WTINIT is input in grams. If IACT = 1, WTINIT is input in Curies.
IWTYPE(J) =	Waste form type for waste form J.

Assignment of waste types to a specific container is done using subroutine READN. This subroutine reads the following five values repeatedly until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

NI = Compressed element number of the first element in the sequence.

NSEQ = NSEQ + 1 container type definitions will be generated.
 NAD = Increment of NI for each of the NSEQ + 1 nodes.
 NITYP = Type of container type assigned to node NI.
 NTYPAD = Increment of NITYP for each of the NSEQ + 1 nodes.

Waste type, IWTYP(I) is calculated from the equation:

$$IWTYP(NI + N * NAD) = NITYP + N * NTYPAD$$

where N ranges from 0 to NSEQ.

Format:

```

      read(5,9) set21a
      write(4,9)set21a
c-----
      DO 507 J=1,NWTYPE
        read(5,9) label
        write(4,9)label
      do 6666 iso = 1, niso
        PARTK0(J,iso) = 0.0
        PARTKI(J,iso) = 0.0
        PARTD(J,iso) = 0.0
c-----
c  read contaminant material dependent quantities
c-----
        read(5,9) label
        write(4,9)label
        read(5,*) sfra(j,iso),pfra(j,iso),bfra(j,iso),
1 deff(j,iso), disol(j,iso)
        write(4,26)sfra(j,iso),pfra(j,iso),bfra(j,iso),
1 deff(j,iso),disol(j,iso)
        read(5,9) blank
        write(4,9)blank
c-----
        read(5,9) label
        write(4,9)label
        read(5,*) partk0(j,iso),partki(j,iso),partd(j,iso)
        write(4,26)partk0(j,iso),partki(j,iso),partd(j,iso)
        read(5,9) blank
        write(4,9)blank
      6666  continue
c-----
        read(5,9) label
        write(4,9)label
        read(5,*) POREL(J),VOLWF(J),VRATIO(J)
        write(4,26) POREL(J),VOLWF(J),VRATIO(J)
        read(5,9) blank
        write(4,9)blank
      507  CONTINUE
c-----
c
c ***** DATA SET 21B: READ INITIAL MASSES AT EACH WASTE ELEMENT
c

```

```

C-----
      read(5,9) set21b
      write(4,9) set21b
do 5555 iso = 1, niso
      read(5,9) label
      write(4,9) label
      read(5,9) label
      write(4,9) label
      READ(5,*) (WTINIT(I,iso),I=1,NCON)
      write(4,26)(WTINIT(I,iso),I=1,NCON)
      read(5,9) blank
      write(4,9) blank
5555      continue
C-----
C
C ***** DATA SET 21C: READ WASTE TYPE ASSIGNMENTS
C-----
      read(5,9) set21c
      write(4,9) set21c
      read(5,9) label
      write(4,9) label
nset21 = 21
CALL READN(IWTYPE,MXWtyp,NCON,nset21)
      read(5,9) blank
      write(4,9) blank
C

```

Example:

```

      SET 21:  WASTE FORM RELEASE PARAMETERS
      NWTYPE = 1
      SFRACT(I)  PFRACT(I)  BFRACT(I)  DEFF(I)  DISOL(I)      ISO = 1
      0.333D0    0.333D0    0.333D0    1.0D-8    1.0D-03
'BLANK'
      PARTK0(I)  PARTKI(I)  PARTKD(I)
      0.0D0      0.0D0      0.0D0
'BLANK'
      SFRACT(I)  PFRACT(I)  BFRACT(I)  DEFF(I)  DISOL(I)      ISO = 2
      0.333D0    0.333D0    0.333D0    1.0D-8    1.0D-03
'BLANK'
      PARTK0(I)  PARTKI(I)  PARTKD(I)
      0.0D0      0.0D0      0.0D0
'BLANK'
      SFRACT(I)  PFRACT(I)  BFRACT(I)  DEFF(I)  DISOL(I)      ISO = 3
      0.333D0    0.333D0    0.333D0    1.0D-8    1.0D-03
'BLANK'
      PARTK0(I)  PARTKI(I)  PARTKD(I)
      0.0D0      0.0D0      0.0D0
'BLANK'
      POREL      VOLWF      VRATIO
      25.0D0      1.0D6      1.0
'BLANK'

```

```

C ***** DATA SET 21B: INITIAL MASSES OF EACH WASTE ELEMENT
      ISO =1
      WTINIT1,X1      X2      X3      X4      X5      X6      X7      X8      X9      3.0D0
      3.0D0 3.0D0 3.0D0 3.0D0 3.0D0
'BLANK'
      ISO = 2
      WTINIT1,X1      X2      X3      X4      X5      X6      X7      X8      X9      0.0D0
      0.0D0 0.0D0 0.0D0 0.0D0 0.0D0
'BLANK'
      ISO =3
      WTINIT1,X1      X2      X3      X4      X5      X6      X7      X8      X9      0.0D0
      0.0D0 0.0D0 0.0D0 0.0D0 0.0D0
'BLANK'
C ***** DATA SET 21C: READ WASTE TYPE ASSIGNMENTS
      MI      NSEQ      MAD      MITYP      MTPAD
      1      5      1      1      0
      0      0      0      0      0
'BLANK'

```

Comments

In the preceding example, there is only one waste form type with three contaminants. For each waste type, the waste form geometry parameters, POREL, VOLWF, and VRATIO are input after the contaminant specific release rate properties are input for each contaminant. If there had been multiple waste form types, data set 21A is repeated once for each waste type. Then, initial inventories, data set 21B, are input.

6.22 DATA SET 22: Output Control Parameters

This data set is divided into three subsets. The first subset contains the information required to define the time step at which output occurs and the types of output for the main output file. The second subset is not used in BLT-MS and is reserved for BLT-EC. Nevertheless, three alpha-numeric input lines are required. The third subset collects the information for defining trace files.

The output control array, KPR, is dimensioned to accept 1000 values representing the output requested at each time step. If more than 1000 time steps are anticipated, (NTI > 1000 in data set 5), the user must input only 1000 values. The selection for output control is repeated for each 1000 points. For example, output control at time step 1200 would be determined by the value of the 200th value in the array KPR.

Definitions:

- KPRO = Printer control for steady-state and initial conditions:
0 = print nothing
1 = print flow, total flow rate and information concerning time of the container breach, cumulative and instantaneous releases from the waste forms
2 = print (1) above plus concentrations at each location.
3 = print (2) above plus material flux at each location.
- KPR(I) = Printer control for time step I, one value required for each time step up to 1000 time steps. Values have a definition identical to KPRO.

Reading of KPRO and KPR is achieved with a formatted read statement which reads in 80 integer values per line.

Blank values are treated as zero. Therefore, the number of lines of input required is $1 + \text{INT}((\text{NTI} + 1)/80)$ where INT is the integer value of that division. For example, 273 time steps necessitates 274 input values, or 4 lines of 80 input values.

Trace File Parameters:

NTRC = Number of nodes with a concentration trace
 NTRF = Number of nodes with a flux trace
 NSTPTR = Number of time steps between output to the trace files

When a trace file is requested at a node, a separate trace file is written for each contaminant. The file name for the concentration trace files is TRACECN*.DAT and for the flux trace files is TRACEFX*.DAT. Where the * changes from 0 - 9 depending upon the isotope. Isotope 1 concentration versus time information can be found in TRACECN1.DAT. Similar numbering is used up to isotope 9. Isotope 10 information can be found on TRACECN0.DAT.

NTRCEC(I) = Global node number of the Ith concentration trace profile.

NTRCEF(I) = Global node number of the Ith flux trace profile.

Format:

```

      read(5,9) set22a
      write(4,9)set22a
      read(5,9) label
      write(4,9)label
      read(5,9) label
      write(4,9)label
      READ (5,30) KPRO,(KPR(I),I=1,NTI)
      write(4,30) KPRO,(KPR(I),I=1,NTI)
      read(5,9) blank
      write(4,9)blank
C-----
C ***** DATA SET 22B: dummy for BLTMS-not used
C-----
      read(5,9) set22b
      write(4,9)set22b
      read(5,9) label
      write(4,9)label
      read(5,9) blank
      write(4,9)blank
C-----
C ***** DATA SET 22C: TRACE FILE-CONTROL  part of old set 5
C-----
      read(5,9) set22c
      write(4,9)set22c
      read(5,9) label
      write(4,9)label
      read (5,*) NTRC,NTRF,NSTPTR
      write(4,10) NTRC,NTRF,NSTPTR
      read(5,9) blank
      write(4,9)blank
C-----
      IF(NTRC .GT. 0) then
        read(5,9) label
        write(4,9)label

```

```

        READ(5,*) (NTRCEC(I),I=1,NTRC)
        write(4,10)(NTRCEC(I),I=1,NTRC)
        read(5,9) blank
        write(4,9)blank
    endif
C-----
    IF(NTRF .GT. 0) then
        read(5,9) label
        write(4,9)label
        READ(5,*) (NTRCEF(I),I=1,NTRf)
        write(4,10)(NTRCEF(I),I=1,NTRf)
        read(5,9) blank
        write(4,9)blank
    endif

```

Example:

```

        SET 22:  PRINTER CONTROL PARAMETERS
Set 22A: Printer Control parameters
Kpr0  Kpr(1)  Kpr(2)  Kpr(3)  Kpr(4)  Kpr(5)  Kpr(6)
022   2      0      0 0      0      0      0
0     2      222      0      0      0      0
0     2      0      0      0      0
0     2      2      0
'BLANK'
C ***** DATA SET 22B: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE
        NOT USED IN BLTMS
'BLANK'
C ***** DATA SET 22C: TRACE FILES-NO OF CONC. AND FLUX NODE NUMBERS & NODE NOS
        NTRC  NTRF  NSTPTR
        8     0     1
'BLANK'
Concentration trace information-Global node numbers  NTRCEC(k)
    2    32    62    92   122   152   182   212
'BLANK'

```

Comments

In the preceding example, 8 concentration traces were requested and 0 flux traces. Since flux traces were not requested input is not required on their locations. If the number of flux traces requested was greater than zero, data similar to the concentration traces would be required. Also, the read statement for KPR is formatted and blanks are treated as a value of zero.

6.23 DATA SET 23: Velocity and Moisture Content

If the velocity input control variable, KVI, is less than or equal to 0, Darcy flux and moisture content are input in this data set. If KVI is greater than 0, velocity, pressure head, total head, and moisture content are read from a file which is typically created by FEMWATER. The Darcy flux has units of cm/s, and the moisture content is dimensionless.

Definitions:

- VX(I) = Darcy flux in the X-direction at node I (cm/s).
- VZ(I) = Darcy flux in the Z-direction at node I (cm/s). It is recommended to define the lower left hand corner of the modeled domain as the minimum value for X and Z. In this case, a negative Z flux implies downward flow.
- TH(IQ,J) = Moisture content at nodal point IQ, in element J. Moisture content is defined at each nodal point in the finite element grid. In quadrilateral elements there are four moisture content values associated with each element.

VX and VZ values are input on the same input line. The read statement is repeated until the value for the first parameter is zero. Non-blank values must be input for all parameters because of the free-format read statement.

The variables are:

Velocity Definition:

- NI = Node number of the first node in the sequence.
- NSEQ = NSEQ + 1 nodal velocity values will be generated.
- NAD = Increment of NI for each of the NSEQ + 1 nodes.
- VXNI = X-Darcy velocity component of node NI (cm/s).
- VZNI = Z-Darcy velocity component of node NI (cm/s).
- VXAD = Increment of the X-Darcy flux for each of the NSEQ + 1 nodes (cm/s).
- VZAD = Increment of the Z-Darcy flux for each of the NSEQ + 1 nodes (cm/s).

The Darcy flux in the X-direction, VX, and the Darcy flux in the Z-direction are calculated from:

$$\begin{aligned} \text{VX}(\text{NI} + \text{N} * \text{NAD}) &= \text{VXNI} + \text{N} * \text{VXAD} \\ \text{VZ}(\text{NI} + \text{N} * \text{NAD}) &= \text{VZNI} + \text{N} * \text{VZAD} \end{aligned}$$

where N ranges from 0 to NSEQ.

Moisture Content Definition:

The moisture content is defined with the following input. Again, the read statement is repeated until a zero value appears for the first parameter. The free-format read necessitates input of all values requested.

- NI = Element number of the first element in the sequence.
- NSEQ = NSEQ + 1 moisture content values will be generated.
- NAD = Increment of the element number for each of the NSEQ + 1 elements.
- THNI = Moisture content for element NI (dimensionless).
- THNIAD = Increment of the moisture content for each of the NSEQ + 1 elements (dimensionless).

The moisture content for each element is calculated as:

$$\text{TH}(\text{IQ}, \text{NI} + \text{N} * \text{NAD}) = \text{THNI} + \text{N} * \text{THNIAD}$$

where N ranges from 0 to NSEQ.

Format:


```

        if(kvi.gt.0) then
            read(5,9) set23a
            write(4,9)set23a
            read(5,9) label
            write(4,9)label
            read(5,9) blank
C
C ----- READ INITIAL VELOCITY, PRESSURE HEAD, TOTAL HEAD, AND
C ----- MOISTURE CONTENT VIA LOGICAL UNIT 1 IF KVI.GT. 0
C
        READ(1,3333) TIMEM,(H(NP),NP=1,NNP),(HT(NP),NP=1,NNP),
        1 ((TH(IQ,M), IQ=1,4),M=1,NEL),(VX(NP),NP=1,NNP), 2 (VZ(NP),NP=1,NNP)
        3333 FORMAT(5E14.7)
C-----
        timem = timem
        else
C
C----- READ VELOCITY VIA CARDS IF KVILE.0)
        read(5,9) set23b
        write(4,9)set23b
        read(5,9) label
        write(4,9)label
210 continue
        READ (5,*) NI,NSEQ,NAD,VXNI,VZNI,VXAD,VZAD
        IF(NI.EQ.0) GO TO 250
C
        NJ=NI+NSEQ
        DO 220 NP=NI,NJ
        I=NI+(NP-NI)*NAD
        VX(I)=VXNI+VXAD*FLOAT(NP-NI)
        VZ(I)=VZNI+VZAD*FLOAT(NP-NI)
220 CONTINUE
        GO TO 210
250 CONTINUE
C
        read(5,9) blank
        write(4,9)blank
C
C----- READ MOISTURE CONTENT IF KVILE.0
C
        read(5,9) label
        write(4,9)label
260 continue
        READ(5,*) NI,NSEQ,NAD,THNI,THNIAD
        IF(NI.EQ.0) GO TO 290
        NJ=NI+NSEQ
        DO 280 NP=NI,NJ
        I=NI+(NP-NI)*NAD
        DO 270 IQ=1,4
            TH(IQ,I)=THNI+THNIAD*FLOAT(NP-NI)
270 CONTINUE
280 CONTINUE
        GO TO 260

```

290 CONTINUE

read(5,9) blank

write(4,9)blank

Example:

```
C ***** DATA SET 23B: VELOCITY AND MOISTURE CONTENT
  Ni Nseq  Nad   Vxni      Vzni      Vxad  Vzad
  1  212   1  +2.316d-04  0.0d-00  0.0    0.0
  0  0     0   0         0         0     0
SET 23B Moisture content:
  Ni  Nseq  Nad  Thni      Thniad
  1   139   1   0.2       0.0
  0   0     0   0         0
'BLANK'
```

Comment

In this problem there are 213 nodes and 140 elements. Therefore, the preceding input specifies a Darcy flux in the X-direction of $2.315\text{E-}4$ cm/s for all 213 nodes and a moisture content of 0.2 in all 140 elements.

Table 6.3 Example BLT-MS Input, CHAIN7.DAT

```

C ***** DATA SET 1: PROBLEM IDENTIFICATION AND DESCRIPTION-- BLTMS-DATA
  1 Prob2: Three species decay chain. Containers

C ***** DATA SET 2: INTEGER PARAMETERS FOR VELOCITY INPUT AND STEADY STATE
      KVI      KSS
      -1       1

C ***** DATA SET 3: INTEGER PARAMETERS FOR CONTAINERS AND WASTE
      NISO      NCON      NCTYPE      NWTYPE      IDIFF      IACT
      3         6         2         1         3         0

C ***** DATA SET 4: INTEGRATION INTEGER PARAMETERS
      ILUMP      IMID      IWET      IOPTIM      IVML
      1         0         1         1         0

C ***** DATA SET 5: INTEGER SOLUTION CONTROL PARAMETERS
      NTI      NDTCHG
      273      1

C ***** DATA SET 6: GRID AND ELEMENT PARAMETERS
      NNP      NEL      NMAT      NCM      KMESH
      213      140      1         0         0

C ***** DATA SET 7A: DIRICHLET INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NDNP(I)    NDPR(I)    NDDP(I)
      0          0          0
      0          0          0
      0          0          0

C ***** DATA SET 7B: CAUCHY INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NCNP(I)    NCES(I)    NCPR(I)    NCDP(I)
      3          2          1          4
      3          2          1          4
      3          2          1          4

C ***** DATA SET 7C: NEUMANN INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NNNP(I)    NNES(I)    NNPR(I)    NNDP(I)
      3          2          1          4
      3          2          1          4
      3          2          1          4

C ***** DATA SET 8: INTEGER PARAMETERS FOR SOURCES
      NSEL(I)    NSPR(I)    NSDP(I)    volume/element sources
      0          0          0          AM241
      0          0          0          PU241
      0          0          0          PU240

      NWNP(I)    NWPR(I)    NWDP(I)    well/point source
      0          0          0
      0          0          0
      0          0          0

C ***** DATA SET 9: CONTAMINANT MATERIAL INFORMATION
      Contam(I)  ATM(I)      T 1/2 (I)  CSAT(I)
      Am241      241.00      4.33D2     1.000
      Pu241      241.00      15.000     1.000

```

Table 6.3 Example BLT-MS Input, CHAIN7.DAT (continued)

```

Pu240      240.00      6.54D3      1.000

DECAY CHAIN INFORMATION:
NUMBER OF CHAINS
1

LENGTH OF CHAIN
3

COMPONENTS OF THE CHAIN (Numerical order Am241 = 1; Pu241=2; PU240=3
1      2      3

BRANCHING FRACTIONS OF THE CHAIN (need length of chain - 1 values)
1.0      1.0
C ***** DATA SET 10: TIME INTEGRATION CONTROL PARAMETERS
      DELT(yrs) CHNG      DELMAX(yr) TMAX(yrs) W      WV
      1.000000 0.0D0      1.00      300.0      1.0D0      1.0D00

Set 10a: DELTA T CHANGES at year(s):
      3.15E02

C ***** DATA SET 11: REAL PARAMETERS FOR NONLINEAR SOLVE
      DUMMY SET: NOT USED IN BLTMS

C ***** DATA SET 12: NODAL POINT COORDINATE read if KVI le 0; kmsh ge 0
WIDTH OF THE WASTE CONTAINING REGION MODELED (CM)
100.0

ni nseq  nad      fni      fad      frd
1   2   1      0.0      00.0      0.0
4   2   1     100.0      00.0      0.0
7   2   1     200.0      00.0      0.0
10  2   1     300.0      00.0      0.0
13  2   1     400.0      00.0      0.0
16  2   1     500.0      00.0      0.0
19  2   1     600.0      00.0      0.0
22  2   1     700.0      00.0      0.0
25  2   1     800.0      00.0      0.0
28  2   1     900.0      00.0      0.0
31  2   1    1000.0      00.0      0.0
34  2   1    1100.0      0.00      0.0
37  2   1    1200.0      0.00      0.0
40  2   1    1300.0      0.00      0.0
43  2   1    1400.0      0.00      0.0
46  2   1    1500.0      0.00      0.0
49  2   1    1600.0      0.00      0.0
52  2   1    1700.0      0.00      0.0
55  2   1    1800.0      0.00      0.0
58  2   1    1900.0      0.00      0.0
61  2   1    2000.0      0.00      0.0
64  2   1    2100.0      0.00      0.0
67  2   1    2200.0      0.00      0.0
70  2   1    2300.0      0.00      0.0
73  2   1    2400.0      0.00      0.0
76  2   1    2500.0      0.00      0.0

```

Table 6.3 Example BLT-MS Input, CHAIN7.DAT (continued)

79	2	1	2600.0	0.00	0.0
82	2	1	2700.0	0.00	0.0
85	2	1	2800.0	0.00	0.0
88	2	1	2900.0	0.00	0.0
91	2	1	3000.0	0.00	0.0
94	2	1	3100.0	0.00	0.0
97	2	1	3200.0	0.00	0.0
100	2	1	3300.0	0.00	0.0
103	2	1	3400.0	0.00	0.0
106	2	1	3500.0	0.00	0.0
109	2	1	3600.0	0.00	0.0
112	2	1	3700.0	0.00	0.0
115	2	1	3800.0	0.00	0.0
118	2	1	3900.0	0.00	0.0
121	2	1	4000.0	0.00	0.0
124	2	1	4100.0	0.00	0.0
127	2	1	4200.0	0.00	0.0
130	2	1	4300.0	0.00	0.0
133	2	1	4400.0	0.00	0.0
136	2	1	4500.0	0.00	0.0
139	2	1	4600.0	0.00	0.0
142	2	1	4700.0	0.00	0.0
145	2	1	4800.0	0.00	0.0
148	2	1	4900.0	0.00	0.0
151	2	1	5000.0	0.00	0.0
154	2	1	5100.0	0.00	0.0
157	2	1	5200.0	0.00	0.0
160	2	1	5300.0	0.00	0.0
163	2	1	5400.0	0.00	0.0
166	2	1	5500.0	0.00	0.0
169	2	1	5600.0	0.00	0.0
172	2	1	5700.0	0.00	0.0
175	2	1	5800.0	0.00	0.0
178	2	1	5900.0	0.00	0.0
181	2	1	6000.0	0.00	0.0
184	2	1	6100.0	0.00	0.0
187	2	1	6200.0	0.00	0.0
190	2	1	6300.0	0.00	0.0
193	2	1	6400.0	0.00	0.0
196	2	1	6500.0	0.00	0.0
199	2	1	6600.0	0.00	0.0
202	2	1	6700.0	0.00	0.0
205	2	1	6800.0	0.00	0.0
208	2	1	6900.0	0.00	0.0
211	2	1	7000.0	0.00	0.0
0	0	0	0	0	0.0

Set12A: z-coordinates

ni	nseq	nad	fni	fad	frd
1	70	3	0.0	00.0	0.0
2	70	3	100.0	00.0	0.0
3	70	3	200.0	00.0	0.0
0	0	0	0	0	0.0

DATA SET12b: ELEMENT INDICES AND MATERIAL TYPES VIA CARDS IF KVI.LE. 0

mi ie(mi,i), i=1,5;-
 1 1 4 5 2 1

Table 6.3 Example BLT-MS Input, CHAIN7.DAT (continued)

```
modl nlay
  2    70
```

DATA SET 13: Material Properties

```
Set 13A: Prop(J,k), j =1, NMPPM(NO. of material properties=5), k = 1, NMAT
mol-dif-co density long-disp trans-disp soil porosity
0.0d00      2.34      259.0      25.90      0.2      k=1
```

```
Prop1(1,k,i) Prop1(2,k,i) Prop1(3,k,i)
KD liquid-degr solid-degr
4.0D2      0.0D0      0.0D0      k=1,i=1
4.0D2      0.0D0      0.0D0      i=2
4.0D2      0.0D0      0.0D0      i=3
```

DATA SET 14: Material type reassignment
Data set not used in this simulation.

