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BLT-EC (Breach, Leach and Transport-Equilibrium Chemistry) Data Input Guide

A Computer Model for Simulating Release and Coupled Geochemical Transport of Contaminants from a Subsurface Disposal Facility

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ABSTRACT

The BLT-EC computer code has been developed, implemented, and tested. BLT-EC is a two-dimensional finite element computer code capable of simulating the time-dependent release and reactive transport of aqueous phase species in a subsurface soil system. BLT-EC contains models to simulate the processes (container degradation, waste-form performance, transport, chemical reactions, and radioactive production and decay) most relevant to estimating the release and transport of contaminants from a subsurface disposal system. Water flow is provided 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, and solubility. Transport considers the processes of advection