DATA SET 15: Input for initial or Pre-initial Conditions

	NI	NNODE	NAD	RNI	RAD	RRD
AM241	1	212	1	0.0	0.0	0.0
	0	0	0	0	0	0
PU241	1	212	1	0.0	0.0	0.0
	0	0	0	0	0	0
PU240	1	212	1	0.0	0.0	0.0
	0	0	0	0	0	0

SET 16: Cauchy Boundary Conditions

AM-241 boundary conditions: units of time and rates is years

```
Tqcbf(j,i) Qcbf(j,i) Tqcbf(j,i) Qcbf(j,i)
0.0 -0.000e3 91.11 -0.000E3 200.0 -0.000e3 277.0 -0.000e3
```

Set 16a: Cauchy Nodes- left side layer- NPCB
1 2 3

```
Ni Nseq Nad Nityp Ntypad: Set 16b: Type Cauchy Node DEFINITION
1 2 1 1 0
0 0 0 0 0
```

```
Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad: ELEMENT SIDE DEFINITION
1 1 1 1 2 1 1 1 1
0 0 0 0 0 0 0 0 0
```

Pu-241 boundary conditions: units of time and rates is years

```
Tqcbf(j,i) Qcbf(j,i) Tqcbf(j,i) Qcbf(j,i)
0.0 -0.00e-0 91.11 -0.000e-0 200.0 -0.000e-6 277.0 -0.000e-6
```

Set 16a: Cauchy Nodes- left side layer- NPCB
1 2 3

```
Ni Nseq Nad Nityp Ntypad: Set 16b: Type Cauchy Node DEFINITION
1 2 1 1 0
0 0 0 0 0
```

Table 6.3 Example BLT-MS Input, CHAIN7.DAT (continued)

Mi	Nseq	M	Is1	Is2	Miad	Mad	Islad	Is2ad:	ELEMENT SIDE DEFINITION
1	1	1	1	2	1	1	1	1	
0	0	0	0	0	0	0	0	0	

Pu-240 boundary conditions: units of time and rates is years
Tqcbf(j,i) Qcbf(j,i) Tqcbf(j,i) Qcbf(j,i)
0.0 -0.000e0 91.11 -0.000e-0 200.0 -0.000e-0 277.0 -0.000e-0

Set 16a: Cauchy Nodes- left side layer- NPCB
1 2 3

Ni	Nseq	Nad	Nityp	Ntypad:	Set 16b: Type Cauchy Node DEFINITION
1	2	1	1	0	
0	0	0	0	0	

Mi	Nseq	M	Is1	Is2	Miad	Mad	Islad	Is2ad:	ELEMENT SIDE DEFINITION
1	1	1	1	2	1	1	1	1	
0	0	0	0	0	0	0	0	0	

Set 16b: Neumann Boundary Conditions
Am-241 boundary conditions :units of time and rates is years
Am-241: Tqnbfbf(j,i) Qnbfbf(j,i) Tqnbfbf(j,i) Qnbfbf(j,i)
0.0 0.0000 91.1 0.0000 200.0 0.0000 300.0 0.0000

Am-241: Set 16a: Neuman Nodes- right side layer- NPNB
211 212 213

Ni	Nseq	Nad	Nityp	Ntypad:	set 16 b: Type Neumann modes
1	2	1	1	0	
0	0	0	0	0	

Am-241	Mi	Nseq	M	Is1	Is2	Miad	Mad	Islad	Is2ad :
	1	1	139	1	2	1	1	1	
	0	0	0	0	0	0	0	0	

Pu-241 boundary conditions :units of time and rates is years
Pu-241: Tqnbfbf(j,i) Qnbfbf(j,i) Tqnbfbf(j,i) Qnbfbf(j,i)
0.0 0.0000 91.1 0.0000 200.0 0.0000 300.0 0.0000

Pu-241: Set 16a: Neuman Nodes- right side layer- NPNB
211 212 213

Ni	Nseq	Nad	Nityp	Ntypad:	set 16 b: Type Neumann modes
1	2	1	1	0	
0	0	0	0	0	

Pu-241	Mi	Nseq	M	Is1	Is2	Miad	Mad	Islad	Is2ad :
	1	1	139	1	2	1	1	1	
	0	0	0	0	0	0	0	0	

PU-240 boundary conditions.
Tqnbfbf(j,i) Qnbfbf(j,i) Tqnbfbf(j,i) Qnbfbf(j,i) : units of time and rates is years
0.0 0.000-0 91.1 0.000-0 200.0 0.000-0 300.0 0.000-0

Pu-240: right side layer-
211 212 213

Table 6.3 Example BLT-MS Input, CHAIN7.DAT (continued)

Ni Nseq Nad Nityp Ntypad: set 16 b: Type Neumann modes
 1 2 1 1 0
 0 0 0 0 0

Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad : Neumann element sides
 1 1 139 1 2 1 1 1 1
 0 0 0 0 0 0 0 0 0

SET 17: DIRICHLET BOUNDARY CONDITIONS
 NOT USED IN THIS PROBLEM

SET 18: EXTERNAL ELEMENT SOURCE/SINK
 NOT USED IN THIS PROBLEM

SET 19: WELL POINT SOURCE/SINK
 NOT USED IN THIS PROBLEM

SET 20: WASTE CONTAINER PARAMETERS

THICK	PITN	PITK	AREA	ASCALE	PITS
1.000D0	0.01D0	0.007D0	2.1D4	0.2D0	5.0D3
GRATE	CLAY	SPH	IAER		
0.317D-09	0.15D0	6.0D0	2		
THICK	PITN	PITK	AREA	ASCALE	PITS
1.000D0	0.01D0	0.007D0	2.1D4	0.2D0	5.0D3
GRATE	CLAY	SPH	IAER		
0.317D+09	0.15D0	6.0D0	2		

(10) NELCON (1) (2) (3) (4) (5) (6) (7) (8) (9)
 21 22 41 42 61 62

MI	MSEQ	MAD	MITYPE	MTYPAD
1	3	1	1	0
5	1	1	2	0
0	0	0	0	0

SET 21: WASTE FORM RELEASE PARAMETERS

NWTYPE = 1

SFRACT(I)	PFRACT(I)	BFRACT(I)	DEFF(I)	DISOL(I)	ISO = 1
0.333D0	0.333D0	0.333D0	1.0D-8	1.0D-03	
PARTK0(I)	PARTKI(I)	PARTKD(I)			
0.0D0	0.0D0	0.0D0			
SFRACT(I)	PFRACT(I)	BFRACT(I)	DEFF(I)	DISOL(I)	ISO = 2
0.333D0	0.333D0	0.333D0	1.0D-8	1.0D-03	
PARTK0(I)	PARTKI(I)	PARTKD(I)			
0.0D0	0.0D0	0.0D0			
SFRACT(I)	PFRACT(I)	BFRACT(I)	DEFF(I)	DISOL(I)	ISO = 3
0.333D0	0.333D0	0.333D0	1.0D-8	1.0D-03	

Table 6.3 Example BLT-MS Input, CHAIN7.DAT (continued)

PARTK0(I)	PARTKI(I)	PARTKD(I)							
0.0D0	0.0D0	0.0D0							
POREL	VOLWF	VRATIO							
25.0D0	1.0D6	1.0							

C ***** DATA SET 21B: INITIAL MASSES OF EACH WASTE ELEMENT

ISO =1

WTINIT1,X1	X2	X3	X4	X5	X6	X7	X8	X9	X10
3.0D0	3.0D0	3.0D0	3.0D0	3.0D0	3.0D0				

ISO = 2

WTINIT1,X1	X2	X3	X4	X5	X6	X7	X8	X9	X10
0.0D0	0.0D0	0.0D0	0.0D0	0.0D0	0.0D0				

ISO =3

WTINIT1,X1	X2	X3	X4	X5	X6	X7	X8	X9	X10
0.0D0	0.0D0	0.0D0	0.0D0	0.0D0	0.0D0				

C ***** DATA SET 21C: READ WASTE TYPE ASSIGNMENTS

MI	NSEQ	MAD	MITYP	MTYPAD
1	5	1	1	0
0	0	0	0	0

SET 22: PRINTER CONTROL PARAMETERS

Set 22A: Printer Control parameters

Kpr0	Kpr(1)	Kpr(2)	Kpr(3)	Kpr(4)	Kpr(5)	Kpr(6)	--Kpr(ntl)
022	2	0	0	0	0	0	0
0	2	222		0	0		0
0	2			0			0
0	2		2				

C ***** DATA SET 22B: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
NOT USED IN BLTMS

C ***** DATA SET 22C: TRACE FILES-NO OF CONC. AND FLUX NODE NUMBERS & NODE
NO'S

NTRC	NTRF	NSTPTR
8	4	1

Concentration trace information-Global node numbers NTRCEC(k)

2	32	62	92	122	152	182	212
---	----	----	----	-----	-----	-----	-----

Flux trace nodes

2	32	62	92
---	----	----	----

C ***** DATA SET 23B: VELOCITY AND MOISTURE CONTENT

Ni	Nseq	Nad	Vxni	Vzni	Vxad	Vzad
1	212	1	+2.316d-04	0.0d-00	0.0	0.0
0	0	0	0	0	0	0

SET 18B:

Ni	Nseq	Nad	Thni	Thniad
1	139	1	0.2	0.0
0	0	0	0	0

7 BLT-MS OUTPUT FILES

BLT-MS creates several output files. The exact number depends on whether containers are simulated, whether trace files have been requested through input, and the number of contaminants in the simulation. Table 7.1 lists the various output files that may be created by BLT-MS. At a minimum, two output files will be created, the main BLT-MS output file, and INPTECHO.DAT, a file which provides an immediate echo print of the BLT-MS input file as it is read. INPTECHO.DAT is extremely useful in detecting errors in input that cause the program to fail. At a maximum, BLT-MS can create forty-two separate output files. For DOS based users, this will cause a problem if the number of files specified in CONFIG.SYS is less than 50. In addition to the two files already discussed, BLT-MS may create a concentration trace file, flux trace file, waste form release rate file, and waste form cumulative mass release file for each isotope. The waste form files are created every time waste forms are simulated. The trace files are created if requested by input (Data Set 22 of the BLT-MS input, variables NTRC and NTRF). With the exception of the main output file, the file names are fixed by BLT-MS and the files will be overwritten every time the code is executed. Renaming of the files is necessary if they are to be used at a later time after subsequent BLT-MS simulations. This section will describe each of the output files, their naming convention, and their structure.

Table 7.1 BLT-MS Output Files

File Name	Contents
INPTECHO.DAT	List of input file as it is read.
User Specified	Primary BLT-MS output file. It prints out the input with text to identify the parameters. Plus, it prints concentrations, fluxes, and waste form release rates as specified through the printer control parameters in Data Set 22, variable, KPR.
LEACHRL?.DAT*	Lists the time, cumulative mass released from the waste form, the mass release by mechanism (rinse, diffusion, degradation), the mass release rate (total and by mechanism), the breached area of the container, and the element number of the container for each element with a waste container.
LEACHMS?.DAT*	Lists the time, mass remaining in the waste form, mass released from the waste form, and the mass decayed over the time step for each release mechanism, and the waste container location.
TRACECN?.DAT*	Lists the time and concentration for specified nodal locations.
TRACEFX?.DAT*	Lists the flux in the x and z-direction for specified nodal locations.

* For each of these types of files, one file is created for each contaminant in the simulation. The first contaminant would have its information stored in LEACHRL1.DAT, etc. The second contaminant in LEACHRL2.DAT and so on.

7.1 Input Check File (INPTECHO.DAT)

A complete example of the file INPTECHO.DAT is supplied in Appendix A. This file contains output written immediately after reading the BLT-MS input file. Therefore, it is quite useful for debugging invalid input. In some cases, all of the input is not printed in the INPTECHO.DAT file. This is done to save space and does not influence the ability to determine the last read statement executed in BLT-MS. The primary output file is not as reliable for locating the source of improper input as INPTECHO.DAT because it does not always create output immediately after reading information. Often, processing occurs between the read statement and the write statement when generating the primary output file.

7.2 Primary Output File

The primary output file name is specified by the user when using BLT-MS. In the first section of the primary output file, the input after some processing is printed. Identifiers are supplied to assist the code user in interpretation of the choices defined by input. Processing of input is limited to expanding information supplied for automatic definition into the form needed for the calculation. For example, if the Darcy flux in the z-direction for all 100 nodes in a simulation was equal, one input record could be used to specify the Darcy flux at all points (Data Set 23 in section 6.23). In this example, the following line of input would achieve the desired results:

```
1 99 1 -2.5E-7 0.0 0.0 0.0
```

In the primary output file, the x and z Darcy flux at each nodal location are explicitly stated. Similar remarks apply to all variables that use formulas (as discussed in section 6) to generate input (for example, element indices, assignment of material types, waste container types, waste form types, and moisture content).

After completion of the review of the input, output from the calculation is presented. The amount of information is controlled by the print control variable, KPR (data set 22 in section 6.22). KPR may change with each time step. If KPR is zero, no output is generated in the primary output file at that time. If KPR is 1, a system flow table, container performance data, and the waste form release rates and cumulative mass released for each release mechanism are printed. The system flow table provides the mass flow rate and cumulative mass flow out of the boundary nodes of the system, introduced into the system through sources, and lost to radioactive decay. If KPR is 2, the above is printed and the contaminant concentration at each nodal location is printed for each contaminant. If KPR is 3 all of the above is printed and the contaminant flux in the x and z-direction at each spatial location is printed for each contaminant. The output is formatted to print all of the information requested pertaining to a single contaminant before moving to the next contaminant.

A partial example of the primary output file is provided in Appendix B.

The primary output file is used extensively by the program BLTPLOT. BLTPLOT reads the nodal information, material definition, waste container location, waste container and waste form type information, Darcy flux, moisture content, and concentrations at each output time. Any changes in the formatting or order of the output may require changes to the BLTPLOT code.

7.3 Waste Form Release Rate Files (LEACHRL?.DAT)

A LEACHRL output file contains information on cumulative mass release and mass release rates for each release mechanism and each waste form. An individual LEACHRL file is created for each contaminant in the simulation. Data are written to this file at the output times defined using the logic for calculating when TRACE files (section 7.5 and 7.6) are written. An input variable, NSTPTR (Data Set 22), defines the number of time steps between output. Output is generated every NSTPTR time steps. For example, if NSTPTR is one, output is generated at each time step.

Each LEACHRL file contains a title line which identifies the contaminant and the BLT-MS input file used in creating this file. This is followed by a blank line. The following line provides eleven identifiers for the data that follows. The identifiers pertain to the waste form located in the finite element domain at the location identified by the variable NELCON and are:

<u>Identifier</u>	<u>Definition</u>
Time (yr)	Simulation time in years
Cumr	Cumulative mass released
Trinse	Cumulative rinse mass released
Tdif	Cumulative diffusion mass released
Tdis	Cumulative degradation mass released
Sosl	Total mass release rate

Rinser Rinse mass release rate
 Diffr Diffusion mass release rate
 Disr Degradation mass release rate
 Barea Container breached area
 Nelcon Finite element containing the waste form

Beneath the identifiers the data generated by BLT-MS is printed. An example of a LEACHRL file is presented in Table 7.2.

Table 7.2 Example of LEACHRL Output File

Isotope =	Am241	Input file	= chain7.dat								
Time (yr)	Cumr	Trinse	Tdif	Tdis	Sosl	Rinser	Diffr	Disr	Barea	Nelcon	
1.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
1.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
1.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
1.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
1.00	1.026E+00	9.990E-01	2.586E-02	9.990E-04	3.251E-14	3.166E-14	8.196E-16	3.166E-17	2.100E+04	61	
1.00	1.026E+00	9.990E-01	2.586E-02	9.990E-04	3.251E-14	3.166E-14	8.196E-16	3.166E-17	2.100E+04	62	
2.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
2.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
2.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
2.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
2.00	1.038E+00	9.990E-01	3.676E-02	1.996E-03	3.767E-16	3.507E-30	3.451E-16	3.161E-17	2.100E+04	61	
2.00	1.038E+00	9.990E-01	3.676E-02	1.996E-03	3.767E-16	3.507E-30	3.451E-16	3.161E-17	2.100E+04	62	
3.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
3.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
3.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
3.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
3.00	1.047E+00	9.990E-01	4.512E-02	2.992E-03	2.967E-16	0.000E+00	2.651E-16	3.156E-17	2.100E+04	61	
3.00	1.047E+00	9.990E-01	4.512E-02	2.992E-03	2.967E-16	0.000E+00	2.651E-16	3.156E-17	2.100E+04	62	
4.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
4.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
4.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
4.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
4.00	1.055E+00	9.990E-01	5.217E-02	3.986E-03	2.549E-16	0.000E+00	2.234E-16	3.150E-17	2.100E+04	61	
4.00	1.055E+00	9.990E-01	5.217E-02	3.986E-03	2.549E-16	0.000E+00	2.234E-16	3.150E-17	2.100E+04	62	
5.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
5.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
5.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
5.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
5.00	1.062E+00	9.990E-01	5.838E-02	4.979E-03	2.281E-16	0.000E+00	1.967E-16	3.145E-17	2.100E+04	61	
5.00	1.062E+00	9.990E-01	5.838E-02	4.979E-03	2.281E-16	0.000E+00	1.967E-16	3.145E-17	2.100E+04	62	
6.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
6.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
6.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
6.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
6.00	1.069E+00	9.990E-01	6.399E-02	5.970E-03	2.091E-16	0.000E+00	1.777E-16	3.140E-17	2.100E+04	61	
6.00	1.069E+00	9.990E-01	6.399E-02	5.970E-03	2.091E-16	0.000E+00	1.777E-16	3.140E-17	2.100E+04	62	
7.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
7.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
7.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
7.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
7.00	1.075E+00	9.990E-01	6.914E-02	6.960E-03	1.947E-16	0.000E+00	1.633E-16	3.135E-17	2.100E+04	61	
7.00	1.075E+00	9.990E-01	6.914E-02	6.960E-03	1.947E-16	0.000E+00	1.633E-16	3.135E-17	2.100E+04	62	
8.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
8.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
8.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
8.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
8.00	1.081E+00	9.990E-01	7.394E-02	7.947E-03	1.833E-16	0.000E+00	1.520E-16	3.130E-17	2.100E+04	61	
8.00	1.081E+00	9.990E-01	7.394E-02	7.947E-03	1.833E-16	0.000E+00	1.520E-16	3.130E-17	2.100E+04	62	
9.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
9.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
9.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
9.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
9.00	1.086E+00	9.990E-01	7.844E-02	8.934E-03	1.740E-16	0.000E+00	1.427E-16	3.125E-17	2.100E+04	61	
9.00	1.086E+00	9.990E-01	7.844E-02	8.934E-03	1.740E-16	0.000E+00	1.427E-16	3.125E-17	2.100E+04	62	
10.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	21	
10.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	22	
10.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	41	
10.00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	42	
10.00	1.092E+00	9.990E-01	8.305E-02	9.918E-03	1.772E-16	0.000E+00	1.460E-16	3.120E-17	2.100E+04	61	
10.00	1.092E+00	9.990E-01	8.305E-02	9.918E-03	1.772E-16	0.000E+00	1.460E-16	3.120E-17	2.100E+04	62	

When multiple contaminants are simulated, the first contaminant LEACHRL file is named LEACHRL1.DAT. The second is LEACHRL2.DAT. This continues until all contaminants have a unique LEACHRL file. The maximum number of contaminants permitted in BLT-MS is ten. In this case, LEACHRL0.DAT would be used to store information pertaining to the tenth contaminant.

LEACHRL files can be used in BLTPLOT to display the cumulative mass released from each waste form by release rate mechanism.

7.4 Waste Form Mass Balance Files (LEACHMS?.DAT)

A LEACHMS output file contains information on mass available for release, mass released, and decay mass over a time step for each release mechanism and each waste form. An individual LEACHMS file is created for each contaminant in the simulation. Data are written to this file at the output times defined using the logic for calculating when TRACE files (section 7.5 and 7.6) are written as discussed in section 7.3.

Each LEACHMS file contains a title line which identifies the contaminant and the BLT-MS input file used in creating this file. This is followed by a blank line. The following line provides eleven identifiers for the data that follows. The identifiers pertain to the waste form located in the finite element domain at the location identified by the variable NELCON and are

<u>Identifier</u>	<u>Definition</u>
Time (yr)	Simulation time
Asmass	Mass available for release due to rinse limited by partitioning
Rsmass	Cumulative mass released due to rinse processes
Dsmass	Mass available for rinse release that decays over the time step
Apmloc	Mass available for release through diffusion processes
Rpmass	Cumulative mass released due to diffusion processes
Dpmass	Mass available for diffusion release that decays over a time step
Abmass	Mass available for release due to degradation processes
Rbmass	Cumulative mass released through the degradation process
Dbmass	Mass available for degradation release that decays over a time step
Nelcon	Finite element that contains the waste form

Beneath the identifiers the data generated by BLT-MS is printed. An example of a LEACHMS file is presented in Table 7.3.

When multiple contaminants are simulated, the naming convention is similar to that for the LEACHMS files discussed in section 7.3.

7.5 Concentration Trace Files (TRACECN?.DAT)

Concentration trace files contain the concentration as a function of time at nodes selected through input in data set 22 (section 6.22). A unique concentration trace file is written for each contaminant in the simulation. Data are written to this file at the output times defined using the logic as discussed in section 7.3.

The first line of the file always contains the problem title as specified via input and the contaminant name. The second line contains the number of traces in the file and the name of the input used to create this output file. Following this, there is one line for each trace which specifies the node and the X, and Z co-ordinates of the node. This is followed by an alpha-numeric line with a column label for the time and the units for the concentration. After this, the data follow. The file is formatted to print the simulation time first, followed by up to six concentration values per line. Therefore, if the number of traces exceeds six, multiple lines are used for the output at each time step. Concentration values are aligned such that the concentration at trace node 7 is beneath the concentration at trace node 1 and so on. An example of a concentration trace

file is presented in Table 7.4.

Table 7.3 Example of LEACHMS Output File

Isotope = Time (yr)	Am241 Asmass	Input file Rsmass	= chain7.dat Dsmass	Apmloc	Rpmass	Dpmass	Abmass	Rbmass	Dbmass	Nelcon
1.00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	21
1.00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	22
1.00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	41
1.00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	9.990E-01	0.000E+00	0.000E+00	42
1.00	1.108E-16	9.990E-01	1.776E-19	9.563E-01	2.586E-02	1.530E-03	9.964E-01	9.990E-04	1.594E-03	61
1.00	1.108E-16	9.990E-01	1.776E-19	9.563E-01	2.586E-02	1.530E-03	9.964E-01	9.990E-04	1.594E-03	62
2.00	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	21
2.00	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	22
2.00	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	41
2.00	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	9.974E-01	0.000E+00	1.598E-03	42
2.00	0.000E+00	1.107E-16	0.000E+00	9.513E-01	1.089E-02	1.522E-03	9.948E-01	9.974E-04	1.591E-03	61
2.00	0.000E+00	1.107E-16	0.000E+00	9.513E-01	1.089E-02	1.522E-03	9.948E-01	9.974E-04	1.591E-03	62
3.00	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	21
3.00	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	22
3.00	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	41
3.00	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	9.958E-01	0.000E+00	1.595E-03	42
3.00	0.000E+00	0.000E+00	0.000E+00	9.452E-01	8.367E-03	1.512E-03	9.922E-01	9.958E-04	1.587E-03	61
3.00	0.000E+00	0.000E+00	0.000E+00	9.452E-01	8.367E-03	1.512E-03	9.922E-01	9.958E-04	1.587E-03	62
4.00	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	21
4.00	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	22
4.00	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	41
4.00	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	9.942E-01	0.000E+00	1.593E-03	42
4.00	0.000E+00	0.000E+00	0.000E+00	9.390E-01	7.050E-03	1.502E-03	9.897E-01	9.942E-04	1.583E-03	61
4.00	0.000E+00	0.000E+00	0.000E+00	9.390E-01	7.050E-03	1.502E-03	9.897E-01	9.942E-04	1.583E-03	62
5.00	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	21
5.00	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	22
5.00	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	41
5.00	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	9.926E-01	0.000E+00	1.590E-03	42
5.00	0.000E+00	0.000E+00	0.000E+00	9.328E-01	6.206E-03	1.492E-03	9.871E-01	9.926E-04	1.579E-03	61
5.00	0.000E+00	0.000E+00	0.000E+00	9.328E-01	6.206E-03	1.492E-03	9.871E-01	9.926E-04	1.579E-03	62
6.00	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	21
6.00	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	22
6.00	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	41
6.00	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	9.910E-01	0.000E+00	1.588E-03	42
6.00	0.000E+00	0.000E+00	0.000E+00	9.268E-01	5.607E-03	1.482E-03	9.845E-01	9.910E-04	1.575E-03	61
6.00	0.000E+00	0.000E+00	0.000E+00	9.268E-01	5.607E-03	1.482E-03	9.845E-01	9.910E-04	1.575E-03	62
7.00	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	21
7.00	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	22
7.00	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	41
7.00	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	9.895E-01	0.000E+00	1.585E-03	42
7.00	0.000E+00	0.000E+00	0.000E+00	9.209E-01	5.153E-03	1.473E-03	9.819E-01	9.895E-04	1.571E-03	61
7.00	0.000E+00	0.000E+00	0.000E+00	9.209E-01	5.153E-03	1.473E-03	9.819E-01	9.895E-04	1.571E-03	62
8.00	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	21
8.00	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	22
8.00	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	41
8.00	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	9.879E-01	0.000E+00	1.583E-03	42
8.00	0.000E+00	0.000E+00	0.000E+00	9.151E-01	4.796E-03	1.464E-03	9.794E-01	9.879E-04	1.567E-03	61
8.00	0.000E+00	0.000E+00	0.000E+00	9.151E-01	4.796E-03	1.464E-03	9.794E-01	9.879E-04	1.567E-03	62
9.00	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	21
9.00	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	22
9.00	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	41
9.00	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	9.863E-01	0.000E+00	1.580E-03	42
9.00	0.000E+00	0.000E+00	0.000E+00	9.094E-01	4.504E-03	1.455E-03	9.768E-01	9.863E-04	1.562E-03	61
9.00	0.000E+00	0.000E+00	0.000E+00	9.094E-01	4.504E-03	1.455E-03	9.768E-01	9.863E-04	1.562E-03	62
10.00	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	21
10.00	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	22
10.00	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	41
10.00	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	9.847E-01	0.000E+00	1.578E-03	42
10.00	0.000E+00	0.000E+00	0.000E+00	9.039E-01	4.608E-03	1.446E-03	9.743E-01	9.847E-04	1.558E-03	61
10.00	0.000E+00	0.000E+00	0.000E+00	9.039E-01	4.608E-03	1.446E-03	9.743E-01	9.847E-04	1.558E-03	62

Table 7.4 Example of a Concentration Trace File with Eight Trace Locations

Prob2: Three species decay chain. Containers Am241
 NUMBER OF CONCENTRATION TRACES = 8 Input file chain7.dat

Node and (X,Z) Locations:	2	(0.00E+00 , 1.00E+02)
Node and (X,Z) Locations:	32	(1.00E+03 , 1.00E+02)
Node and (X,Z) Locations:	62	(2.00E+03 , 1.00E+02)
Node and (X,Z) Locations:	92	(3.00E+03 , 1.00E+02)
Node and (X,Z) Locations:	122	(4.00E+03 , 1.00E+02)
Node and (X,Z) Locations:	152	(5.00E+03 , 1.00E+02)
Node and (X,Z) Locations:	182	(6.00E+03 , 1.00E+02)
Node and (X,Z) Locations:	212	(7.00E+03 , 1.00E+02)

TIME (YRS) Concentrations (units are in gm/cm3)

1.00E+00	4.25E-38	3.66E-29	5.96E-20	9.71E-11	1.34E-16	3.91E-24
	1.14E-31	6.28E-39				
2.00E+00	1.00E-36	5.97E-28	5.32E-19	1.48E-10	9.96E-16	5.79E-23
	2.53E-30	1.86E-37				
3.00E+00	1.23E-35	5.10E-27	2.58E-18	1.72E-10	4.09E-15	4.52E-22
	2.91E-29	2.82E-36				
4.00E+00	1.03E-34	3.03E-26	9.00E-18	1.82E-10	1.23E-14	2.47E-21
	2.31E-28	2.92E-35				
5.00E+00	6.70E-34	1.41E-25	2.53E-17	1.84E-10	3.01E-14	1.06E-20
	1.42E-27	2.33E-34				
6.00E+00	3.59E-33	5.50E-25	6.11E-17	1.82E-10	6.37E-14	3.80E-20
	7.17E-27	1.52E-33				
7.00E+00	1.65E-32	1.85E-24	1.31E-16	1.77E-10	1.21E-13	1.19E-19
	3.12E-26	8.49E-33				
8.00E+00	6.66E-32	5.55E-24	2.56E-16	1.71E-10	2.11E-13	3.31E-19
	1.20E-25	4.15E-32				
9.00E+00	2.42E-31	1.51E-23	4.62E-16	1.66E-10	3.43E-13	8.42E-19
	4.15E-25	1.82E-31				
1.00E+01	8.05E-31	3.80E-23	7.85E-16	1.60E-10	5.29E-13	1.98E-18
	1.31E-24	7.23E-31				
1.10E+01	2.47E-30	8.88E-23	1.27E-15	1.54E-10	7.76E-13	4.33E-18
	3.84E-24	2.65E-30				
1.20E+01	7.07E-30	1.95E-22	1.95E-15	1.49E-10	1.09E-12	8.95E-18
	1.05E-23	8.99E-30				
1.30E+01	1.90E-29	4.07E-22	2.88E-15	1.44E-10	1.49E-12	1.76E-17
	2.70E-23	2.86E-29				
1.40E+01	4.83E-29	8.08E-22	4.13E-15	1.40E-10	1.97E-12	3.29E-17
	6.58E-23	8.56E-29				
1.50E+01	1.17E-28	1.54E-21	5.73E-15	1.35E-10	2.54E-12	5.91E-17
	1.52E-22	2.43E-28				
1.60E+01	2.70E-28	2.81E-21	7.75E-15	1.31E-10	3.21E-12	1.02E-16
	3.38E-22	6.57E-28				
1.70E+01	5.98E-28	4.95E-21	1.02E-14	1.28E-10	3.97E-12	1.71E-16
	7.20E-22	1.70E-27				
1.80E+01	1.28E-27	8.47E-21	1.32E-14	1.24E-10	4.82E-12	2.78E-16
	1.48E-21	4.20E-27				
1.90E+01	2.63E-27	1.41E-20	1.68E-14	1.21E-10	5.76E-12	4.40E-16
	2.92E-21	1.00E-26				
2.00E+01	5.24E-27	2.27E-20	2.10E-14	1.18E-10	6.79E-12	6.78E-16
	5.62E-21	2.31E-26				

The concentration trace files are read by the graphics program BLTPLOT. Graphs of concentration versus time at each trace node can be generated by BLTPLOT. Any changes to the format of this file will require similar changes in BLTPLOT.

7.6 Flux Trace Files (TRACEFX?.DAT)

Flux trace files contain the flux in the X and Z-directions as a function of time at nodes selected through input in data set 22 (section 6.22). A unique flux trace file is written for each contaminant in the simulation. Data are written to this file at the output times defined using the logic as discussed in section 7.3.

Flux trace files are similar in format to the concentration trace files. The first line of the file always contains the problem title as specified via input and the contaminant name. The second line contains the number of traces in the file and the name of the input used to create this output file. Following this, there is one line for each trace which specifies the node and the X, and Z co-ordinates of the node. This is followed by an alpha-numeric line with a column label for the time and the units for the flux. After this, the data follow. The file is formatted to print the simulation time first, followed by up to three pairs of flux values. The first value is the X-direction flux for the first flux trace node. The second value is the Z-direction flux for the first flux trace node. The process is repeated with up to three flux pairs per line. When more than three flux pairs are requested, multiple lines of output are generated for each simulation time. An example of a flux trace file is presented in Table 7.5.

The flux trace files are read by the graphics program BLTPLOT. A graph of the flux in the X and Z-direction versus time at each trace node can be generated by BLTPLOT. Any changes to the format of this file will require similar changes in BLTPLOT.

Table 7.5 Example Flux Trace File with Four Flux Trace Nodes

Prob2: Three species decay chain. Containers
NUMBER OF FLUX TRACES = 4 Input file chain7.dat
Node and (X,Z) Locations: 2 (0.00E+00 , 1.00E+02)
Node and (X,Z) Locations: 32 (1.00E+03 , 1.00E+02)
Node and (X,Z) Locations: 62 (2.00E+03 , 1.00E+02)
Node and (X,Z) Locations: 92 (3.00E+03 , 1.00E+02)
TIME (YRS) FLUX - X; FLUX - Z (units are in gm/cm2/yr)

1.00E+00	-3.50E-30	3.72E-48	-9.18E-25	9.76E-43	-4.81E-19	5.11E-37
	-3.45E-13	-1.66E-31				
2.00E+00	-1.71E-30	-7.50E-48	-4.49E-25	-1.97E-42	-2.36E-19	-1.04E-36
	-2.33E-13	-1.43E-30				
3.00E+00	-8.50E-31	1.03E-47	-2.23E-25	2.71E-42	-1.19E-19	1.36E-36
	-1.61E-13	-3.65E-30				
4.00E+00	-4.33E-31	4.67E-47	-1.14E-25	1.22E-41	-6.72E-20	6.34E-36
	-1.13E-13	-3.04E-30				
5.00E+00	-2.31E-31	3.91E-48	-6.08E-26	1.02E-42	-5.26E-20	-1.47E-37
	-8.09E-14	-3.17E-30				
6.00E+00	-1.33E-31	-3.44E-47	-3.53E-26	-9.02E-42	-6.65E-20	-5.97E-36
	-5.91E-14	-5.37E-30				
7.00E+00	-8.45E-32	9.71E-48	-2.37E-26	2.50E-42	-1.11E-19	-2.47E-36
	-4.40E-14	-5.16E-30				
8.00E+00	-6.01E-32	5.97E-47	-2.03E-26	1.55E-41	-1.96E-19	-9.88E-37
	-3.32E-14	-5.49E-30				
9.00E+00	-4.75E-32	1.69E-47	-2.47E-26	3.77E-42	-3.34E-19	-1.20E-35
	-2.55E-14	-5.74E-30				
1.00E+01	-4.20E-32	-1.90E-46	-4.11E-26	-5.12E-41	-5.42E-19	-5.23E-35
	-1.99E-14	-7.36E-30				
1.10E+01	-3.91E-32	-1.32E-46	-7.92E-26	-3.79E-41	-8.38E-19	-5.56E-35
	-1.57E-14	-7.21E-30				
1.20E+01	-3.84E-32	-4.28E-46	-1.59E-25	-1.18E-40	-1.24E-18	-1.17E-34
	-1.24E-14	-7.69E-30				
1.30E+01	-4.05E-32	7.59E-46	-3.13E-25	1.79E-40	-1.77E-18	-2.65E-35
	-9.92E-15	-7.46E-30				
1.40E+01	-4.82E-32	-2.72E-46	-6.01E-25	-1.03E-40	-2.45E-18	-1.69E-34
	-7.94E-15	-7.96E-30				
1.50E+01	-6.76E-32	6.71E-46	-1.11E-24	1.06E-40	-3.28E-18	-1.45E-34
	-6.36E-15	-7.79E-30				
1.60E+01	-1.11E-31	-8.39E-46	-1.99E-24	-3.11E-40	-4.29E-18	-3.65E-34
	-5.08E-15	-8.76E-30				
1.70E+01	-2.04E-31	2.99E-46	-3.43E-24	-6.07E-41	-5.47E-18	-3.52E-34
	-4.04E-15	-7.10E-30				
1.80E+01	-3.92E-31	-2.21E-45	-5.75E-24	-7.62E-40	-6.85E-18	-6.50E-34
	-3.18E-15	-8.24E-30				
1.90E+01	-7.60E-31	-7.50E-46	-9.36E-24	-6.40E-40	-8.40E-18	-8.89E-34
	-2.46E-15	-7.56E-30				
2.00E+01	-1.46E-30	4.58E-45	-1.48E-23	1.73E-40	-1.01E-17	-5.55E-34
	-1.87E-15	-7.50E-30				

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8 BLTPLOT: A GRAPHICAL POST-PROCESSOR FOR BLT-MS AND BLT-EC

BLT-MS and BLT-EC generate large quantities of numeric output. It is not practical to examine this output without the aid of an interpreter that translates the numeric output into a graphical display. This can be accomplished through spreadsheet programs. However, to ease the burden on the user, BLTPLOT was specifically written to read information from BLT-MS and BLT-EC output files and provide graphical output.

BLTPLOT is a FORTRAN computer program that was created to enable output from the programs BLT-MS and BLT-EC to be readily analyzed graphically on a video display device. BLTPLOT runs on DOS or in a full screen DOS window under Windows (3.1 WFW 3.11, or 95). BLTPLOT uses multiple colors to depict the features of the output. In addition, these plots may be saved as PostScript files which are copies of the displayed graphical output. PostScript files can be generated for black and white printers as well as color printers. The Post Script file can also be imported directly into WordPerfect as an image. The program BLTPLOT is menu driven to provide easy access to the various display options. On screen help is displayed with all menu items to assist the user in selection of the proper choice from the menu.

BLTPLOT has the following plotting capabilities:

- A) System Maps:
 - 1. A material location plot with unique colors to depict regions of dissimilar material type.
 - 2. A container location plot with unique colors to depict each container type
 - 3. A waste form location map with unique colors to depict each waste form type.
- B) Contour Maps with different colors to depict the different levels for:
 - 1. Moisture content
 - 2. X-direction Darcy flux
 - 3. Z-direction Darcy flux
 - 4. Pressure head
 - 5. Total head
 - 6. Concentration of each contaminant at selected times. For BLT-EC, the user is allowed to plot total concentration, dissolved concentration, precipitated concentration, adsorbed concentration, and Kd.
- C) Vector plots of the total Darcy flux at each location. The magnitude and direction of the Darcy flux are depicted through arrows of different size and colors.
- D) X-Y plots for:
 - 1. Concentration at user specified locations
 - 2. Flux at user specified locations
 - 3. Cumulative mass released for each waste form by release mechanism (rinse, diffusion, degradation).

The program relies on calls to graphics library provided as part of the MS FORTRAN package for its video displays. The video display and the PostScript files are generated by calls to the NASADIG [NASA, 1994] library of routines.

The following sections describe the use of BLTPLOT as it applies to BLT-MS files..

8.1 BLTPLOT Configuration Files

BLTPLOT determines the names of the output files that are read and screen plotting parameters from a configuration file. These files always have an extension of ".CNF". When the program begins, the user is presented with a menu of available configuration files in the working directory.

A configuration file is presented in Table 8.1.

Table 8.1 Example of the Configuration File, BLTMS.CNF

	MS: type of data to be plotted
	T: t superimposes grid over the plot
	F: t adjusts x and y scale to fill the screen
	T: t plots velocity-arrow outline in white
	1.500E-01: character height in inches
	2.100E-01: velocity arrow length in inches
aux_in.dat	: Name of the file output from FEMWATER
	: Name of the BLT restart file
	: Name of the BLT input file
leachr11.dat	: Name of the BLT waste-leaching output file
bltms.out	: Name of the BLT output file
tracecn1.dat	: Name of the Concentration trace file
tracefx1.dat	: Name of the Mass-Flux BLTMS output file
	7: Function number (F) to plot;
	0 - Material number,
	1 - Water content,
	2 - X velocity,
	3 - Y velocity,
	4 - Total velocity,
	5 - Total head,
	6 - Pressure head,
	7 - Concentration,
	8 - Container type,
	9 - Waste type.
	1.000E-10: Interval for plotting function

Table 8.1 contains the following information:

A two letter code, MS or EC, which specifies whether the data to be displayed come from the program BLT-MS or BLT-EC.

Several logical variables used for display options:

fill screen:	a logical variable that if true will cause differing scaling in the x and y direction such that the viewing window will essentially fill the screen.
overlay grid:	a logical variable that if true will cause the finite element grid to be plotted as an overlay to the plot.
outline arrow:	a logical variable that if true will cause the program to outline arrows in white if drawing velocity vectors.

Two real variables for the size of the characters and arrow:

character size: a real variable that represents the height of characters in inches used during plotting and graphing.

arrow size: a real variable that represents the maximum dimension (in inches) of arrows used to represent velocity vectors during plotting. Velocity less than maximum are scaled to the maximum magnitude of velocity and the maximum arrow size.

Several character variables used to define the names of the files read as input. If a file name is left blank, BLTPLOT automatically skips through the sections of the code that use that particular file and does not permit the user to select options supplied by the missing file. For example, the FEMWATER output file provides the pressure head. If it is not specified, the option to plot pressure head is not displayed in BLTPLOT. The files potentially used for plotting are:

- a) FEMWATER output: the name of the file output by FEMWATER that is used as input for the BLT-MS run to supply pressure head and total head.
- b) BLT-MS or BLT-EC restart file: Historical and not used in this version of the program.
- c) BLT-MS or BLT-EC input file: Historical and not used in this version of the program.
- d) BLT-MS output: the name of the file created for listing the BLT-MS output.
or
BLT-EC output : the name of the file created for listing the BLT-EC output.
- e) Leaching file: the name of the file created by BLT-MS containing the mass released as a function of time from each waste form. Generally, this will be LEACHRL?.DAT. Where the "?" is a number between 0 and 9 that represents the number of the isotope. The capability to plot leaching file output from BLT-EC has not been implemented into BLTPLOT.
- f) Trace concentration: the name of the file created by BLT-MS containing the concentration as a function of time at specific nodes. Generally, this will be TRACECN?.DAT. Where the "?" represents the number of the isotope. The capability to plot concentration trace files generated by BLT-EC has not been implemented into BLTPLOT.
- g) Trace Mass-flux file: the name of the file created by BLT-MS containing the flux as a function of time at specific nodes. Generally, this will be TRACEFX?.DAT. Where the "?" represents the number of the isotope. The capability to plot concentration trace files generated by BLT-EC has not been implemented into BLTPLOT.

BLTPLOT permits the user to select the contaminant for which a plot will be generated. Therefore, for the leaching and trace files any number can be used in place of the question mark. BLTPLOT will select the correct file based on input that requests the plotting of a given contaminant. This will be true as long as the file name contains eight characters before the extension and the eighth character must be a number.

The list of files is followed by an integer flag indicating the default value for the function to plot. The selection of which function to plot can be changed during use of BLTPLOT. This is followed by the list of available functions:

- 0 - Material number,
- 1 - Water content,
- 2 - X velocity,

- 3 - Y velocity,
- 4 - Total velocity,
- 5 - Total head,
- 6 - Pressure head,
- 7 - Concentration,
- 8 - Container type,
- 9 - Waste type.

The final line in the configuration file contains the default contour interval. This value is reset when the selection of plot variables is made.

8.2 Use of BLTPLOT

When BLTPLOT is started, it displays a menu of available configuration files in the current working directory. These are files with the extension 'CNF'. A maximum of twenty configuration files can be used. In addition, a menu item of 'New' is available for defining a new configuration file. Generally it is best to have BLTPLOT installed in the same directory as the output files generated by BLT-MS or BLT-EC.

After defining a new configuration file or selecting an existing file, BLTPLOT reads the specified input file(s) and prints the main menu on the screen. Movement between choices is accomplished by either typing the first letter of the choice to be used or by using the arrow keys on the keyboard. The Enter key implements the selected choice. The main menu displays the following five choices:

Configure Options Graph Function Exit

Configure	to select or modify the configuration file used
Options	to adjust the contour interval options and choose the orientation and type (color or B&W) of the PostScript output file.
Graph	(when appropriate) to select a graph of a time trace of a function for a specific node or element.
Function	to select (and plot) a function. The available functions were listed above in Table 8.1.
Exit	to exit the program.

8.2.1 Configure Option

The Configure option allows modification of the current configuration file, or selection of a new file as discussed above. The information is entered on an input form with data checking where possible and an on screen help for each item.

8.2.2 Options Option

The Options option allows selection of the choice of contour colors for the first negative contour interval and the choice of the PostScript output file format. Finite element programs such as BLT-MS and BLT-EC sometimes predict negative concentrations which are small relative to the peak concentrations. Away from the source, the concentrations can oscillate between negative and positive values. This leads to a striped contour plot. To avoid this behavior, negative values with values less than the first positive contour interval can be plotted with the same color as the positive values. For example, if the first positive contour interval is from 0 to 10^{-11} . The user can request that all values with an absolute value less than 10^{-11} be plotted with the same color. If the predicted concentration is negative and the absolute value exceeds the value of the first positive contour interval, a unique contour color will be used to highlight the regions of negative values.

This typically indicates a problem with the simulation (i.e., numerical stability limits exceeded) and changes should be made in the input file.

The PostScript printer options permit selection of color or black and white printers with either portrait or landscape orientation. For color plots, the number of different contour colors is 14. If more than 14 color contours are requested, the color sequence is repeated. For black and white printers, the number of different contour shadings is four. For output to postscript printers select the portrait orientation. Landscape orientation is appropriate if the files are to be read in by other software that reads PostScript files. For output that will be used in WordPerfect, select landscape orientation with a black and white printer. The PostScript file can be imported as an image. It is important to recognize that BLTPLOT generates PostScript files and not Encapsulated PostScript files, (EPS files). While EPS files are more widely accepted by commercially available software, the routines used to generate the files were not capable of creating EPS files.

8.2.3 Graph Option

The Graph option allows X-Y plots of selected variables. When the Graph option is selected, BLTPLOT first displays a sub-menu with up to four choices. If trace and leaching files are not specified in the configuration file, this graph option is not enabled.

Leaching Concentration Flux Quit

The number of choices depends on the files specified in the configuration file. Leaching refers to mass released from each waste form. Concentration refers to the concentration at selected nodes stored in the concentration trace files. Flux refers to the flux at selected nodes stored in the flux trace files. These three functions are plotted as a function of time. Quit returns to the main menu.

After selection of the type of plot, BLTPLOT lists all contaminants modeled in the simulation and requires selection of a single contaminant. After selection of a contaminant for plotting, a list of all the elements (leaching) or node locations (concentrations and mass flux) where information is available is shown on the screen as a menu. Also included in the location menu are the following options:

Map, PlotOptn, Contaminant, Hard Copy, and Done.

Map	prints a map with labeled element or node locations for all locations associated with the plot information.
Plot Options	for graphs include the ability to alter the following axis parameters.
tmin:	minimum value of time for the horizontal axis.
tmax:	maximum value of time for the horizontal axis.
ymin:	minimum value on the vertical axis.
ymax:	maximum value on the vertical axis.

Depending on the selected plot, ymin and ymax may refer to the mass released from the waste form, concentration, or flux.

Contaminant permits selection of a different contaminant for plotting.

Hard Copy generates a PostScript file based on the options set in the Options option of the main menu. The file name is the first six letters of the configuration file name followed by two digits and an extension of PS. For example, if the configuration file name is CHAIN7.CNF, the first hard copy file name would be CHAIN700.PS. The second file would

be CHAIN701.PS and so on. A check is performed to prevent overwriting of existing PS files. The name for the PS file generated by BLTPLOT is printed on the visual display. In addition, the name of the file and the type of plot and the data it contains are listed in the BLTPLOT.LOG file. BLTPLOT.LOG will be overwritten each time BLTPLOT is started and a PostScript file is generated. If several PostScript files are generated in a single use of BLTPLOT, they will all be contained in BLTPLOT.LOG.

Done returns to the submenu which permits selection of Leaching, Concentration, or Flux graphs.

If a node number is selected, a plot is generated on the screen. After viewing the plot, the user is instructed to strike any key to return to the menu listing all of the nodes and the plot options.

8.2.4 Function Option

The function option permits selection among a number of different functions to be plotted. These functions include:

- Material number,
- Water content,
- X velocity,
- Y velocity,
- Total velocity,
- Total head,
- Pressure head,
- Concentration,
- Container type,
- Waste type.

In any particular application of BLTPLOT, some of the preceding values may not be available for plotting. Specifically, unless an auxiliary file for FEMWATER output is specified in the configuration file, the total head and pressure head will not be listed as plotting options.

The concentration plots depend on the contaminant of interest. All other plots are independent of the contaminant.

For plots that are contaminant independent, upon selection a plot is immediately generated. After viewing the plot, a sub-menu appears with the following choices: **PlotOptn**, **HardCopy**, **Function**, and **Quit**.

PlotOptn for contaminant independent plots, this option allows selection of the contour intervals as follows:

minimum contour:	minimum value of variable to be colored.
maximum contour:	maximum value of variable to be colored.
contour interval:	interval of variable to be represented as a uniform color.

HardCopy makes a hard copy (as previously discussed).

Function changes the function to be plotted.

Quit returns to the main menu.

For concentration contour plots, all contaminants simulated in the problem are listed and the user is first asked to select which contaminant to represent in the plot. Second, the list of times at which information has been stored for plotting is displayed along with the options to change the plotting parameters, change the contaminant, generate a hard copy, or quit

and return to the main menu. If a time is selected, a plot is generated and displayed. After viewing the plot, control is returned to this menu.

If **PlotOptn** is used with a concentration contour, an additional menu is presented. Concentration contours may be plotted based on the value of the concentration at the nodes or as the Log of the concentration. The new menu is thus **Linear** and **Log**. If Log is chosen, the plot will be automatically generated for the current contaminant at the currently chosen time. Once a linear or log contour has been completed, further selections of PlotOptn will allow the modification of the minimum, maximum, and contour interval values in the chosen variable type (linear or log). For log plots, the interval is also the log of concentration. For example, if the minimum log value was -10 and the maximum log value was -6, a contour interval of 1 would provide contours at -10, -9, -8, -7, and -6. Non-integer contour intervals are permitted.

When limiting the contour range, all values above the maximum specified value are plotted as one color, all values below the minimum specified value are also plotted as a unique color.

8.2.5 Exit Option

Option to exit the program and return to DOS.

9 CONCLUSIONS

The BLT-MS computer code has been developed, implemented, and tested. BLT-MS is a two-dimensional finite element computer code capable of simulating the time evolution of concentration resulting from the time-dependent release and transport of aqueous phase species in a subsurface soil system. BLT-MS contains models to simulate the processes (water flow, container degradation, waste form performance, transport, and radioactive production and decay) most relevant to estimating the release and transport of contaminants from a subsurface disposal system.

BLT-MS is an extension of the BLT code [Sullivan and Suen, 1989]. The major difference between the two codes is the ability to simulate multiple contaminants in a single simulation. This permits simulation of radioactive production and decay of species in the waste form prior to release and during transport. Other changes from the BLT computer code include improved treatment of releases from the waste form, and improvements to the waste form rinse with partitioning and degradation models.

To facilitate creation of an input file, the code BLTMSIN has been written. BLTMSIN is a menu driven program that guides the user through all of the steps required to create BLT-MS input. Upon completion of these steps, BLTMSIN will create an annotated BLT-MS input file. The annotations define the input data used by BLT-MS and provide the code user with an easy method to understand the input values. This is particularly useful when modifying an existing input file.

To permit rapid analysis of the output data created by BLT-MS, a graphics program, BLTPLOT has been written. BLTPLOT is capable of providing two-dimensional contour plots of: a) the concentration for each contaminant at specified times, b) moisture content, and c) Darcy flux in each direction. BLTPLOT also provides two-dimensional system maps of container location, waste form type, and material regions with different transport properties. BLTPLOT also provides X-Y plots of a) the concentration (or flux) as a function of time at specified nodes for each contaminant, and b) cumulative mass released from each waste form for each contaminant.

BLT-MS has been verified through comparison with other computer codes and analytical solutions to certain problems. The models for production through radioactive decay have been verified in both the waste form and the transport segments of the code. Although BLT-MS has been verified, this does not mean that the code applies to all situations. Prior to use of BLT-MS, a conceptual model of the system should be developed. This conceptual model should include all of the processes and events that impact on release and transport of the contaminant. If BLT-MS simulates these processes, it may be applied to the problem. In addition, as with all computer models, the validity of the projections rely heavily on the validity of the model parameters. Often, large uncertainties exist over the proper choice of the model parameters. It is crucial to document and support the choice of the model parameters. Model projections are only as good as the model input parameters.

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APPENDIX A

EXAMPLE OF INPTECHO.DAT FILE

The following is an example of the INPTECHO.DAT file.

```

C ***** DATA SET 1: PROBLEM IDENTIFICATION AND DESCRIPTION-- BLTMS-DATA
  1 Prob2: Three species decay chain. Containers

C ***** DATA SET 2: INTEGER PARAMETERS FOR VELOCITY INPUT AND STEADY STATE
      KVI      KSS
-1      1

C ***** DATA SET 3: INTEGER PARAMETERS FOR CONTAINERS AND WASTE
      NISO      NCON      NCTYPE      NWTYPER      IDIFF      IACT
  3      6      2      1      2      0

C ***** DATA SET 4: INTEGRATION INTEGER PARAMETERS
      ILUMP      IMID      IWET      IOPTIM      IVML
  1      0      1      1      0

C ***** DATA SET 5: INTEGER SOLUTION CONTROL PARAMETERS
      NTI      NDTCHG
273      1

C ***** DATA SET 6: GRID AND ELEMENT PARAMETERS
      NNP      NEL      NMAT      NCM      KMESH
213 140      1      0      0

C ***** DATA SET 7A: DIRICHLET INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NDNP(I)      NDPR(I)      NDDP(I)
  0      0      0
  0      0      0
  0      0      0

C ***** DATA SET 7B: CAUCHY INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NCNP(I)      NCES(I)      NCPR(I)      NCDP(I)
  3      2      1      4
  3      2      1      4
  3      2      1      4

C ***** DATA SET 7C: NEUMANN INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
      NNNP(I)      NNES(I)      NNPR(I)      NNDP(I)
  3      2      1      4
  3      2      1      4
  3      2      1      4

C ***** DATA SET 8: INTEGER PARAMETERS FOR SOURCES
      NSEL(I)      NSPR(I)      NSDP(I)      volume/element sources
  0      0      0
  0      0      0

```


0 0 0

NWNP(I) NWPR(I) NWDP(I) well/point source
0 0 0
0 0 0
0 0 0

C ***** DATA SET 9: CONTAMINANT MATERIAL INFORMATION

	Contam(I)	ATM(I)	T 1/2 (I)	CSAT(I)
Am241	0.24E+03	0.43E+03	0.10E+01	
Pu241	0.24E+03	0.15E+02	0.10E+01	
Pu240	0.24E+03	0.65E+10	0.10E+01	

DECAY CHAIN INFORMATION:
NUMBER OF CHAINS

1

LENGTH OF CHAIN

3

COMPONENTS OF THE CHAIN (Numerical order Am241 = 1; Pu241=2; PU240=3
1 2 3

BRANCHING FRACTIONS OF THE CHAIN (need length of chain - 1 values)
0.10E+01 0.10E+01

C ***** DATA SET 10: TIME INTEGRATION CONTROL PARAMETERS

DELT(yrs)	CHNG	DELMAX(yr)	TMAX(yrs)	W	WV
0.10E+01	0.00E+00	0.10E+01	0.30E+03	0.10E+01	0.10E+01

Set 10a: DELTA T CHANGES at year(s):
0.31E+03

C ***** DATA SET 11: REAL PARAMETERS FOR NONLINEAR SOLVE
DUMMY SET: NOT USED IN BLTMS

C ***** DATA SET 12: NODAL POINT COORDINATE read if KVI le 0; kmsh ge 0
WIDTH OF THE WASTE CONTAINING REGION MODELED (CM)
0.10E+03

ni	nseq	nad	fni	fad	frd
Set12A: z-coordinates					
ni	nseq	nad	fni	fad	frd

DATA SET12b: ELEMENT INDICES AND MATERIAL TYPES VIA CARDS IF KVI.LE. 0
mi ie(mi,i), i=1,5;-

modl nlay

DATA SET 13: Material Properties

Set 13A: Prop(J,k), j =1, NMPPM(NO. of material properties=5), k = 1, NMAT
mol-dif-co density long-disp trans-disp soil porosity
0.00E+00 0.23E+01 0.26E+03 0.26E+02 0.20E+00

Set 13b: Prop1(j,k,i) j=1,NMPPM1(=3), k=1,NMAT,i= 1, niso
KD liquid-degr solid-degr
0.40E+03 0.00E+00 0.00E+00

0.40E+03 0.00E+00 0.00E+00
0.40E+03 0.00E+00 0.00E+00

DATA SET 14: Material type reassignment
Data set not used in this simulation.

0

DATA SET 15: Input for initial or Pre-initial Conditions
NI NNODE NAD RNI RAD RRD
AM241
PU241
PU240

SET 16: Cauchy Boundary Conditions
AM-241 boundary conditions: units of time and rates is years
Tqcbf(j,i) Qcbf(j,i) Tqcbf(j,i) Qcbf(j,i)
0.000E+00 0.000E+00 9.111E+01 0.000E+00 2.000E+02 0.000E+00
2.770E+02 0.000E+00

Set 16a: Cauchy Nodes- left side layer- NPCB
1 2 3

Ni Nseq Nad Nityp Ntypad: Set 16b: Type Cauchy Node DEFINITION

Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad: ELEMENT SIDE DEFINITION
1 1 1 1 2 1 1 1 1

Pu-241 boundary conditions: units of time and rates is years
Tqcbf(j,i) Qcbf(j,i) Tqcbf(j,i) Qcbf(j,i)
0.000E+00 0.000E+00 9.111E+01 0.000E+00 2.000E+02 0.000E+00
2.770E+02 0.000E+00

Set 16a: Cauchy Nodes- left side layer- NPCB
1 2 3

Ni Nseq Nad Nityp Ntypad: Set 16b: Type Cauchy Node DEFINITION

Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad: ELEMENT SIDE DEFINITION
1 1 1 1 2 1 1 1 1

Pu-240 boundary conditions: units of time and rates is years
Tqcbf(j,i) Qcbf(j,i) Tqcbf(j,i) Qcbf(j,i)
0.000E+00 0.000E+00 9.111E+01 0.000E+00 2.000E+02 0.000E+00
2.770E+02 0.000E+00

Set 16a: Cauchy Nodes- left side layer- NPCB
1 2 3

Ni Nseq Nad Nityp Ntypad: Set 16b: Type Cauchy Node DEFINITION

Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad: ELEMENT SIDE DEFINITION
1 1 1 1 2 1 1 1 1

Set 16b: Neumann Boundary Conditions
Am-241 boundary conditions :units of time and rates is years
Am-241: Tqnbfb(j,i) Qnbfb(j,i) Tqnbfb(j,i) Qnbfb(j,i)
0.000E+00 0.000E+00 9.110E+01 0.000E+00 2.000E+02 0.000E+00
3.000E+02 0.000E+00

Am-241: Set 16a: Neuman Nodes- right side layer- NPNB
 211 212 213

Ni Nseq Nad Nityp Ntypad: set 16 b: Type Neumann modes

Am-241 Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad :
 1 1 139 1 2 1 1 1 1

Pu-241 boundary conditions :units of time and rates is years
 Pu-241: Tqnbj(j,i) Qnbj(j,i) Tqnbj(j,i) Qnbj(j,i)
 0.000E+00 0.000E+00 9.110E+01 0.000E+00 2.000E+02 0.000E+00
 3.000E+02 0.000E+00

Pu-241: Set 16a: Neuman Nodes- right side layer- NPNB
 211 212 213

Ni Nseq Nad Nityp Ntypad: set 16 b: Type Neumann modes

Pu-241 Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad :
 1 1 139 1 2 1 1 1 1

PU-240 boundary conditions.
 Tqnbj(j,i) Qnbj(j,i) Tqnbj(j,i) Qnbj(j,i) : units of time and rates is years
 0.000E+00 0.000E+00 9.110E+01 0.000E+00 2.000E+02 0.000E+00
 3.000E+02 0.000E+00

Pu-240: right side layer-
 211 212 213

Ni Nseq Nad Nityp Ntypad: set 16 b: Type Neumann modes

Mi Nseq M Is1 Is2 Miad Mad Islad Is2ad : Neumann element sides
 1 1 139 1 2 1 1 1 1

SET 17: DIRICHLET BOUNDARY CONDITONS
 NOT USED IN THIS PROBLEM

SET 18: EXTERNAL ELEMENT SOURCE/SINK
 NOT USED IN THIS PROBLEM

SET 19: WELL POINT SOURCE/SINK
 NOT USED IN THIS PROBLEM

SET 20: WASTE CONTAINER PARAMETERS

THICK	PITN	PITK	AREA	ASCALE	PITS
1.000E+00	1.000E-02	7.000E-03	2.100E+04	2.000E-01	5.000E+03

GRATE	CLAY	SPH	IAER
3.170E-10	1.500E-01	6.000E+00	2.000E+00

THICK	PITN	PITK	AREA	ASCALE	PITS
1.000E+00	1.000E-02	7.000E-03	2.100E+04	2.000E-01	5.000E+03

C ***** DATA SET 22B: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
NOT USED IN BLTMS

C ***** DATA SET 22C: TRACE FILES-NO OF CONC. AND FLUX NODE NUMBERS & NODES
NTRC NTRF NSTPTR
8 0 1

Concentration trace information-Global node numbers NTRCEC(k)
2 32 62 92 122 152 182 212

C ***** DATA SET 23B: VELOCITY AND MOISTURE CONTENT
Ni Nseq Nad Vxni Vzni Vxad Vzad
SET 18B:
Ni Nseq Nad Thni Thniad

APPENDIX B

PARTIAL PRIMARY OUTPUT FILE GENERATED BY BLT-MS

This appendix presents the output generated through the input check in BLT-MS and the output at the first and last time steps of the problem described in the input file CHAIN7.DAT. Intermediate time steps have not been included to save space.

PROBLEM 1 Prob2: Three species decay chain. Containers

**** BASIC INTEGER PARAMETERS ****

NUMBER OF NODAL POINTS. 213
 NUMBER OF ELEMENTS. 140
 NUMBER OF DIFFERENT MATERIALS 1
 NUMBER OF CORRECTION MATERIALS. 0
 VELOCITY INPUT CONTROL. -1
 GRID CONTROL: =0 READ cards; =1, automatic generation 0

**** NUMERICAL MODEL SELECTION PARAMETERS ****

STEADY-STATE CALCULATION. . . KSS . . . 1; 1=NO, 0=YES
 UPSTREAM WEIGHTING INDICATOR, IWET. . . 1; 0=GALERKIN, 1=UPSTREAM
 LUMPING INDICATOR, ILUMP. 1; 0=NO, 1=YES
 TIME-DIFFERENCE INDICATOR, IMID 0; 0=NO, 1=YES
 WEIGHTING FACTOR OPTIMIZING INDICATOR . 1; 0=NO, 1=YES
 IS FLUX-SOLVING MATRIX LUMPED? 0; 0=NO, 1=YES

**** CONTAMINANT INFORMATION ****

FLAG FOR MASS INPUT (MASS=0, ACTIVITY=1) 0

NUCLIDE	ATM	DECAY-CONSTANT	CSAT
-----	---	-----	----
Am241	241.	5.073E-11	1.000E+00
Pu241	241.	1.464E-09	1.000E+00
Pu240	240.	3.358E-12	1.000E+00

**** DECAY CHAINS ****

NUMBER OF DECAY CHAINS (0=NO, > 1=YES) . . 1

DECAY CHAIN NUMBER 1 - LENGTH OF CHAIN IS 3

Chain 1: Am241 DECAYS TO Pu241 WITH A BRANCHING FRACTION OF 1.000
 Chain 1: Pu241 DECAYS TO Pu240 WITH A BRANCHING FRACTION OF 1.000

**** TIME STEP PARAMETERS ****

NUMBER OF TIME INCREMENTS 273

TIME INCREMENT. 1.000E+00
 MULTIPLIER FOR INCREASING DELT. 0.000E+00
 MAXIMUM VALUE OF DELT 1.000E+00
 MAXIMUM VALUE OF TIME 3.000E+02
 TIME-INTEGRATION PARAMETER. 1.000E+00
 NO. OF TIMES TO SETTING INITIAL DELT .. 1

TIME OF CHANGING DELT
 3.150E+02

*** COMPUTED BOUNDARY ELEMENT SIDE INFORMATION ***

MP	M	NP1	NP2	L1	L2	DLB(MP)	DCOSXB(MP)	DCOSZB(MP)
1	1	1	4	1	2	1.000E+02	0.000E+00	-1.000E+00
2	1	2	1	4	1	1.000E+02	-1.000E+00	-6.123E-17
3	2	6	3	3	4	1.000E+02	-5.421E-20	1.000E+00
4	2	3	2	4	1	1.000E+02	-1.000E+00	-6.123E-17
5	3	4	7	1	2	1.000E+02	0.000E+00	-1.000E+00
6	4	9	6	3	4	1.000E+02	-5.421E-20	1.000E+00
7	5	7	10	1	2	1.000E+02	0.000E+00	-1.000E+00
8	6	12	9	3	4	1.000E+02	-5.421E-20	1.000E+00
9	7	10	13	1	2	1.000E+02	0.000E+00	-1.000E+00
10	8	15	12	3	4	1.000E+02	-5.421E-20	1.000E+00
11	9	13	16	1	2	1.000E+02	0.000E+00	-1.000E+00
12	10	18	15	3	4	1.000E+02	-5.421E-20	1.000E+00
13	11	16	19	1	2	1.000E+02	0.000E+00	-1.000E+00
14	12	21	18	3	4	1.000E+02	-5.421E-20	1.000E+00
15	13	19	22	1	2	1.000E+02	0.000E+00	-1.000E+00
16	14	24	21	3	4	1.000E+02	-5.421E-20	1.000E+00
17	15	22	25	1	2	1.000E+02	0.000E+00	-1.000E+00
18	16	27	24	3	4	1.000E+02	-5.421E-20	1.000E+00
19	17	25	28	1	2	1.000E+02	0.000E+00	-1.000E+00
20	18	30	27	3	4	1.000E+02	-5.421E-20	1.000E+00
21	19	28	31	1	2	1.000E+02	0.000E+00	-1.000E+00
22	20	33	30	3	4	1.000E+02	-5.421E-20	1.000E+00
23	21	31	34	1	2	1.000E+02	0.000E+00	-1.000E+00
24	22	36	33	3	4	1.000E+02	-5.421E-20	1.000E+00
25	23	34	37	1	2	1.000E+02	0.000E+00	-1.000E+00
26	24	39	36	3	4	1.000E+02	-5.421E-20	1.000E+00
27	25	37	40	1	2	1.000E+02	0.000E+00	-1.000E+00
28	26	42	39	3	4	1.000E+02	-5.421E-20	1.000E+00
29	27	40	43	1	2	1.000E+02	0.000E+00	-1.000E+00
30	28	45	42	3	4	1.000E+02	-5.421E-20	1.000E+00
31	29	43	46	1	2	1.000E+02	0.000E+00	-1.000E+00
32	30	48	45	3	4	1.000E+02	-5.421E-20	1.000E+00
33	31	46	49	1	2	1.000E+02	0.000E+00	-1.000E+00
34	32	51	48	3	4	1.000E+02	-5.421E-20	1.000E+00
35	33	49	52	1	2	1.000E+02	0.000E+00	-1.000E+00
36	34	54	51	3	4	1.000E+02	-5.421E-20	1.000E+00
37	35	52	55	1	2	1.000E+02	0.000E+00	-1.000E+00
38	36	57	54	3	4	1.000E+02	-5.421E-20	1.000E+00
39	37	55	58	1	2	1.000E+02	0.000E+00	-1.000E+00
40	38	60	57	3	4	1.000E+02	-5.421E-20	1.000E+00
41	39	58	61	1	2	1.000E+02	0.000E+00	-1.000E+00
42	40	63	60	3	4	1.000E+02	-5.421E-20	1.000E+00
43	41	61	64	1	2	1.000E+02	0.000E+00	-1.000E+00

44	42	66	63	3	4	1.000E+02	-5.421E-20	1.000E+00
45	43	64	67	1	2	1.000E+02	0.000E+00	-1.000E+00
46	44	69	66	3	4	1.000E+02	-5.421E-20	1.000E+00
47	45	67	70	1	2	1.000E+02	0.000E+00	-1.000E+00
48	46	72	69	3	4	1.000E+02	-5.421E-20	1.000E+00
49	47	70	73	1	2	1.000E+02	0.000E+00	-1.000E+00
50	48	75	72	3	4	1.000E+02	-5.421E-20	1.000E+00
51	49	73	76	1	2	1.000E+02	0.000E+00	-1.000E+00
52	50	78	75	3	4	1.000E+02	-5.421E-20	1.000E+00
53	51	76	79	1	2	1.000E+02	0.000E+00	-1.000E+00
54	52	81	78	3	4	1.000E+02	-5.421E-20	1.000E+00
55	53	79	82	1	2	1.000E+02	0.000E+00	-1.000E+00
56	54	84	81	3	4	1.000E+02	-5.421E-20	1.000E+00
57	55	82	85	1	2	1.000E+02	0.000E+00	-1.000E+00
58	56	87	84	3	4	1.000E+02	-5.421E-20	1.000E+00
59	57	85	88	1	2	1.000E+02	0.000E+00	-1.000E+00
60	58	90	87	3	4	1.000E+02	-5.421E-20	1.000E+00
61	59	88	91	1	2	1.000E+02	0.000E+00	-1.000E+00
62	60	93	90	3	4	1.000E+02	-5.421E-20	1.000E+00
63	61	91	94	1	2	1.000E+02	0.000E+00	-1.000E+00
64	62	96	93	3	4	1.000E+02	-5.421E-20	1.000E+00
65	63	94	97	1	2	1.000E+02	0.000E+00	-1.000E+00
66	64	99	96	3	4	1.000E+02	-5.421E-20	1.000E+00
67	65	97	100	1	2	1.000E+02	0.000E+00	-1.000E+00
68	66	102	99	3	4	1.000E+02	-5.421E-20	1.000E+00
69	67	100	103	1	2	1.000E+02	0.000E+00	-1.000E+00
70	68	105	102	3	4	1.000E+02	-5.421E-20	1.000E+00
71	69	103	106	1	2	1.000E+02	0.000E+00	-1.000E+00
72	70	108	105	3	4	1.000E+02	-5.421E-20	1.000E+00
73	71	106	109	1	2	1.000E+02	0.000E+00	-1.000E+00
74	72	111	108	3	4	1.000E+02	-5.421E-20	1.000E+00
75	73	109	112	1	2	1.000E+02	0.000E+00	-1.000E+00
76	74	114	111	3	4	1.000E+02	-5.421E-20	1.000E+00
77	75	112	115	1	2	1.000E+02	0.000E+00	-1.000E+00
78	76	117	114	3	4	1.000E+02	-5.421E-20	1.000E+00
79	77	115	118	1	2	1.000E+02	0.000E+00	-1.000E+00
80	78	120	117	3	4	1.000E+02	-5.421E-20	1.000E+00
81	79	118	121	1	2	1.000E+02	0.000E+00	-1.000E+00
82	80	123	120	3	4	1.000E+02	-5.421E-20	1.000E+00
83	81	121	124	1	2	1.000E+02	0.000E+00	-1.000E+00
84	82	126	123	3	4	1.000E+02	-5.421E-20	1.000E+00
85	83	124	127	1	2	1.000E+02	0.000E+00	-1.000E+00
86	84	129	126	3	4	1.000E+02	-5.421E-20	1.000E+00
87	85	127	130	1	2	1.000E+02	0.000E+00	-1.000E+00
88	86	132	129	3	4	1.000E+02	-5.421E-20	1.000E+00
89	87	130	133	1	2	1.000E+02	0.000E+00	-1.000E+00
90	88	135	132	3	4	1.000E+02	-5.421E-20	1.000E+00
91	89	133	136	1	2	1.000E+02	0.000E+00	-1.000E+00
92	90	138	135	3	4	1.000E+02	-5.421E-20	1.000E+00
93	91	136	139	1	2	1.000E+02	0.000E+00	-1.000E+00
94	92	141	138	3	4	1.000E+02	-5.421E-20	1.000E+00
95	93	139	142	1	2	1.000E+02	0.000E+00	-1.000E+00
96	94	144	141	3	4	1.000E+02	-5.421E-20	1.000E+00
97	95	142	145	1	2	1.000E+02	0.000E+00	-1.000E+00
98	96	147	144	3	4	1.000E+02	-5.421E-20	1.000E+00
99	97	145	148	1	2	1.000E+02	0.000E+00	-1.000E+00
100	98	150	147	3	4	1.000E+02	-5.421E-20	1.000E+00

*** COMPUTED BOUNDARY ELEMENT SIDE INFORMATION

MP	M	NP1	NP2	L1	L2	DLB(MP)	DCOSXB(MP)	DCOSZB(MP)
101	99	148	151	1	2	1.000E+02	0.000E+00	-1.000E+00
102	100	153	150	3	4	1.000E+02	-5.421E-20	1.000E+00
103	101	151	154	1	2	1.000E+02	0.000E+00	-1.000E+00
104	102	156	153	3	4	1.000E+02	-5.421E-20	1.000E+00
105	103	154	157	1	2	1.000E+02	0.000E+00	-1.000E+00
106	104	159	156	3	4	1.000E+02	-5.421E-20	1.000E+00
107	105	157	160	1	2	1.000E+02	0.000E+00	-1.000E+00
108	106	162	159	3	4	1.000E+02	-5.421E-20	1.000E+00
109	107	160	163	1	2	1.000E+02	0.000E+00	-1.000E+00
110	108	165	162	3	4	1.000E+02	-5.421E-20	1.000E+00
111	109	163	166	1	2	1.000E+02	0.000E+00	-1.000E+00
112	110	168	165	3	4	1.000E+02	-5.421E-20	1.000E+00
113	111	166	169	1	2	1.000E+02	0.000E+00	-1.000E+00
114	112	171	168	3	4	1.000E+02	-5.421E-20	1.000E+00
115	113	169	172	1	2	1.000E+02	0.000E+00	-1.000E+00
116	114	174	171	3	4	1.000E+02	-5.421E-20	1.000E+00
117	115	172	175	1	2	1.000E+02	0.000E+00	-1.000E+00
118	116	177	174	3	4	1.000E+02	-5.421E-20	1.000E+00
119	117	175	178	1	2	1.000E+02	0.000E+00	-1.000E+00
120	118	180	177	3	4	1.000E+02	-5.421E-20	1.000E+00
121	119	178	181	1	2	1.000E+02	0.000E+00	-1.000E+00
122	120	183	180	3	4	1.000E+02	-5.421E-20	1.000E+00
123	121	181	184	1	2	1.000E+02	0.000E+00	-1.000E+00
124	122	186	183	3	4	1.000E+02	-5.421E-20	1.000E+00
125	123	184	187	1	2	1.000E+02	0.000E+00	-1.000E+00
126	124	189	186	3	4	1.000E+02	-5.421E-20	1.000E+00
127	125	187	190	1	2	1.000E+02	0.000E+00	-1.000E+00
128	126	192	189	3	4	1.000E+02	-5.421E-20	1.000E+00
129	127	190	193	1	2	1.000E+02	0.000E+00	-1.000E+00
130	128	195	192	3	4	1.000E+02	-5.421E-20	1.000E+00
131	129	193	196	1	2	1.000E+02	0.000E+00	-1.000E+00
132	130	198	195	3	4	1.000E+02	-5.421E-20	1.000E+00
133	131	196	199	1	2	1.000E+02	0.000E+00	-1.000E+00
134	132	201	198	3	4	1.000E+02	-5.421E-20	1.000E+00
135	133	199	202	1	2	1.000E+02	0.000E+00	-1.000E+00
136	134	204	201	3	4	1.000E+02	-5.421E-20	1.000E+00
137	135	202	205	1	2	1.000E+02	0.000E+00	-1.000E+00
138	136	207	204	3	4	1.000E+02	-5.421E-20	1.000E+00
139	137	205	208	1	2	1.000E+02	0.000E+00	-1.000E+00
140	138	210	207	3	4	1.000E+02	-5.421E-20	1.000E+00
141	139	208	211	1	2	1.000E+02	0.000E+00	-1.000E+00
142	139	211	212	2	3	1.000E+02	1.000E+00	-6.123E-17
143	140	212	213	2	3	1.000E+02	1.000E+00	-6.123E-17
144	140	213	210	3	4	1.000E+02	-5.421E-20	1.000E+00

FACILITY WIDTH (cm) - 1.00E+02

**** NODAL COORDINATE ****

NODE	X	Z	NODE	X	Z
1	0.000E+00	0.000E+00	2	0.000E+00	1.000E+02

3	0.000E+00	2.000E+02	4	1.000E+02	0.000E+00
5	1.000E+02	1.000E+02	6	1.000E+02	2.000E+02
7	2.000E+02	0.000E+00	8	2.000E+02	1.000E+02
9	2.000E+02	2.000E+02	10	3.000E+02	0.000E+00
11	3.000E+02	1.000E+02	12	3.000E+02	2.000E+02
13	4.000E+02	0.000E+00	14	4.000E+02	1.000E+02
15	4.000E+02	2.000E+02	16	5.000E+02	0.000E+00
17	5.000E+02	1.000E+02	18	5.000E+02	2.000E+02
19	6.000E+02	0.000E+00	20	6.000E+02	1.000E+02
21	6.000E+02	2.000E+02	22	7.000E+02	0.000E+00
23	7.000E+02	1.000E+02	24	7.000E+02	2.000E+02
25	8.000E+02	0.000E+00	26	8.000E+02	1.000E+02
27	8.000E+02	2.000E+02	28	9.000E+02	0.000E+00
29	9.000E+02	1.000E+02	30	9.000E+02	2.000E+02
31	1.000E+03	0.000E+00	32	1.000E+03	1.000E+02
33	1.000E+03	2.000E+02	34	1.100E+03	0.000E+00
35	1.100E+03	1.000E+02	36	1.100E+03	2.000E+02
37	1.200E+03	0.000E+00	38	1.200E+03	1.000E+02
39	1.200E+03	2.000E+02	40	1.300E+03	0.000E+00
41	1.300E+03	1.000E+02	42	1.300E+03	2.000E+02
43	1.400E+03	0.000E+00	44	1.400E+03	1.000E+02
45	1.400E+03	2.000E+02	46	1.500E+03	0.000E+00
47	1.500E+03	1.000E+02	48	1.500E+03	2.000E+02
49	1.600E+03	0.000E+00	50	1.600E+03	1.000E+02
51	1.600E+03	2.000E+02	52	1.700E+03	0.000E+00
53	1.700E+03	1.000E+02	54	1.700E+03	2.000E+02
55	1.800E+03	0.000E+00	56	1.800E+03	1.000E+02
57	1.800E+03	2.000E+02	58	1.900E+03	0.000E+00
59	1.900E+03	1.000E+02	60	1.900E+03	2.000E+02
61	2.000E+03	0.000E+00	62	2.000E+03	1.000E+02
63	2.000E+03	2.000E+02	64	2.100E+03	0.000E+00
65	2.100E+03	1.000E+02	66	2.100E+03	2.000E+02
67	2.200E+03	0.000E+00	68	2.200E+03	1.000E+02
69	2.200E+03	2.000E+02	70	2.300E+03	0.000E+00
71	2.300E+03	1.000E+02	72	2.300E+03	2.000E+02
73	2.400E+03	0.000E+00	74	2.400E+03	1.000E+02
75	2.400E+03	2.000E+02	76	2.500E+03	0.000E+00
77	2.500E+03	1.000E+02	78	2.500E+03	2.000E+02
79	2.600E+03	0.000E+00	80	2.600E+03	1.000E+02
81	2.600E+03	2.000E+02	82	2.700E+03	0.000E+00
83	2.700E+03	1.000E+02	84	2.700E+03	2.000E+02
85	2.800E+03	0.000E+00	86	2.800E+03	1.000E+02
87	2.800E+03	2.000E+02	88	2.900E+03	0.000E+00
89	2.900E+03	1.000E+02	90	2.900E+03	2.000E+02
91	3.000E+03	0.000E+00	92	3.000E+03	1.000E+02
93	3.000E+03	2.000E+02	94	3.100E+03	0.000E+00
95	3.100E+03	1.000E+02	96	3.100E+03	2.000E+02
97	3.200E+03	0.000E+00	98	3.200E+03	1.000E+02
99	3.200E+03	2.000E+02	100	3.300E+03	0.000E+00

**** NODAL COORDINATE ****

NODE	X	Z	NODE	X	Z
----	-	-	----	-	-
101	3.300E+03	1.000E+02	102	3.300E+03	2.000E+02
103	3.400E+03	0.000E+00	104	3.400E+03	1.000E+02
105	3.400E+03	2.000E+02	106	3.500E+03	0.000E+00

107	3.500E+03	1.000E+02	108	3.500E+03	2.000E+02
109	3.600E+03	0.000E+00	110	3.600E+03	1.000E+02
111	3.600E+03	2.000E+02	112	3.700E+03	0.000E+00
113	3.700E+03	1.000E+02	114	3.700E+03	2.000E+02
115	3.800E+03	0.000E+00	116	3.800E+03	1.000E+02
117	3.800E+03	2.000E+02	118	3.900E+03	0.000E+00
119	3.900E+03	1.000E+02	120	3.900E+03	2.000E+02
121	4.000E+03	0.000E+00	122	4.000E+03	1.000E+02
123	4.000E+03	2.000E+02	124	4.100E+03	0.000E+00
125	4.100E+03	1.000E+02	126	4.100E+03	2.000E+02
127	4.200E+03	0.000E+00	128	4.200E+03	1.000E+02
129	4.200E+03	2.000E+02	130	4.300E+03	0.000E+00
131	4.300E+03	1.000E+02	132	4.300E+03	2.000E+02
133	4.400E+03	0.000E+00	134	4.400E+03	1.000E+02
135	4.400E+03	2.000E+02	136	4.500E+03	0.000E+00
137	4.500E+03	1.000E+02	138	4.500E+03	2.000E+02
139	4.600E+03	0.000E+00	140	4.600E+03	1.000E+02
141	4.600E+03	2.000E+02	142	4.700E+03	0.000E+00
143	4.700E+03	1.000E+02	144	4.700E+03	2.000E+02
145	4.800E+03	0.000E+00	146	4.800E+03	1.000E+02
147	4.800E+03	2.000E+02	148	4.900E+03	0.000E+00
149	4.900E+03	1.000E+02	150	4.900E+03	2.000E+02
151	5.000E+03	0.000E+00	152	5.000E+03	1.000E+02
153	5.000E+03	2.000E+02	154	5.100E+03	0.000E+00
155	5.100E+03	1.000E+02	156	5.100E+03	2.000E+02
157	5.200E+03	0.000E+00	158	5.200E+03	1.000E+02
159	5.200E+03	2.000E+02	160	5.300E+03	0.000E+00
161	5.300E+03	1.000E+02	162	5.300E+03	2.000E+02
163	5.400E+03	0.000E+00	164	5.400E+03	1.000E+02
165	5.400E+03	2.000E+02	166	5.500E+03	0.000E+00
167	5.500E+03	1.000E+02	168	5.500E+03	2.000E+02
169	5.600E+03	0.000E+00	170	5.600E+03	1.000E+02
171	5.600E+03	2.000E+02	172	5.700E+03	0.000E+00
173	5.700E+03	1.000E+02	174	5.700E+03	2.000E+02
175	5.800E+03	0.000E+00	176	5.800E+03	1.000E+02
177	5.800E+03	2.000E+02	178	5.900E+03	0.000E+00
179	5.900E+03	1.000E+02	180	5.900E+03	2.000E+02
181	6.000E+03	0.000E+00	182	6.000E+03	1.000E+02
183	6.000E+03	2.000E+02	184	6.100E+03	0.000E+00
185	6.100E+03	1.000E+02	186	6.100E+03	2.000E+02
187	6.200E+03	0.000E+00	188	6.200E+03	1.000E+02
189	6.200E+03	2.000E+02	190	6.300E+03	0.000E+00
191	6.300E+03	1.000E+02	192	6.300E+03	2.000E+02
193	6.400E+03	0.000E+00	194	6.400E+03	1.000E+02
195	6.400E+03	2.000E+02	196	6.500E+03	0.000E+00
197	6.500E+03	1.000E+02	198	6.500E+03	2.000E+02
199	6.600E+03	0.000E+00	200	6.600E+03	1.000E+02

**** NODAL COORDINATE ****

NODE	X	Z	NODE	X	Z
----	-	-	----	-	-
201	6.600E+03	2.000E+02	202	6.700E+03	0.000E+00
203	6.700E+03	1.000E+02	204	6.700E+03	2.000E+02
205	6.800E+03	0.000E+00	206	6.800E+03	1.000E+02
207	6.800E+03	2.000E+02	208	6.900E+03	0.000E+00
209	6.900E+03	1.000E+02	210	6.900E+03	2.000E+02

211 7.000E+03 0.000E+00 212 7.000E+03 1.000E+02
 213 7.000E+03 2.000E+02

**** MATERIAL PROPERTIES ****

MAT. NO.	DIFF-COEF	RHOB	LONG-DSP	TRANS-DSP	POR
1	0.000E+00	2.340E+00	2.590E+02	2.590E+01	2.000E-01

**** MATERIAL-RADIONUCLIDE PROPERTIES ****

MAT. NO.	ISO-NO.	RADNUC	KD	LIQ-DEGR	SOLID-DEGR
1	1	Am241	4.000E+02	0.000E+00	0.000E+00
1	2	Pu241	4.000E+02	0.000E+00	0.000E+00
1	3	Pu240	4.000E+02	0.000E+00	0.000E+00

**** ELEMENT DATA: GLOBAL INDICES OF ELEMENT NODES ****

ELM	NOD1	2	3	4	MTYP	ELM	NOD1	2	3	4	MTYP
1	1	4	5	2	1	2	2	5	6	3	1
3	4	7	8	5	1	4	5	8	9	6	1
5	7	10	11	8	1	6	8	11	12	9	1
7	10	13	14	11	1	8	11	14	15	12	1
9	13	16	17	14	1	10	14	17	18	15	1
11	16	19	20	17	1	12	17	20	21	18	1
13	19	22	23	20	1	14	20	23	24	21	1
15	22	25	26	23	1	16	23	26	27	24	1
17	25	28	29	26	1	18	26	29	30	27	1
19	28	31	32	29	1	20	29	32	33	30	1
21	31	34	35	32	1	22	32	35	36	33	1
23	34	37	38	35	1	24	35	38	39	36	1
25	37	40	41	38	1	26	38	41	42	39	1
27	40	43	44	41	1	28	41	44	45	42	1
29	43	46	47	44	1	30	44	47	48	45	1
31	46	49	50	47	1	32	47	50	51	48	1
33	49	52	53	50	1	34	50	53	54	51	1
35	52	55	56	53	1	36	53	56	57	54	1
37	55	58	59	56	1	38	56	59	60	57	1
39	58	61	62	59	1	40	59	62	63	60	1
41	61	64	65	62	1	42	62	65	66	63	1
43	64	67	68	65	1	44	65	68	69	66	1
45	67	70	71	68	1	46	68	71	72	69	1
47	70	73	74	71	1	48	71	74	75	72	1
49	73	76	77	74	1	50	74	77	78	75	1
51	76	79	80	77	1	52	77	80	81	78	1
53	79	82	83	80	1	54	80	83	84	81	1
55	82	85	86	83	1	56	83	86	87	84	1
57	85	88	89	86	1	58	86	89	90	87	1
59	88	91	92	89	1	60	89	92	93	90	1
61	91	94	95	92	1	62	92	95	96	93	1
63	94	97	98	95	1	64	95	98	99	96	1
65	97	100	101	98	1	66	98	101	102	99	1
67	100	103	104	101	1	68	101	104	105	102	1
69	103	106	107	104	1	70	104	107	108	105	1
71	106	109	110	107	1	72	107	110	111	108	1

73	109	112	113	110	1	74	110	113	114	111	1
75	112	115	116	113	1	76	113	116	117	114	1
77	115	118	119	116	1	78	116	119	120	117	1
79	118	121	122	119	1	80	119	122	123	120	1
81	121	124	125	122	1	82	122	125	126	123	1
83	124	127	128	125	1	84	125	128	129	126	1
85	127	130	131	128	1	86	128	131	132	129	1
87	130	133	134	131	1	88	131	134	135	132	1
89	133	136	137	134	1	90	134	137	138	135	1
91	136	139	140	137	1	92	137	140	141	138	1
93	139	142	143	140	1	94	140	143	144	141	1
95	142	145	146	143	1	96	143	146	147	144	1
97	145	148	149	146	1	98	146	149	150	147	1
99	148	151	152	149	1	100	149	152	153	150	1

**** ELEMENT DATA: GLOBAL INDICES OF ELEMENT NODES ****

ELM	NOD1	2	3	4	MTYP	ELM	NOD1	2	3	4	MTYP
101	151	154	155	152	1	102	152	155	156	153	1
103	154	157	158	155	1	104	155	158	159	156	1
105	157	160	161	158	1	106	158	161	162	159	1
107	160	163	164	161	1	108	161	164	165	162	1
109	163	166	167	164	1	110	164	167	168	165	1
111	166	169	170	167	1	112	167	170	171	168	1
113	169	172	173	170	1	114	170	173	174	171	1
115	172	175	176	173	1	116	173	176	177	174	1
117	175	178	179	176	1	118	176	179	180	177	1
119	178	181	182	179	1	120	179	182	183	180	1
121	181	184	185	182	1	122	182	185	186	183	1
123	184	187	188	185	1	124	185	188	189	186	1
125	187	190	191	188	1	126	188	191	192	189	1
127	190	193	194	191	1	128	191	194	195	192	1
129	193	196	197	194	1	130	194	197	198	195	1
131	196	199	200	197	1	132	197	200	201	198	1
133	199	202	203	200	1	134	200	203	204	201	1
135	202	205	206	203	1	136	203	206	207	204	1
137	205	208	209	206	1	138	206	209	210	207	1
139	208	211	212	209	1	140	209	212	213	210	1

IHALFB = 4 IBAND = 9 IHBP = 5

**** CAUCHY BOUNDARY CONDITIONS ****

Radionuclide Am241 isotope 1

PROFILE NO. 1

TIME	FLUX	TIME	FLUX	TIME	FLUX
----	----	----	----	----	----
0.000E+00	0.000E+00	9.111E+01	0.000E+00	2.000E+02	0.000E+00
2.770E+02	0.000E+00				

GLOBAL NODAL NUMBER AND PROFILE TYPE OF CAUCHY BOUNDARY NODES

I NPCB CTYP	I NPCB CTYP	I NPCB CTYP	I NPCB CTYP
1 1 1	2 2 1	3 3 1	

Radionuclide Am241 isotope 1

CAUCHY ELEMENT SIDE DATA

MP	M CNP1 CNP2	MP	M CNP1 CNP2	MP	M CNP1 CNP2
1	1 1 2	2	2 2 3		

*** COMPUTED CAUCHY ELEMENT SIDE INFORMATION ***

MP	M CNP1 CNP2 L1 L2	MP	M CNP1 CNP2 L1 L2	MP	M CNP1 CNP2 L1 L2
1	1 2 1 4 1	2	2 3 2 4 1		

**** CAUCHY BOUNDARY CONDITIONS ****

Radionuclide Pu241 isotope 2

PROFILE NO. 1

TIME	FLUX	TIME	FLUX	TIME	FLUX
----	----	----	----	----	----
0.000E+00	0.000E+00	9.111E+01	0.000E+00	2.000E+02	0.000E+00
2.770E+02	0.000E+00				

GLOBAL NODAL NUMBER AND PROFILE TYPE OF CAUCHY BOUNDARY NODES

I NPCB CTYP	I NPCB CTYP	I NPCB CTYP	I NPCB CTYP
1 1 1	2 2 1	3 3 1	

Radionuclide Pu241 isotope 2

CAUCHY ELEMENT SIDE DATA

MP	M CNP1 CNP2	MP	M CNP1 CNP2	MP	M CNP1 CNP2
1	1 1 2	2	2 2 3		

*** COMPUTED CAUCHY ELEMENT SIDE INFORMATION ***

MP	M	CNP1	CNP2	L1	L2	MP	M	CNP1	CNP2	L1	L2	MP	M	CNP1	CNP2	L1	L2
1	1	2	1	4	1	2	2	3	2	4	1						

**** CAUCHY BOUNDARY CONDITIONS ****

Radionuclide Pu240 isotope 3

PROFILE NO. 1

TIME	FLUX	TIME	FLUX	TIME	FLUX
----	----	----	----	----	----
0.000E+00	0.000E+00	9.111E+01	0.000E+00	2.000E+02	0.000E+00
2.770E+02	0.000E+00				

GLOBAL NODAL NUMBER AND PROFILE TYPE OF CAUCHY BOUNDARY NODES

I	NPCB	CTYP	I	NPCB	CTYP	I	NPCB	CTYP	I	NPCB	CTYP
1	1	1	2	2	1	3	3	1			

Radionuclide Pu240 isotope 3

CAUCHY ELEMENT SIDE DATA

MP	M	CNP1	CNP2	MP	M	CNP1	CNP2	MP	M	CNP1	CNP2
1	1	1	2	2	2	2	3				

*** COMPUTED CAUCHY ELEMENT SIDE INFORMATION ***

MP	M	CNP1	CNP2	L1	L2	MP	M	CNP1	CNP2	L1	L2	MP	M	CNP1	CNP2	L1	L2
1	1	2	1	4	1	2	2	3	2	4	1						

**** NEUMANN BOUNDARY CONDITIONS ****

Radionuclide Am241 isotope 1

PROFILE NO. 1

TIME	FLUX	TIME	FLUX	TIME	FLUX
----	----	----	----	----	----

0.000E+00 0.000E+00 9.110E+01 0.000E+00 2.000E+02 0.000E+00
 3.000E+02 0.000E+00

GLOBAL NODAL NUMBER AND PROFILE TYPE OF NEUMAN BOUNDARY NODES

I NPNB NTYP	I NPNB NTYP	I NPNB NTYP	I NPNB NTYP
1 211 1	2 212 1	3 213 1	

Radionuclide Am241 isotope 1

NEUMANN ELEMENT SIDE DATA

MP	M	CNP1	CNP2	MP	M	CNP1	CNP2	MP	M	CNP1	CNP2
1	139	1	2	2	140	2	3				

*** COMPUTED NEUMANN ELEMENT SIDE INFORMATION ***

MP	M	CNP1	CNP2	L1	L2	DL(MP)	DCOSXN(MP)	DCOSZN(MP)
1	139	1	2	2	3	1.000E+02	1.000E+00	-6.123E-17
2	140	2	3	2	3	1.000E+02	1.000E+00	-6.123E-17

**** NEUMANN BOUNDARY CONDITIONS ****

Radionuclide Pu241 isotope 2

PROFILE NO. 1

TIME	FLUX	TIME	FLUX	TIME	FLUX
----	----	----	----	----	----
0.000E+00	0.000E+00	9.110E+01	0.000E+00	2.000E+02	0.000E+00
3.000E+02	0.000E+00				

GLOBAL NODAL NUMBER AND PROFILE TYPE OF NEUMAN BOUNDARY NODES

I NPNB NTYP	I NPNB NTYP	I NPNB NTYP	I NPNB NTYP
1 211 1	2 212 1	3 213 1	

Radionuclide Pu241 isotope 2

NEUMANN ELEMENT SIDE DATA

MP	M	CNP1	CNP2	MP	M	CNP1	CNP2	MP	M	CNP1	CNP2
----	---	------	------	----	---	------	------	----	---	------	------

1 139 1 2 2 140 2 3

*** COMPUTED NEUMANN ELEMENT SIDE INFORMATION ***

MP	M	CNP1	CNP2	L1	L2	DL(MP)	DCOSXN(MP)	DCOSZN(MP)
1	139	1	2	2	3	1.000E+02	1.000E+00	-6.123E-17
2	140	2	3	2	3	1.000E+02	1.000E+00	-6.123E-17

**** NEUMANN BOUNDARY CONDITIONS ****

Radionuclide Pu240 isotope 3

PROFILE NO. 1

TIME	FLUX	TIME	FLUX	TIME	FLUX
----	----	----	----	----	----
0.000E+00	0.000E+00	9.110E+01	0.000E+00	2.000E+02	0.000E+00
3.000E+02	0.000E+00				

GLOBAL NODAL NUMBER AND PROFILE TYPE OF NEUMAN BOUNDARY NODES

I	NPNB	NTYP	I	NPNB	NTYP	I	NPNB	NTYP	I	NPNB	NTYP
1	211	1	2	212	1	3	213	1			

Radionuclide Pu240 isotope 3

NEUMANN ELEMENT SIDE DATA

MP	M	CNP1	CNP2	MP	M	CNP1	CNP2	MP	M	CNP1	CNP2
1	139	1	2	2	140	2	3				

*** COMPUTED NEUMANN ELEMENT SIDE INFORMATION ***

MP	M	CNP1	CNP2	L1	L2	DL(MP)	DCOSXN(MP)	DCOSZN(MP)
1	139	1	2	2	3	1.000E+02	1.000E+00	-6.123E-17
2	140	2	3	2	3	1.000E+02	1.000E+00	-6.123E-17

*** CONTAINER/PACKAGE INFORMATION ****

TYPE	THICKNESS	PARAM_N	PARAM_K	AREA	ASCALE
1	1.000E+00	1.000E-02	7.000E-03	2.100E+04	2.000E-01

PITS	GRATE	CLAY	SOIL-PH	AERA_IND
5.000E+03	3.170E-10	1.500E-01	6.000E+00	2

TYPE	THICKNESS	PARAM_N	PARAM_K	AREA	ASCALE
2	1.000E+00	1.000E-02	7.000E-03	2.100E+04	2.000E-01

PITS	GRATE	CLAY	SOIL-PH	AERA_IND
5.000E+03	3.170E+08	1.500E-01	6.000E+00	2

GLOBAL ELEMENT NUMBER AND CONTAINER/PACKAGE TYPE SOURCE

I	ELEMENT NO.	TYPE
1	21	1
2	22	1
3	41	1
4	42	1
5	61	2
6	62	2

**** WASTE FORM INFORMATION ****

FLAG FOR DIFFUSION SOLUTION (0 - 5) . . . 3

Am241 isotope no = 1

TYPE	SURF_FRACT	PORE_FRACT	BULK_FRACT	EFFECT_D	FRACT_REL_RATE
1	3.330E-01	3.330E-01	3.330E-01	1.000E-08	1.000E-03

TYPE	PORE_LEN	VOL_WF	KD(0)	KD(INF)	KD-DECAY	VOL_RATIO
1	2.500E+01	1.000E+06	0.000E+00	0.000E+00	0.000E+00	1.000E+00

Pu241 isotope no = 2

TYPE	SURF_FRACT	PORE_FRACT	BULK_FRACT	EFFECT_D	FRACT_REL_RATE
1	3.330E-01	3.330E-01	3.330E-01	1.000E-08	1.000E-03

TYPE	PORE_LEN	VOL_WF	KD(0)	KD(INF)	KD-DECAY	VOL_RATIO
1	2.500E+01	1.000E+06	0.000E+00	0.000E+00	0.000E+00	1.000E+00

Pu240 isotope no = 3

TYPE	SURF_FRACT	PORE_FRACT	BULK_FRACT	EFFECT_D	FRACT_REL_RATE
1	3.330E-01	3.330E-01	3.330E-01	1.000E-08	1.000E-03

TYPE	PORE_LEN	VOL_WF	KD(0)	KD(INF)	KD-DECAY	VOL_RATIO
1	2.500E+01	1.000E+06	0.000E+00	0.000E+00	0.000E+00	1.000E+00

Am241 isotope no = 1

GLOBAL ELEMENT NO. AND WASTE TYPE SOURCE

I	ELEMENT_NO.	WF_TYPE	SURF_MASS	PORE_MASS	BULK_MASS	TOTAL_MASS
1	21	1	9.990E-01	9.990E-01	9.990E-01	3.000E+00
2	22	1	9.990E-01	9.990E-01	9.990E-01	3.000E+00
3	41	1	9.990E-01	9.990E-01	9.990E-01	3.000E+00
4	42	1	9.990E-01	9.990E-01	9.990E-01	3.000E+00
5	61	1	9.990E-01	9.990E-01	9.990E-01	3.000E+00
6	62	1	9.990E-01	9.990E-01	9.990E-01	3.000E+00

Pu241 isotope no = 2

GLOBAL ELEMENT NO. AND WASTE TYPE SOURCE

I	ELEMENT_NO.	WF_TYPE	SURF_MASS	PORE_MASS	BULK_MASS	TOTAL_MASS
1	21	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	22	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
3	41	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4	42	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
5	61	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
6	62	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Pu240 isotope no = 3

GLOBAL ELEMENT NO. AND WASTE TYPE SOURCE

I	ELEMENT_NO.	WF_TYPE	SURF_MASS	PORE_MASS	BULK_MASS	TOTAL_MASS
1	21	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	22	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
3	41	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4	42	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
5	61	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
6	62	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00

**** LINE-PRINT OUTPUT CONTROL AND STORAGE****

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0 2 2 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2 0 0 0 0 0 0 0 0 2 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 2

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NUMBER OF CONCENTRATION TRACE PROFILES      8
NUMBER OF FLUX TRACE PROFILES . . . . .    4
NUMBER OF TIME STEPS BETWEEN TRACES . .    1

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NODE NUMBERS FOR CONCENTRATION TRACES

2 32 62 92 122 152 182 212

NODE NUMBERS FOR FLUX TRACES

2 32 62 92

INITIAL VELOCITY PROFILES

NODE	VX	VZ	NODE	VX	VZ	NODE	VX	VZ
1	2.316E-04	0.000E+00	2	2.316E-04	0.000E+00	3	2.316E-04	0.000E+00
4	2.316E-04	0.000E+00	5	2.316E-04	0.000E+00	6	2.316E-04	0.000E+00
7	2.316E-04	0.000E+00	8	2.316E-04	0.000E+00	9	2.316E-04	0.000E+00
10	2.316E-04	0.000E+00	11	2.316E-04	0.000E+00	12	2.316E-04	0.000E+00
13	2.316E-04	0.000E+00	14	2.316E-04	0.000E+00	15	2.316E-04	0.000E+00
16	2.316E-04	0.000E+00	17	2.316E-04	0.000E+00	18	2.316E-04	0.000E+00
19	2.316E-04	0.000E+00	20	2.316E-04	0.000E+00	21	2.316E-04	0.000E+00
22	2.316E-04	0.000E+00	23	2.316E-04	0.000E+00	24	2.316E-04	0.000E+00
25	2.316E-04	0.000E+00	26	2.316E-04	0.000E+00	27	2.316E-04	0.000E+00
28	2.316E-04	0.000E+00	29	2.316E-04	0.000E+00	30	2.316E-04	0.000E+00
31	2.316E-04	0.000E+00	32	2.316E-04	0.000E+00	33	2.316E-04	0.000E+00
34	2.316E-04	0.000E+00	35	2.316E-04	0.000E+00	36	2.316E-04	0.000E+00
37	2.316E-04	0.000E+00	38	2.316E-04	0.000E+00	39	2.316E-04	0.000E+00
40	2.316E-04	0.000E+00	41	2.316E-04	0.000E+00	42	2.316E-04	0.000E+00
43	2.316E-04	0.000E+00	44	2.316E-04	0.000E+00	45	2.316E-04	0.000E+00
46	2.316E-04	0.000E+00	47	2.316E-04	0.000E+00	48	2.316E-04	0.000E+00
49	2.316E-04	0.000E+00	50	2.316E-04	0.000E+00	51	2.316E-04	0.000E+00
52	2.316E-04	0.000E+00	53	2.316E-04	0.000E+00	54	2.316E-04	0.000E+00
55	2.316E-04	0.000E+00	56	2.316E-04	0.000E+00	57	2.316E-04	0.000E+00
58	2.316E-04	0.000E+00	59	2.316E-04	0.000E+00	60	2.316E-04	0.000E+00
61	2.316E-04	0.000E+00	62	2.316E-04	0.000E+00	63	2.316E-04	0.000E+00
64	2.316E-04	0.000E+00	65	2.316E-04	0.000E+00	66	2.316E-04	0.000E+00
67	2.316E-04	0.000E+00	68	2.316E-04	0.000E+00	69	2.316E-04	0.000E+00
70	2.316E-04	0.000E+00	71	2.316E-04	0.000E+00	72	2.316E-04	0.000E+00
73	2.316E-04	0.000E+00	74	2.316E-04	0.000E+00	75	2.316E-04	0.000E+00
76	2.316E-04	0.000E+00	77	2.316E-04	0.000E+00	78	2.316E-04	0.000E+00
79	2.316E-04	0.000E+00	80	2.316E-04	0.000E+00	81	2.316E-04	0.000E+00
82	2.316E-04	0.000E+00	83	2.316E-04	0.000E+00	84	2.316E-04	0.000E+00
85	2.316E-04	0.000E+00	86	2.316E-04	0.000E+00	87	2.316E-04	0.000E+00
88	2.316E-04	0.000E+00	89	2.316E-04	0.000E+00	90	2.316E-04	0.000E+00
91	2.316E-04	0.000E+00	92	2.316E-04	0.000E+00	93	2.316E-04	0.000E+00
94	2.316E-04	0.000E+00	95	2.316E-04	0.000E+00	96	2.316E-04	0.000E+00
97	2.316E-04	0.000E+00	98	2.316E-04	0.000E+00	99	2.316E-04	0.000E+00
100	2.316E-04	0.000E+00	101	2.316E-04	0.000E+00	102	2.316E-04	0.000E+00
103	2.316E-04	0.000E+00	104	2.316E-04	0.000E+00	105	2.316E-04	0.000E+00
106	2.316E-04	0.000E+00	107	2.316E-04	0.000E+00	108	2.316E-04	0.000E+00
109	2.316E-04	0.000E+00	110	2.316E-04	0.000E+00	111	2.316E-04	0.000E+00
112	2.316E-04	0.000E+00	113	2.316E-04	0.000E+00	114	2.316E-04	0.000E+00
115	2.316E-04	0.000E+00	116	2.316E-04	0.000E+00	117	2.316E-04	0.000E+00
118	2.316E-04	0.000E+00	119	2.316E-04	0.000E+00	120	2.316E-04	0.000E+00
121	2.316E-04	0.000E+00	122	2.316E-04	0.000E+00	123	2.316E-04	0.000E+00
124	2.316E-04	0.000E+00	125	2.316E-04	0.000E+00	126	2.316E-04	0.000E+00
127	2.316E-04	0.000E+00	128	2.316E-04	0.000E+00	129	2.316E-04	0.000E+00
130	2.316E-04	0.000E+00	131	2.316E-04	0.000E+00	132	2.316E-04	0.000E+00
133	2.316E-04	0.000E+00	134	2.316E-04	0.000E+00	135	2.316E-04	0.000E+00

136	2.316E-04	0.000E+00	137	2.316E-04	0.000E+00	138	2.316E-04	0.000E+00
139	2.316E-04	0.000E+00	140	2.316E-04	0.000E+00	141	2.316E-04	0.000E+00
142	2.316E-04	0.000E+00	143	2.316E-04	0.000E+00	144	2.316E-04	0.000E+00
145	2.316E-04	0.000E+00	146	2.316E-04	0.000E+00	147	2.316E-04	0.000E+00
148	2.316E-04	0.000E+00	149	2.316E-04	0.000E+00	150	2.316E-04	0.000E+00
151	2.316E-04	0.000E+00	152	2.316E-04	0.000E+00	153	2.316E-04	0.000E+00
154	2.316E-04	0.000E+00	155	2.316E-04	0.000E+00	156	2.316E-04	0.000E+00
157	2.316E-04	0.000E+00	158	2.316E-04	0.000E+00	159	2.316E-04	0.000E+00
160	2.316E-04	0.000E+00	161	2.316E-04	0.000E+00	162	2.316E-04	0.000E+00
163	2.316E-04	0.000E+00	164	2.316E-04	0.000E+00	165	2.316E-04	0.000E+00
166	2.316E-04	0.000E+00	167	2.316E-04	0.000E+00	168	2.316E-04	0.000E+00
169	2.316E-04	0.000E+00	170	2.316E-04	0.000E+00	171	2.316E-04	0.000E+00
172	2.316E-04	0.000E+00	173	2.316E-04	0.000E+00	174	2.316E-04	0.000E+00
175	2.316E-04	0.000E+00	176	2.316E-04	0.000E+00	177	2.316E-04	0.000E+00
178	2.316E-04	0.000E+00	179	2.316E-04	0.000E+00	180	2.316E-04	0.000E+00
181	2.316E-04	0.000E+00	182	2.316E-04	0.000E+00	183	2.316E-04	0.000E+00
184	2.316E-04	0.000E+00	185	2.316E-04	0.000E+00	186	2.316E-04	0.000E+00
187	2.316E-04	0.000E+00	188	2.316E-04	0.000E+00	189	2.316E-04	0.000E+00
190	2.316E-04	0.000E+00	191	2.316E-04	0.000E+00	192	2.316E-04	0.000E+00
193	2.316E-04	0.000E+00	194	2.316E-04	0.000E+00	195	2.316E-04	0.000E+00
196	2.316E-04	0.000E+00	197	2.316E-04	0.000E+00	198	2.316E-04	0.000E+00
199	2.316E-04	0.000E+00	200	2.316E-04	0.000E+00	201	2.316E-04	0.000E+00
202	2.316E-04	0.000E+00	203	2.316E-04	0.000E+00	204	2.316E-04	0.000E+00
205	2.316E-04	0.000E+00	206	2.316E-04	0.000E+00	207	2.316E-04	0.000E+00
208	2.316E-04	0.000E+00	209	2.316E-04	0.000E+00	210	2.316E-04	0.000E+00
211	2.316E-04	0.000E+00	212	2.316E-04	0.000E+00	213	2.316E-04	0.000E+00

MOISTURE CONTENT IN EACH ELEMENT

Element	Loc 1	Loc 2	Loc 3	Loc 4
1	2.000E-01	2.000E-01	2.000E-01	2.000E-01
2	2.000E-01	2.000E-01	2.000E-01	2.000E-01
3	2.000E-01	2.000E-01	2.000E-01	2.000E-01
4	2.000E-01	2.000E-01	2.000E-01	2.000E-01
5	2.000E-01	2.000E-01	2.000E-01	2.000E-01
6	2.000E-01	2.000E-01	2.000E-01	2.000E-01
7	2.000E-01	2.000E-01	2.000E-01	2.000E-01
8	2.000E-01	2.000E-01	2.000E-01	2.000E-01
9	2.000E-01	2.000E-01	2.000E-01	2.000E-01
10	2.000E-01	2.000E-01	2.000E-01	2.000E-01
11	2.000E-01	2.000E-01	2.000E-01	2.000E-01
12	2.000E-01	2.000E-01	2.000E-01	2.000E-01
13	2.000E-01	2.000E-01	2.000E-01	2.000E-01
14	2.000E-01	2.000E-01	2.000E-01	2.000E-01
15	2.000E-01	2.000E-01	2.000E-01	2.000E-01
16	2.000E-01	2.000E-01	2.000E-01	2.000E-01
17	2.000E-01	2.000E-01	2.000E-01	2.000E-01
18	2.000E-01	2.000E-01	2.000E-01	2.000E-01
19	2.000E-01	2.000E-01	2.000E-01	2.000E-01
20	2.000E-01	2.000E-01	2.000E-01	2.000E-01
21	2.000E-01	2.000E-01	2.000E-01	2.000E-01
22	2.000E-01	2.000E-01	2.000E-01	2.000E-01
23	2.000E-01	2.000E-01	2.000E-01	2.000E-01
24	2.000E-01	2.000E-01	2.000E-01	2.000E-01
25	2.000E-01	2.000E-01	2.000E-01	2.000E-01
26	2.000E-01	2.000E-01	2.000E-01	2.000E-01
27	2.000E-01	2.000E-01	2.000E-01	2.000E-01
28	2.000E-01	2.000E-01	2.000E-01	2.000E-01

NUREG/CR-6492

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SYSTEM-FLOW TABLE 1 AT TIME =1.000E+00 years , DELT =1.000E+00 ITIM = 1

TYPE OF FLOW	RATE M/T/L	INC.FLOW M/L	TOTAL FLOW M/L
1. THROUGH DIRICHLET BOUNDARY NODES . . .	0.0000E+00	0.0000E+00	0.0000E+00
2. THROUGH CAUCHY BOUNDARY NODES . . .	0.0000E+00	0.0000E+00	0.0000E+00
3. THROUGH NEUMANN BOUNDARY NODES . . .	0.0000E+00	0.0000E+00	0.0000E+00
4. THROUGH SEEPAGE NODES	0.0000E+00	0.0000E+00	0.0000E+00
5. THROUGH INFILTRATION NODES	0.0000E+00	0.0000E+00	0.0000E+00
6. THROUGH UNSPECIFIED NODES (NUMERICAL) .	0.0000E+00	0.0000E+00	0.0000E+00
7. NET FLOW THROUGH ENTIRE BOUNDARY NODES	0.0000E+00	0.0000E+00	0.0000E+00
8. INCREASE IN MATERIAL CONTENT (LIQUID) .	1.3867E-13	4.3761E-06	4.3761E-06
9. INCREASE IN MATERIAL CONTENT (SOLID) .	6.4898E-10	2.0480E-02	2.0480E-02
10. RADIOACTIVE LOSSES (LIQUID AND SOLID) .	1.0391E-12	1.6396E-05	1.6396E-05
11. LOSS TO COMP. OF SKELTON	0.0000E+00	0.0000E+00	0.0000E+00
12. LOSS THROUGH DISSOLVED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
13. LOSS THROUGH ADSORBED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
14. ARTIFICIAL SOURCES/SINKS	-3.9009E-08	-1.2310E+00	-1.2310E+00

*** NOTE: (+) = OUT FROM, (-) = INTO THE REGION.

Am241 isotope = 1

CONTAINER BREACH

ELEMENT	CONTAINER TYPE	TIME BREACH	BREACHED AREA	CONTAINER AREA	RATIO
61	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00
62	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00

Am241 SOURCE TERM TO THE TRANSPORT CALCULATION --- IN GM/CM-CM-CM-S

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL REL RATE	RINSE REL RATE	DIFFUSION REL RATE	DISSOLUTION REL RATE
61	2	1	6.42E-14	6.25E-14	1.62E-15	6.25E-17
62	2	1	6.42E-14	6.25E-14	1.62E-15	6.25E-17

CUMULATIVE RELEASE FROM THE WASTE FORM AVAILABLE FOR TRANSPORT ---- IN GRAMS

CONTAMINANT Am241	ELEMENT	CUM. REL
	61	1.03E+00
	62	1.03E+00

Am241 CUMULATIVE MASS RELEASED FROM THE WASTE FORM ---- IN GRAMS

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL RELEASED	RINSE RELEASE	DIFFUSION RELEASE	DISSOLUTION RELEASE
61	2	1	1.03E+00	9.99E-01	2.59E-02	9.99E-04
62	2	1	1.03E+00	9.99E-01	2.59E-02	9.99E-04

Am241 isotope = 1

OUTPUT TABLE 1 CONCENTRATIONS (GM/CM3) AT TIME =1.000E+00 years
(DELT =1.000E+00)

*** ITIME = 1

NODE I CONCENTRATION (GM/CM3) AT NODES I,I+1,...,I+5

1	4.2462E-38	4.2462E-38	4.2462E-38	1.9083E-37	1.9083E-37	1.9083E-37
7	1.5628E-36	1.5628E-36	1.5628E-36	1.3030E-35	1.3030E-35	1.3030E-35
13	1.0868E-34	1.0868E-34	1.0868E-34	9.0645E-34	9.0645E-34	9.0645E-34
19	7.5604E-33	7.5604E-33	7.5604E-33	6.3058E-32	6.3058E-32	6.3058E-32
25	5.2595E-31	5.2595E-31	5.2595E-31	4.3868E-30	4.3868E-30	4.3868E-30
31	3.6589E-29	3.6589E-29	3.6589E-29	3.0517E-28	3.0517E-28	3.0517E-28
37	2.5454E-27	2.5454E-27	2.5454E-27	2.1230E-26	2.1230E-26	2.1230E-26
43	1.7707E-25	1.7707E-25	1.7707E-25	1.4769E-24	1.4769E-24	1.4769E-24
49	1.2318E-23	1.2318E-23	1.2318E-23	1.0274E-22	1.0274E-22	1.0274E-22
55	8.5695E-22	8.5695E-22	8.5695E-22	7.1475E-21	7.1475E-21	7.1475E-21
61	5.9615E-20	5.9615E-20	5.9615E-20	4.9723E-19	4.9723E-19	4.9723E-19
67	4.1472E-18	4.1472E-18	4.1472E-18	3.4591E-17	3.4591E-17	3.4591E-17
73	2.8851E-16	2.8851E-16	2.8851E-16	2.4064E-15	2.4064E-15	2.4064E-15
79	2.0071E-14	2.0071E-14	2.0071E-14	1.6740E-13	1.6740E-13	1.6740E-13
85	1.3962E-12	1.3962E-12	1.3962E-12	1.1646E-11	1.1646E-11	1.1646E-11
91	9.7132E-11	9.7132E-11	9.7132E-11	8.1015E-10	8.1015E-10	8.1015E-10
97	1.4290E-10	1.4290E-10	1.4290E-10	2.5207E-11	2.5207E-11	2.5207E-11
103	4.4464E-12	4.4464E-12	4.4464E-12	7.8431E-13	7.8431E-13	7.8431E-13
109	1.3835E-13	1.3835E-13	1.3835E-13	2.4403E-14	2.4403E-14	2.4403E-14
115	4.3045E-15	4.3045E-15	4.3045E-15	7.5929E-16	7.5929E-16	7.5929E-16
121	1.3393E-16	1.3393E-16	1.3393E-16	2.3625E-17	2.3625E-17	2.3625E-17
127	4.1672E-18	4.1672E-18	4.1672E-18	7.3507E-19	7.3507E-19	7.3507E-19
133	1.2966E-19	1.2966E-19	1.2966E-19	2.2871E-20	2.2871E-20	2.2871E-20
139	4.0343E-21	4.0343E-21	4.0343E-21	7.1162E-22	7.1162E-22	7.1162E-22
145	1.2553E-22	1.2553E-22	1.2553E-22	2.2142E-23	2.2142E-23	2.2142E-23
151	3.9056E-24	3.9056E-24	3.9056E-24	6.8893E-25	6.8893E-25	6.8893E-25
157	1.2152E-25	1.2152E-25	1.2152E-25	2.1435E-26	2.1435E-26	2.1435E-26
163	3.7811E-27	3.7811E-27	3.7811E-27	6.6695E-28	6.6695E-28	6.6695E-28
169	1.1765E-28	1.1765E-28	1.1765E-28	2.0752E-29	2.0752E-29	2.0752E-29
175	3.6605E-30	3.6605E-30	3.6605E-30	6.4568E-31	6.4568E-31	6.4568E-31
181	1.1389E-31	1.1389E-31	1.1389E-31	2.0090E-32	2.0090E-32	2.0090E-32
187	3.5437E-33	3.5437E-33	3.5437E-33	6.2508E-34	6.2508E-34	6.2508E-34
193	1.1026E-34	1.1026E-34	1.1026E-34	1.9449E-35	1.9449E-35	1.9449E-35
199	3.4307E-36	3.4307E-36	3.4307E-36	6.0515E-37	6.0515E-37	6.0515E-37

205 1.0679E-37 1.0679E-37 1.0679E-37 1.9183E-38 1.9183E-38 1.9183E-38
 211 6.2800E-39 6.2800E-39 6.2800E-39

In container 1 for isotope 2

AS INPUT, THE WASTE FORM PROPERTIES DO NOT INITIALLY

PERMIT DISSOLUTION OR DIFFUSION --- PLEASE CHECK THE INPUT:

(The code will stop if both sets of transport and mass coefficients are initially 0.
 IN THIS CASE USE THE RINSE MODEL IF THIS IS THE ONLY RELEASE MODE

Note: Mass will diffuse into the waste form if D .NE. 0

In container 1 for isotope 2

AS INPUT, THE WASTE FORM PROPERTIES DO NOT INITIALLY

PERMIT DISSOLUTION OR DIFFUSION --- PLEASE CHECK THE INPUT:

(The code will stop if both sets of transport and mass coefficients are initially 0.
 IN THIS CASE USE THE RINSE MODEL IF THIS IS THE ONLY RELEASE MODE

Note: Mass will diffuse into the waste form if D .NE. 0

SYSTEM-FLOW TABLE 2 AT TIME =1.000E+00 years , DELT =1.000E+00 ITIM = 1

TYPE OF FLOW	RATE M/T/L	INC.FLOW M/L	TOTAL FLOW M/L
1. THROUGH DIRICHLET BOUNDARY NODES . . .	0.0000E+00	0.0000E+00	0.0000E+00
2. THROUGH CAUCHY BOUNDARY NODES . . .	7.0059E-28	1.1055E-20	1.1055E-20
3. THROUGH NEUMANN BOUNDARY NODES . . .	1.6487E-32	2.6015E-25	2.6015E-25
4. THROUGH SEEPAGE NODES	0.0000E+00	0.0000E+00	0.0000E+00
5. THROUGH INFILTRATION NODES	0.0000E+00	0.0000E+00	0.0000E+00
6. THROUGH UNSPECIFIED NODES (NUMERICAL) .	1.1003E-27	1.7361E-20	1.7361E-20
7. NET FLOW THROUGH ENTIRE BOUNDARY NODES	1.8009E-27	2.8416E-20	2.8416E-20
8. INCREASE IN MATERIAL CONTENT (LIQUID) .	2.1448E-16	6.7685E-09	6.7685E-09
9. INCREASE IN MATERIAL CONTENT (SOLID) .	1.0038E-12	3.1677E-05	3.1677E-05
10. RADIOACTIVE LOSSES (LIQUID AND SOLID) .	4.6394E-14	7.3204E-07	7.3204E-07
11. LOSS TO COMP. OF SKELTON	0.0000E+00	0.0000E+00	0.0000E+00
12. LOSS THROUGH DISSOLVED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
13. LOSS THROUGH ADSORBED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
14. ARTIFICIAL SOURCES/SINKS	-9.7530E-09	-3.0778E-01	-3.0778E-01

*** NOTE: (+) = OUT FROM, (-) = INTO THE REGION.

Pu241 isotope = 2

CONTAINER BREACH

ELEMENT	CONTAINER TYPE	TIME BREACH	BREACHED AREA	CONTAINER AREA	RATIO
61	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00
62	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00

Pu241 SOURCE TERM TO THE TRANSPORT CALCULATION --- IN GM/CM-CM-CM-S

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL REL RATE	RINSE REL RATE	DIFFUSION REL RATE	DISSOLUTION REL RATE
61	2	1	5.64E-19	0.00E+00	5.13E-19	5.06E-20
62	2	1	5.64E-19	0.00E+00	5.13E-19	5.06E-20

CUMULATIVE RELEASE FROM THE WASTE FORM AVAILABLE FOR TRANSPORT ---- IN GRAMS

CONTAMINANT Pu241	ELEMENT	CUM. REL
	61	1.78E-05
	62	1.78E-05

Pu241 CUMULATIVE MASS RELEASED FROM THE WASTE FORM ---- IN GRAMS

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL RELEASED	RINSE RELEASE	DIFFUSION RELEASE	DISSOLUTION RELEASE
61	2	1	1.78E-05	0.00E+00	1.62E-05	1.60E-06
62	2	1	1.78E-05	0.00E+00	1.62E-05	1.60E-06

Pu241 isotope = 2

OUTPUT TABLE 2 CONCENTRATIONS (GM/CM3) AT TIME =1.000E+00 years
(DELT =1.000E+00)

*** ITIME = 1

NODE I CONCENTRATION (GM/CM3) AT NODES I,I+1,...,I+5

1	2.0223E-39	2.0223E-39	2.0223E-39	8.9169E-39	8.9169E-39	8.9169E-39
7	7.1557E-38	7.1557E-38	7.1557E-38	5.8425E-37	5.8425E-37	5.8425E-37
13	4.7666E-36	4.7666E-36	4.7666E-36	3.8841E-35	3.8841E-35	3.8841E-35
19	3.1606E-34	3.1606E-34	3.1606E-34	2.5682E-33	2.5682E-33	2.5682E-33
25	2.0835E-32	2.0835E-32	2.0835E-32	1.6873E-31	1.6873E-31	1.6873E-31
31	1.3638E-30	1.3638E-30	1.3638E-30	1.1000E-29	1.1000E-29	1.1000E-29
37	8.8522E-29	8.8522E-29	8.8522E-29	7.1052E-28	7.1052E-28	7.1052E-28
43	5.6866E-27	5.6866E-27	5.6866E-27	4.5366E-26	4.5366E-26	4.5366E-26
49	3.6060E-25	3.6060E-25	3.6060E-25	2.8544E-24	2.8544E-24	2.8544E-24
55	2.2487E-23	2.2487E-23	2.2487E-23	1.7619E-22	1.7619E-22	1.7619E-22

61	1.3715E-21	1.3715E-21	1.3715E-21	1.0595E-20	1.0595E-20	1.0595E-20
67	8.1095E-20	8.1095E-20	8.1095E-20	6.1372E-19	6.1372E-19	6.1372E-19
73	4.5789E-18	4.5789E-18	4.5789E-18	3.3539E-17	3.3539E-17	3.3539E-17
79	2.3966E-16	2.3966E-16	2.3966E-16	1.6536E-15	1.6536E-15	1.6536E-15
85	1.0818E-14	1.0818E-14	1.0818E-14	6.4595E-14	6.4595E-14	6.4595E-14
91	3.1795E-13	3.1795E-13	3.1795E-13	7.4939E-13	7.4939E-13	7.4939E-13
97	3.9646E-13	3.9646E-13	3.9646E-13	1.1506E-13	1.1506E-13	1.1506E-13
103	2.8002E-14	2.8002E-14	2.8002E-14	6.2554E-15	6.2554E-15	6.2554E-15
109	1.3281E-15	1.3281E-15	1.3281E-15	2.7265E-16	2.7265E-16	2.7265E-16
115	5.4646E-17	5.4646E-17	5.4646E-17	1.0758E-17	1.0758E-17	1.0758E-17
121	2.0888E-18	2.0888E-18	2.0888E-18	4.0107E-19	4.0107E-19	4.0107E-19
127	7.6318E-20	7.6318E-20	7.6318E-20	1.4414E-20	1.4414E-20	1.4414E-20
133	2.7049E-21	2.7049E-21	2.7049E-21	5.0488E-22	5.0488E-22	5.0488E-22
139	9.3795E-23	9.3795E-23	9.3795E-23	1.7354E-23	1.7354E-23	1.7354E-23
145	3.1993E-24	3.1993E-24	3.1993E-24	5.8792E-25	5.8792E-25	5.8792E-25
151	1.0773E-25	1.0773E-25	1.0773E-25	1.9692E-26	1.9692E-26	1.9692E-26
157	3.5909E-27	3.5909E-27	3.5909E-27	6.5348E-28	6.5348E-28	6.5348E-28
163	1.1869E-28	1.1869E-28	1.1869E-28	2.1522E-29	2.1522E-29	2.1522E-29
169	3.8962E-30	3.8962E-30	3.8962E-30	7.0432E-31	7.0432E-31	7.0432E-31
175	1.2715E-31	1.2715E-31	1.2715E-31	2.2926E-32	2.2926E-32	2.2926E-32
181	4.1289E-33	4.1289E-33	4.1289E-33	7.4282E-34	7.4282E-34	7.4282E-34
187	1.3351E-34	1.3351E-34	1.3351E-34	2.3972E-35	2.3972E-35	2.3972E-35
193	4.3008E-36	4.3008E-36	4.3008E-36	7.7096E-37	7.7096E-37	7.7096E-37
199	1.3810E-37	1.3810E-37	1.3810E-37	2.4720E-38	2.4720E-38	2.4720E-38
205	4.4236E-39	4.4236E-39	4.4236E-39	8.0592E-40	8.0592E-40	8.0592E-40
211	2.6720E-40	2.6720E-40	2.6720E-40			

In container 1 for isotope 3

AS INPUT, THE WASTE FORM PROPERTIES DO NOT INITIALLY

PERMIT DISSOLUTION OR DIFFUSION --- PLEASE CHECK THE INPUT:

(The code will stop if both sets of transport and mass coefficients are initially 0.
IN THIS CASE USE THE RINSE MODEL IF THIS IS THE ONLY RELEASE MODE

Note: Mass will diffuse into the waste form if D .NE. 0

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IN THIS CASE USE THE RINSE MODEL IF THIS IS THE ONLY RELEASE MODE

Note: Mass will diffuse into the waste form if D .NE. 0

SYSTEM-FLOW TABLE 3 AT TIME =1.000E+00 years , DELT =1.000E+00 ITIM = 1

TYPE OF FLOW	RATE M/T/L	INC.FLOW M/L	TOTAL FLOW M/L
1. THROUGH DIRICHLET BOUNDARY NODES . . .	0.0000E+00	0.0000E+00	0.0000E+00
2. THROUGH CAUCHY BOUNDARY NODES . . .	1.1903E-32	1.8782E-25	1.8782E-25
3. THROUGH NEUMANN BOUNDARY NODES . . .	2.8082E-37	4.4311E-30	4.4311E-30
4. THROUGH SEEPAGE NODES	0.0000E+00	0.0000E+00	0.0000E+00
5. THROUGH INFILTRATION NODES	0.0000E+00	0.0000E+00	0.0000E+00

6. THROUGH UNSPECIFIED NODES (NUMERICAL) . -1.0098E-31 -1.5934E-24 -1.5934E-24
 7. NET FLOW THROUGH ENTIRE BOUNDARY NODES -8.9079E-32 -1.4056E-24 -1.4056E-24
 8. INCREASE IN MATERIAL CONTENT (LIQUID) . 1.0001E-17 3.1560E-10 3.1560E-10
 9. INCREASE IN MATERIAL CONTENT (SOLID) . 4.6804E-14 1.4770E-06 1.4770E-06
 10. RADIOACTIVE LOSSES (LIQUID AND SOLID) . 4.9616E-18 7.8288E-11 7.8288E-11
 11. LOSS TO COMP. OF SKELTON 0.0000E+00 0.0000E+00 0.0000E+00
 12. LOSS THROUGH DISSOLVED PHASE 0.0000E+00 0.0000E+00 0.0000E+00
 13. LOSS THROUGH ADSORBED PHASE 0.0000E+00 0.0000E+00 0.0000E+00
 14. ARTIFICIAL SOURCES/SINKS -1.9468E-13 -6.1436E-06 -6.1436E-06
 *** NOTE: (+) = OUT FROM, (-) = INTO THE REGION.

Pu240 isotope = 3

CONTAINER BREACH

ELEMENT	CONTAINER TYPE	TIME BREACH	BREACHED AREA	CONTAINER AREA	RATIO
61	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00
62	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00

Pu240 SOURCE TERM TO THE TRANSPORT CALCULATION ---- IN GM/CM-CM-CM-S

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL REL RATE	RINSE REL RATE	DIFFUSION REL RATE	DISSOLUTION REL RATE
61	2	1	2.12E-20	0.00E+00	1.90E-20	2.23E-21
62	2	1	2.12E-20	0.00E+00	1.90E-20	2.23E-21

CUMULATIVE RELEASE FROM THE WASTE FORM AVAILABLE FOR TRANSPORT ---- IN GRAMS

CONTAMINANT Pu240	ELEMENT	CUM. REL
	61	6.70E-07
	62	6.70E-07

Pu240 CUMULATIVE MASS RELEASED FROM THE WASTE FORM ---- IN GRAMS

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL RELEASED	RINSE RELEASE	DIFFUSION RELEASE	DISSOLUTION RELEASE
61	2	1	6.70E-07	0.00E+00	5.99E-07	7.05E-08

62 2 1 6.70E-07 0.00E+00 5.99E-07 7.05E-08

Pu240 isotope = 3

OUTPUT TABLE 3 CONCENTRATIONS (GM/CM3) AT TIME =1.000E+00 years
(DELT =1.000E+00)

*** ITIME = 1

NODE I CONCENTRATION (GM/CM3) AT NODES I,I+1,...,I+5

1	2.6372E-39	2.6372E-39	2.6372E-39	1.1237E-38	1.1237E-38	1.1237E-38
7	8.6649E-38	8.6649E-38	8.6649E-38	6.7980E-37	6.7980E-37	6.7980E-37
13	5.3227E-36	5.3227E-36	5.3227E-36	4.1567E-35	4.1567E-35	4.1567E-35
19	3.2368E-34	3.2368E-34	3.2368E-34	2.5128E-33	2.5128E-33	2.5128E-33
25	1.9442E-32	1.9442E-32	1.9442E-32	1.4988E-31	1.4988E-31	1.4988E-31
31	1.1508E-30	1.1508E-30	1.1508E-30	8.7978E-30	8.7978E-30	8.7978E-30
37	6.6935E-29	6.6935E-29	6.6935E-29	5.0654E-28	5.0654E-28	5.0654E-28
43	3.8106E-27	3.8106E-27	3.8106E-27	2.8476E-26	2.8476E-26	2.8476E-26
49	2.1120E-25	2.1120E-25	2.1120E-25	1.5532E-24	1.5532E-24	1.5532E-24
55	1.1311E-23	1.1311E-23	1.1311E-23	8.1442E-23	8.1442E-23	8.1442E-23
61	5.7871E-22	5.7871E-22	5.7871E-22	4.0481E-21	4.0481E-21	4.0481E-21
67	2.7786E-20	2.7786E-20	2.7786E-20	1.8634E-19	1.8634E-19	1.8634E-19
73	1.2138E-18	1.2138E-18	1.2138E-18	7.6135E-18	7.6135E-18	7.6135E-18
79	4.5399E-17	4.5399E-17	4.5399E-17	2.5206E-16	2.5206E-16	2.5206E-16
85	1.2562E-15	1.2562E-15	1.2562E-15	5.2255E-15	5.2255E-15	5.2255E-15
91	1.5315E-14	1.5315E-14	1.5315E-14	2.5649E-14	2.5649E-14	2.5649E-14
97	1.8814E-14	1.8814E-14	1.8814E-14	8.4196E-15	8.4196E-15	8.4196E-15
103	2.8261E-15	2.8261E-15	2.8261E-15	8.1047E-16	8.1047E-16	8.1047E-16
109	2.1089E-16	2.1089E-16	2.1089E-16	5.1385E-17	5.1385E-17	5.1385E-17
115	1.1943E-17	1.1943E-17	1.1943E-17	2.6791E-18	2.6791E-18	2.6791E-18
121	5.8457E-19	5.8457E-19	5.8457E-19	1.2475E-19	1.2475E-19	1.2475E-19
127	2.6146E-20	2.6146E-20	2.6146E-20	5.3973E-21	5.3973E-21	5.3973E-21
133	1.1000E-21	1.1000E-21	1.1000E-21	2.2175E-22	2.2175E-22	2.2175E-22
139	4.4279E-23	4.4279E-23	4.4279E-23	8.7688E-24	8.7688E-24	8.7688E-24
145	1.7239E-24	1.7239E-24	1.7239E-24	3.3670E-25	3.3670E-25	3.3670E-25
151	6.5382E-26	6.5382E-26	6.5382E-26	1.2630E-26	1.2630E-26	1.2630E-26
157	2.4283E-27	2.4283E-27	2.4283E-27	4.6488E-28	4.6488E-28	4.6488E-28
163	8.8651E-29	8.8651E-29	8.8651E-29	1.6845E-29	1.6845E-29	1.6845E-29
169	3.1903E-30	3.1903E-30	3.1903E-30	6.0238E-31	6.0238E-31	6.0238E-31
175	1.1342E-31	1.1342E-31	1.1342E-31	2.1301E-32	2.1301E-32	2.1301E-32
181	3.9906E-33	3.9906E-33	3.9906E-33	7.4594E-34	7.4594E-34	7.4594E-34
187	1.3914E-34	1.3914E-34	1.3914E-34	2.5904E-35	2.5904E-35	2.5904E-35
193	4.8135E-36	4.8135E-36	4.8135E-36	8.9290E-37	8.9290E-37	8.9290E-37
199	1.6536E-37	1.6536E-37	1.6536E-37	3.0578E-38	3.0578E-38	3.0578E-38
205	5.6487E-39	5.6487E-39	5.6487E-39	1.0626E-39	1.0626E-39	1.0626E-39
211	3.6208E-40	3.6208E-40	3.6208E-40			

SYSTEM-FLOW TABLE 28 AT TIME =2.730E+02 years , DELT =1.000E+00 ITIM = 273

TYPE OF FLOW

RATE
M/T/L

INC.FLOW
M/L

TOTAL FLOW
M/L

1.	THROUGH DIRICHLET BOUNDARY NODES	0.0000E+00	0.0000E+00	0.0000E+00
2.	THROUGH CAUCHY BOUNDARY NODES	1.6700E-15	5.2725E-08	7.1013E-06
3.	THROUGH NEUMANN BOUNDARY NODES	2.5550E-13	7.9920E-06	3.2241E-04
4.	THROUGH SEEPAGE NODES	0.0000E+00	0.0000E+00	0.0000E+00
5.	THROUGH INFILTRATION NODES	0.0000E+00	0.0000E+00	0.0000E+00
6.	THROUGH UNSPECIFIED NODES (NUMERICAL) .	-1.3985E-26	-4.4215E-19	-4.3335E-17
7.	NET FLOW THROUGH ENTIRE BOUNDARY NODES	2.5717E-13	8.0448E-06	3.2951E-04
8.	INCREASE IN MATERIAL CONTENT (LIQUID) .	-1.4959E-16	-4.7206E-09	1.3872E-05
9.	INCREASE IN MATERIAL CONTENT (SOLID) .	-7.0007E-13	-2.2093E-05	6.4919E-02
10.	RADIOACTIVE LOSSES (LIQUID AND SOLID) .	3.2938E-12	1.0396E-04	2.1494E-02
11.	LOSS TO COMP. OF SKELTON	0.0000E+00	0.0000E+00	0.0000E+00
12.	LOSS THROUGH DISSOLVED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
13.	LOSS THROUGH ADSORBED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
14.	ARTIFICIAL SOURCES/SINKS	-9.7033E-11	-3.0621E-03	-2.8884E+00

*** NOTE: (+) = OUT FROM, (-) = INTO THE REGION.

Am241 isotope = 1

CONTAINER BREACH

ELEMENT	CONTAINER TYPE	TIME BREACH	BREACHED AREA	CONTAINER AREA	RATIO
21	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
22	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
41	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
42	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
61	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00
62	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00

Am241 SOURCE TERM TO THE TRANSPORT CALCULATION --- IN GM/CM-CM-CM-S

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL REL RATE	RINSE REL RATE	DIFFUSION REL RATE	DISSOLUTION REL RATE
21	1	1	5.26E-17	0.00E+00	3.21E-17	2.05E-17
22	1	1	5.26E-17	0.00E+00	3.21E-17	2.05E-17
41	1	1	5.26E-17	0.00E+00	3.21E-17	2.05E-17
42	1	1	5.26E-17	0.00E+00	3.21E-17	2.05E-17
61	2	1	4.85E-17	0.00E+00	2.80E-17	2.05E-17
62	2	1	4.85E-17	0.00E+00	2.80E-17	2.05E-17

CUMULATIVE RELEASE FROM THE WASTE FORM AVAILABLE FOR TRANSPORT ---- IN GRAMS

CONTAMINANT Am241	ELEMENT	CUM. REL
	21	1.32E+00

22	1.32E+00
41	1.32E+00
42	1.32E+00
61	1.72E+00
62	1.72E+00

Am241 CUMULATIVE MASS RELEASED FROM THE WASTE FORM ---- IN GRAMS

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL RELEASED	RINSE RELEASE	DIFFUSION RELEASE	DISSOLUTION RELEASE
21	1	1	1.32E+00	8.53E-01	3.39E-01	1.30E-01
22	1	1	1.32E+00	8.53E-01	3.39E-01	1.30E-01
41	1	1	1.32E+00	8.53E-01	3.39E-01	1.30E-01
42	1	1	1.32E+00	8.53E-01	3.39E-01	1.30E-01
61	2	1	1.72E+00	9.99E-01	4.98E-01	2.21E-01
62	2	1	1.72E+00	9.99E-01	4.98E-01	2.21E-01

Am241 isotope = 1

OUTPUT TABLE 28 CONCENTRATIONS (GM/CM3) AT TIME =2.730E+02 years
(DELT =1.000E+00)

*** ITIME = 273

NODE I CONCENTRATION (GM/CM3) AT NODES I,I+1,...,I+5

1	7.3999E-13	7.3999E-13	7.3999E-13	1.0806E-12	1.0806E-12	1.0806E-12
7	1.5578E-12	1.5578E-12	1.5578E-12	2.2245E-12	2.2245E-12	2.2245E-12
13	3.1535E-12	3.1535E-12	3.1535E-12	4.4446E-12	4.4446E-12	4.4446E-12
19	6.2353E-12	6.2353E-12	6.2353E-12	8.7164E-12	8.7164E-12	8.7164E-12
25	1.2154E-11	1.2154E-11	1.2154E-11	1.6922E-11	1.6922E-11	1.6922E-11
31	2.3550E-11	2.3550E-11	2.3550E-11	3.2795E-11	3.2795E-11	3.2795E-11
37	3.5043E-11	3.5043E-11	3.5043E-11	3.7592E-11	3.7592E-11	3.7592E-11
43	4.0472E-11	4.0472E-11	4.0472E-11	4.3732E-11	4.3732E-11	4.3732E-11
49	4.7445E-11	4.7445E-11	4.7445E-11	5.1731E-11	5.1731E-11	5.1731E-11
55	5.6776E-11	5.6776E-11	5.6776E-11	6.2875E-11	6.2875E-11	6.2875E-11
61	7.0478E-11	7.0478E-11	7.0478E-11	8.0272E-11	8.0272E-11	8.0272E-11
67	8.2578E-11	8.2578E-11	8.2578E-11	8.4645E-11	8.4645E-11	8.4645E-11
73	8.6472E-11	8.6472E-11	8.6472E-11	8.8090E-11	8.8090E-11	8.8090E-11
79	8.9571E-11	8.9571E-11	8.9571E-11	9.1048E-11	9.1048E-11	9.1048E-11
85	9.2734E-11	9.2734E-11	9.2734E-11	9.4952E-11	9.4952E-11	9.4952E-11
91	9.8185E-11	9.8185E-11	9.8185E-11	1.0314E-10	1.0314E-10	1.0314E-10
97	1.0098E-10	1.0098E-10	1.0098E-10	9.8452E-11	9.8452E-11	9.8452E-11
103	9.5611E-11	9.5611E-11	9.5611E-11	9.2513E-11	9.2513E-11	9.2513E-11
109	8.9220E-11	8.9220E-11	8.9220E-11	8.5796E-11	8.5796E-11	8.5796E-11
115	8.2305E-11	8.2305E-11	8.2305E-11	7.8807E-11	7.8807E-11	7.8807E-11
121	7.5358E-11	7.5358E-11	7.5358E-11	7.2005E-11	7.2005E-11	7.2005E-11
127	6.8785E-11	6.8785E-11	6.8785E-11	6.5724E-11	6.5724E-11	6.5724E-11

133	6.2835E-11	6.2835E-11	6.2835E-11	6.0122E-11	6.0122E-11	6.0122E-11
139	5.7575E-11	5.7575E-11	5.7575E-11	5.5176E-11	5.5176E-11	5.5176E-11
145	5.2902E-11	5.2902E-11	5.2902E-11	5.0723E-11	5.0723E-11	5.0723E-11
151	4.8609E-11	4.8609E-11	4.8609E-11	4.6528E-11	4.6528E-11	4.6528E-11
157	4.4453E-11	4.4453E-11	4.4453E-11	4.2362E-11	4.2362E-11	4.2362E-11
163	4.0238E-11	4.0238E-11	4.0238E-11	3.8071E-11	3.8071E-11	3.8071E-11
169	3.5858E-11	3.5858E-11	3.5858E-11	3.3603E-11	3.3603E-11	3.3603E-11
175	3.1315E-11	3.1315E-11	3.1315E-11	2.9011E-11	2.9011E-11	2.9011E-11
181	2.6709E-11	2.6709E-11	2.6709E-11	2.4430E-11	2.4430E-11	2.4430E-11
187	2.2201E-11	2.2201E-11	2.2201E-11	2.0045E-11	2.0045E-11	2.0045E-11
193	1.7992E-11	1.7992E-11	1.7992E-11	1.6071E-11	1.6071E-11	1.6071E-11
199	1.4320E-11	1.4320E-11	1.4320E-11	1.2786E-11	1.2786E-11	1.2786E-11
205	1.1537E-11	1.1537E-11	1.1537E-11	1.0674E-11	1.0674E-11	1.0674E-11
211	1.0355E-11	1.0355E-11	1.0355E-11			

SYSTEM-FLOW TABLE 29 AT TIME =2.730E+02 years , DELT =1.000E+00 ITIM = 273

TYPE OF FLOW	RATE M/T/L	INC.FLOW M/L	TOTAL FLOW M/L
1. THROUGH DIRICHLET BOUNDARY NODES	0.0000E+00	0.0000E+00	0.0000E+00
2. THROUGH CAUCHY BOUNDARY NODES	3.3859E-15	7.9799E-08	7.3381E-06
3. THROUGH NEUMANN BOUNDARY NODES	5.0329E-13	1.1902E-05	3.3334E-04
4. THROUGH SEEPAGE NODES	0.0000E+00	0.0000E+00	0.0000E+00
5. THROUGH INFILTRATION NODES	0.0000E+00	0.0000E+00	0.0000E+00
6. THROUGH UNSPECIFIED NODES (NUMERICAL) .	2.6556E-26	1.9821E-19	-3.7654E-17
7. NET FLOW THROUGH ENTIRE BOUNDARY NODES	5.0667E-13	1.1982E-05	3.4068E-04
8. INCREASE IN MATERIAL CONTENT (LIQUID) .	-5.3866E-18	-1.6999E-10	4.9808E-07
9. INCREASE IN MATERIAL CONTENT (SOLID) .	-2.5209E-14	-7.9554E-07	2.3310E-03
10. RADIOACTIVE LOSSES (LIQUID AND SOLID) .	3.4140E-12	1.0776E-04	2.1480E-02
11. LOSS TO COMP. OF SKELTON	0.0000E+00	0.0000E+00	0.0000E+00
12. LOSS THROUGH DISSOLVED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
13. LOSS THROUGH ADSORBED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
14. ARTIFICIAL SOURCES/SINKS	-1.7823E-11	-5.6246E-04	-5.6967E-01

*** NOTE: (+) = OUT FROM, (-) = INTO THE REGION.

Pu241 isotope = 2

CONTAINER BREACH

ELEMENT	CONTAINER TYPE	TIME BREACH	BREACHED AREA	CONTAINER AREA	RATIO
21	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
22	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
41	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
42	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
61	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00
62	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00

Pu241 SOURCE TERM TO THE TRANSPORT CALCULATION --- IN GM/CM-CM-CM-S

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL REL RATE	RINSE REL RATE	DIFFUSION REL RATE	DISSOLUTION REL RATE
21	1	1	1.92E-18	0.00E+00	1.15E-18	7.69E-19
22	1	1	1.92E-18	0.00E+00	1.15E-18	7.69E-19
41	1	1	1.92E-18	0.00E+00	1.15E-18	7.69E-19
42	1	1	1.92E-18	0.00E+00	1.15E-18	7.69E-19
61	2	1	1.77E-18	0.00E+00	1.00E-18	7.69E-19
62	2	1	1.77E-18	0.00E+00	1.00E-18	7.69E-19

CUMULATIVE RELEASE FROM THE WASTE FORM AVAILABLE FOR TRANSPORT ---- IN GRAMS

CONTAMINANT Pu241	ELEMENT	CUM. REL
	21	4.80E-02
	22	4.80E-02
	41	4.80E-02
	42	4.80E-02
	61	2.12E-02
	62	2.12E-02

Pu241 CUMULATIVE MASS RELEASED FROM THE WASTE FORM ---- IN GRAMS

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL RELEASED	RINSE RELEASE	DIFFUSION RELEASE	DISSOLUTION RELEASE
21	1	1	4.80E-02	3.09E-02	1.23E-02	4.87E-03
22	1	1	4.80E-02	3.09E-02	1.23E-02	4.87E-03
41	1	1	4.80E-02	3.09E-02	1.23E-02	4.87E-03
42	1	1	4.80E-02	3.09E-02	1.23E-02	4.87E-03
61	2	1	2.12E-02	0.00E+00	1.37E-02	7.49E-03
62	2	1	2.12E-02	0.00E+00	1.37E-02	7.49E-03

Pu241 isotope = 2

OUTPUT TABLE 29 CONCENTRATIONS(GM/CM3) AT TIME =2.730E+02 years
(DELT =1.000E+00)

*** ITIME = 273

NODE I CONCENTRATION (GM/CM3) AT NODES I,I+1,...,I+5

1	2.7635E-14	2.7635E-14	2.7635E-14	3.9951E-14	3.9951E-14	3.9951E-14
7	5.7276E-14	5.7276E-14	5.7276E-14	8.1526E-14	8.1526E-14	8.1526E-14
13	1.1533E-13	1.1533E-13	1.1533E-13	1.6228E-13	1.6228E-13	1.6228E-13
19	2.2734E-13	2.2734E-13	2.2734E-13	3.1731E-13	3.1731E-13	3.1731E-13
25	4.4163E-13	4.4163E-13	4.4163E-13	6.1339E-13	6.1339E-13	6.1339E-13
31	8.5078E-13	8.5078E-13	8.5078E-13	1.1791E-12	1.1791E-12	1.1791E-12
37	1.2597E-12	1.2597E-12	1.2597E-12	1.3512E-12	1.3512E-12	1.3512E-12
43	1.4547E-12	1.4547E-12	1.4547E-12	1.5719E-12	1.5719E-12	1.5719E-12
49	1.7055E-12	1.7055E-12	1.7055E-12	1.8597E-12	1.8597E-12	1.8597E-12
55	2.0413E-12	2.0413E-12	2.0413E-12	2.2603E-12	2.2603E-12	2.2603E-12
61	2.5323E-12	2.5323E-12	2.5323E-12	2.8799E-12	2.8799E-12	2.8799E-12
67	2.9623E-12	2.9623E-12	2.9623E-12	3.0363E-12	3.0363E-12	3.0363E-12
73	3.1019E-12	3.1019E-12	3.1019E-12	3.1602E-12	3.1602E-12	3.1602E-12
79	3.2138E-12	3.2138E-12	3.2138E-12	3.2675E-12	3.2675E-12	3.2675E-12
85	3.3288E-12	3.3288E-12	3.3288E-12	3.4090E-12	3.4090E-12	3.4090E-12
91	3.5247E-12	3.5247E-12	3.5247E-12	3.6996E-12	3.6996E-12	3.6996E-12
97	3.6221E-12	3.6221E-12	3.6221E-12	3.5316E-12	3.5316E-12	3.5316E-12
103	3.4298E-12	3.4298E-12	3.4298E-12	3.3189E-12	3.3189E-12	3.3189E-12
109	3.2011E-12	3.2011E-12	3.2011E-12	3.0785E-12	3.0785E-12	3.0785E-12
115	2.9536E-12	2.9536E-12	2.9536E-12	2.8284E-12	2.8284E-12	2.8284E-12
121	2.7049E-12	2.7049E-12	2.7049E-12	2.5848E-12	2.5848E-12	2.5848E-12
127	2.4693E-12	2.4693E-12	2.4693E-12	2.3596E-12	2.3596E-12	2.3596E-12
133	2.2559E-12	2.2559E-12	2.2559E-12	2.1585E-12	2.1585E-12	2.1585E-12
139	2.0670E-12	2.0670E-12	2.0670E-12	1.9808E-12	1.9808E-12	1.9808E-12
145	1.8990E-12	1.8990E-12	1.8990E-12	1.8206E-12	1.8206E-12	1.8206E-12
151	1.7445E-12	1.7445E-12	1.7445E-12	1.6697E-12	1.6697E-12	1.6697E-12
157	1.5951E-12	1.5951E-12	1.5951E-12	1.5200E-12	1.5200E-12	1.5200E-12
163	1.4437E-12	1.4437E-12	1.4437E-12	1.3659E-12	1.3659E-12	1.3659E-12
169	1.2865E-12	1.2865E-12	1.2865E-12	1.2056E-12	1.2056E-12	1.2056E-12
175	1.1237E-12	1.1237E-12	1.1237E-12	1.0411E-12	1.0411E-12	1.0411E-12
181	9.5858E-13	9.5858E-13	9.5858E-13	8.7697E-13	8.7697E-13	8.7697E-13
187	7.9710E-13	7.9710E-13	7.9710E-13	7.1992E-13	7.1992E-13	7.1992E-13
193	6.4640E-13	6.4640E-13	6.4640E-13	5.7767E-13	5.7767E-13	5.7767E-13
199	5.1504E-13	5.1504E-13	5.1504E-13	4.6025E-13	4.6025E-13	4.6025E-13
205	4.1572E-13	4.1572E-13	4.1572E-13	3.8505E-13	3.8505E-13	3.8505E-13
211	3.7372E-13	3.7372E-13	3.7372E-13			

SYSTEM-FLOW TABLE 30 AT TIME =2.730E+02 years , DELT =1.000E+00 ITIM = 273

TYPE OF FLOW	RATE M/T/L	INC.FLOW M/L	TOTAL FLOW M/L
1. THROUGH DIRICHLET BOUNDARY NODES . . .	0.0000E+00	0.0000E+00	0.0000E+00
2. THROUGH CAUCHY BOUNDARY NODES . . .	7.9866E-17	2.7634E-08	6.9813E-06
3. THROUGH NEUMANN BOUNDARY NODES . . .	1.8148E-14	4.2470E-06	3.1364E-04
4. THROUGH SEEPAGE NODES	0.0000E+00	0.0000E+00	0.0000E+00
5. THROUGH INFILTRATION NODES	0.0000E+00	0.0000E+00	0.0000E+00
6. THROUGH UNSPECIFIED NODES (NUMERICAL) .	-1.1675E-28	-2.2277E-19	-4.2389E-17
7. NET FLOW THROUGH ENTIRE BOUNDARY NODES	1.8228E-14	4.2746E-06	3.2062E-04
8. INCREASE IN MATERIAL CONTENT (LIQUID) .	9.8307E-16	3.1023E-08	7.0000E-06
9. INCREASE IN MATERIAL CONTENT (SOLID) .	4.6008E-12	1.4519E-04	3.2760E-02
10. RADIOACTIVE LOSSES (LIQUID AND SOLID) .	1.1005E-13	3.4651E-06	3.8577E-04
11. LOSS TO COMP. OF SKELTON	0.0000E+00	0.0000E+00	0.0000E+00
12. LOSS THROUGH DISSOLVED PHASE	0.0000E+00	0.0000E+00	0.0000E+00
13. LOSS THROUGH ADSORBED PHASE	0.0000E+00	0.0000E+00	0.0000E+00

14. ARTIFICIAL SOURCES/SINKS -4.5690E-11 -1.4419E-03 -2.8918E-01
 *** NOTE: (+) = OUT FROM, (-) = INTO THE REGION.

Pu240 isotope = 3

CONTAINER BREACH

ELEMENT	CONTAINER TYPE	TIME BREACH	BREACHED AREA	CONTAINER AREA	RATIO
21	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
22	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
41	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
42	1	9.90E+01	2.10E+04	2.10E+04	1.00E+00
61	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00
62	2	0.00E+00	2.10E+04	2.10E+04	1.00E+00

Pu240 SOURCE TERM TO THE TRANSPORT CALCULATION --- IN GM/CM-CM-CM-S

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL REL RATE	RINSE REL RATE	DIFFUSION REL RATE	DISSOLUTION REL RATE
21	1	1	2.64E-17	0.00E+00	1.61E-17	1.03E-17
22	1	1	2.64E-17	0.00E+00	1.61E-17	1.03E-17
41	1	1	2.64E-17	0.00E+00	1.61E-17	1.03E-17
42	1	1	2.64E-17	0.00E+00	1.61E-17	1.03E-17
61	2	1	2.44E-17	0.00E+00	1.41E-17	1.03E-17
62	2	1	2.44E-17	0.00E+00	1.41E-17	1.03E-17

CUMULATIVE RELEASE FROM THE WASTE FORM AVAILABLE FOR TRANSPORT ---- IN GRAMS

CONTAMINANT Pu240	ELEMENT	CUM. REL
	21	2.41E-01
	22	2.41E-01
	41	2.41E-01
	42	2.41E-01
	61	1.15E-01
	62	1.15E-01

Pu240 CUMULATIVE MASS RELEASED FROM THE WASTE FORM ---- IN GRAMS

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL RELEASED	RINSE RELEASE	DIFFUSION RELEASE	DISSOLUTION RELEASE
21	1	1	2.41E-01	1.14E-01	8.71E-02	3.93E-02
22	1	1	2.41E-01	1.14E-01	8.71E-02	3.93E-02
41	1	1	2.41E-01	1.14E-01	8.71E-02	3.93E-02
42	1	1	2.41E-01	1.14E-01	8.71E-02	3.93E-02
61	2	1	1.15E-01	0.00E+00	7.10E-02	4.44E-02
62	2	1	1.15E-01	0.00E+00	7.10E-02	4.44E-02

Pu240 isotope = 3

OUTPUT TABLE 30 CONCENTRATIONS (GM/CM3) AT TIME =2.730E+02 years
(DELT =1.000E+00)

*** ITIME = 273

NODE I CONCENTRATION (GM/CM3) AT NODES I, I+1, ..., I+5

1	3.7953E-13	3.7953E-13	3.7953E-13	5.5348E-13	5.5348E-13	5.5348E-13
7	7.9653E-13	7.9653E-13	7.9653E-13	1.1353E-12	1.1353E-12	1.1353E-12
13	1.6063E-12	1.6063E-12	1.6063E-12	2.2595E-12	2.2595E-12	2.2595E-12
19	3.1638E-12	3.1638E-12	3.1638E-12	4.4145E-12	4.4145E-12	4.4145E-12
25	6.1447E-12	6.1447E-12	6.1447E-12	8.5410E-12	8.5410E-12	8.5410E-12
31	1.1868E-11	1.1868E-11	1.1868E-11	1.6504E-11	1.6504E-11	1.6504E-11
37	1.7629E-11	1.7629E-11	1.7629E-11	1.8905E-11	1.8905E-11	1.8905E-11
43	2.0347E-11	2.0347E-11	2.0347E-11	2.1980E-11	2.1980E-11	2.1980E-11
49	2.3841E-11	2.3841E-11	2.3841E-11	2.5991E-11	2.5991E-11	2.5991E-11
55	2.8523E-11	2.8523E-11	2.8523E-11	3.1585E-11	3.1585E-11	3.1585E-11
61	3.5403E-11	3.5403E-11	3.5403E-11	4.0317E-11	4.0317E-11	4.0317E-11
67	4.1479E-11	4.1479E-11	4.1479E-11	4.2525E-11	4.2525E-11	4.2525E-11
73	4.3453E-11	4.3453E-11	4.3453E-11	4.4279E-11	4.4279E-11	4.4279E-11
79	4.5040E-11	4.5040E-11	4.5040E-11	4.5801E-11	4.5801E-11	4.5801E-11
85	4.6668E-11	4.6668E-11	4.6668E-11	4.7804E-11	4.7804E-11	4.7804E-11
91	4.9449E-11	4.9449E-11	4.9449E-11	5.1956E-11	5.1956E-11	5.1956E-11
97	5.0888E-11	5.0888E-11	5.0888E-11	4.9635E-11	4.9635E-11	4.9635E-11
103	4.8223E-11	4.8223E-11	4.8223E-11	4.6680E-11	4.6680E-11	4.6680E-11
109	4.5036E-11	4.5036E-11	4.5036E-11	4.3325E-11	4.3325E-11	4.3325E-11
115	4.1577E-11	4.1577E-11	4.1577E-11	3.9824E-11	3.9824E-11	3.9824E-11
121	3.8091E-11	3.8091E-11	3.8091E-11	3.6404E-11	3.6404E-11	3.6404E-11
127	3.4781E-11	3.4781E-11	3.4781E-11	3.3235E-11	3.3235E-11	3.3235E-11
133	3.1774E-11	3.1774E-11	3.1774E-11	3.0400E-11	3.0400E-11	3.0400E-11
139	2.9110E-11	2.9110E-11	2.9110E-11	2.7894E-11	2.7894E-11	2.7894E-11
145	2.6741E-11	2.6741E-11	2.6741E-11	2.5638E-11	2.5638E-11	2.5638E-11
151	2.4569E-11	2.4569E-11	2.4569E-11	2.3519E-11	2.3519E-11	2.3519E-11
157	2.2474E-11	2.2474E-11	2.2474E-11	2.1424E-11	2.1424E-11	2.1424E-11
163	2.0358E-11	2.0358E-11	2.0358E-11	1.9272E-11	1.9272E-11	1.9272E-11
169	1.8165E-11	1.8165E-11	1.8165E-11	1.7037E-11	1.7037E-11	1.7037E-11
175	1.5892E-11	1.5892E-11	1.5892E-11	1.4739E-11	1.4739E-11	1.4739E-11
181	1.3586E-11	1.3586E-11	1.3586E-11	1.2445E-11	1.2445E-11	1.2445E-11
187	1.1326E-11	1.1326E-11	1.1326E-11	1.0243E-11	1.0243E-11	1.0243E-11
193	9.2097E-12	9.2097E-12	9.2097E-12	8.2422E-12	8.2422E-12	8.2422E-12
199	7.3589E-12	7.3589E-12	7.3589E-12	6.5844E-12	6.5844E-12	6.5844E-12
205	5.9532E-12	5.9532E-12	5.9532E-12	5.5170E-12	5.5170E-12	5.5170E-12

211 5.3554E-12 5.3554E-12 5.3554E-12

APPENDIX C

LIST OF BLT-MS SUBROUTINES AND THEIR FUNCTION

<u>SUBROUTINE</u>	<u>FUNCTION</u>
GM2DXZ	General program manager. Calls input routines, initializes variables, controls the time sequence of the calculation, calls the breach, leach, and transport routines. Determines if print out is requested.
DATIN1	Reads input for Data Sets 1 - Data Set 15.
DATIN2	Reads input for Data Set 16 - Data Set 22.
BREACH	Calculates fraction of the container that has been breached.
LEACH	Calculates waste form release rates for each container and each isotope.
SUBELER	Apportions the rinse source to specific nodes based on the flow rate.
LEACHFD	Finite-difference leaching model general manager. Calculates waste form mass balances.
FDASSM	Assembles the matrix equations for the finite-difference leaching model.
FDSLTV	Solves the finite-difference leaching equations.
PARTCO	Calculates time-dependent waste form partition coefficient
DECAYIN	Calculates decay and ingrowth of progeny in the waste form.
ASEMBL	Assembles the finite element matrix equations for transport
SURF	Determines the surfaces of the modeled domain. Needed for boundary conditions.
AFABTA	Calculates the finite element weighting functions based on velocity and dispersivity terms.
FLUX	Calculates the contaminant flux at each nodal point
Q4D	Calculates terms for the global finite element matrix equation
Q4	Calculates terms for the global finite element matrix equation
Q4R	Calculates terms for evaluating contaminant flow through the system.
SHAPE	Calculates finite element shape factors
BC	Calculates boundary condition terms for the global matrix equation
Q2NB	Called by subroutine BC to modify Neumann boundary condition nodes
SOLVE	Solves the global matrix equation.
PRINTT	Controls output to the primary output file during the transient calculation.
TRACE	Controls output to the concentration and flux trace files during the transient calculation
INTERP	Interpolates between two points in a table for two dimensional arrays.
INTERP1	Interpolates between two points in a table for three dimensional arrays.
READR	Reads in a sequence of integer and real numbers and generates a one-dimensional array based on these numbers. For example, X and Z nodal locations.
READR1	Reads in a sequence of integer and real numbers and generates a two-dimensional array based on these numbers. For example, initial conditions for all contaminants.
READN	Reads in a sequence of integer values and sets up a one-dimensional array based on these numbers.
READN1	Reads in a sequence of integer values and sets up a two-dimensional array based on these numbers.
INPTR2	Reads in and stores a sequence of real numbers
INPTI	Reads in and stores a sequence of integer numbers.
RNODE	Reads in values to create automatic mesh generation.
RELEM	Generates the finite element mesh based on input values.
SHAP2	Calculates shape factors for finite-element equations when automatic mesh generation is used.

Other elements of BLT-MS

Main Program	Initializes matrix sizes and calls GM2DXZ
BLOCKDATA	Provides data for variably dimensioned arrays
Function ERFCC	Calculate complementary error function.

BIBLIOGRAPHIC DATA SHEET

(See instructions on the reverse)

1. REPORT NUMBER
(Assigned by NRC, Add Vol., Supp., Rev.,
and Addendum Numbers, if any.)NUREG/CR-6492
BNL-NUREG-52509

2. TITLE AND SUBTITLE

BLT-MS (Breach, Leach, and Transport-Multiple Species) Data Input Guide: A Computer
Model for Simulating Release of Contaminant from Subsurface Low-Level Waste Disposal
Facility

3. DATE REPORT PUBLISHED

MONTH

YEAR

November

1996

4. FIN OR GRANT NUMBER

A-3276

5. AUTHOR(S)

T. M. Sullivan, R. J. MacKinnon, R. R. Kinsey, A. Aronson, M. Divadeenam

6. TYPE OF REPORT

Technical

7. PERIOD COVERED (Inclusive Dates)

8. PERFORMING ORGANIZATION - NAME AND ADDRESS (If NRC, provide Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address; if contractor, provide name and mailing address.)

Brookhaven National Laboratory
P.O. Box 5000
Upton, New York 11973Ecodynamics Research Associates, Inc.
P.O. Box 9229
Albuquerque, New Mexico 87103

9. SPONSORING ORGANIZATION - NAME AND ADDRESS (If NRC, type "Same as above"; if contractor, provide NRC Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address.)

U.S. Nuclear Regulatory Commission
Office of Research
Washington, DC 20555

10. SUPPLEMENTARY NOTES

R. Cady, NRC Project Manager

11. ABSTRACT (200 words or less)

The BLT-MS computer code has been developed, implemented, and tested. BLT-MS is a two-dimensional finite element computer code capable of simulating the time evolution of concentration resulting from the time-dependent release and transport of aqueous phase species in a subsurface soil system. BLT-MS contains models to simulate the processes (water flow, container degradation, waste form performance, transport, and radioactive production and decay) most relevant to estimating the release and transport of contaminants from a subsurface disposal system. Water flow is simulated through tabular input or auxiliary files. Container degradation considers localized failure due to pitting corrosion and general failure due to uniform surface degradation processes. Waste form performance considers release to be limited by one of our mechanism: rinse with partitioning, diffusion, uniform surface degradation, or solubility. Radioactive production and decay in the waste form are simulated. Transport considers the processes of advection, dispersion, diffusion, radioactive production and decay, reversible linear sorption, and sources (waste forms releases). To improve the usefulness of BLT-MS a pre-processor, BLTMSIN, which assists in the creation of input files, and a post-processor, BLTPLOT, which provides a visual display of the data have been developed. This document reviews the models implemented in BLT-MS and serves as a guide to creating input files for BLT-MS.

12. KEY WORDS/DESCRIPTORS (List words or phrases that will assist researchers in locating the report.)

Computerized Simulation - Underground Disposal, Radioactive Waste Disposal - Computer Codes,
Radioactive Waste Disposal - Underground Disposal, B Codes, BNL, Containers, Contamination,
Fission Product Release, Finite Element Method, Flow Models, Isotope Production, Nuclear Decay,
Radioactive Waste Facilities, Radionuclide Migration, Simulation, Transport

13. AVAILABILITY STATEMENT

Unclassified

14. SECURITY CLASSIFICATION

(This Page)

Unclassified

(This Report)

Unclassified

15. NUMBER OF PAGES

170

16. PRICE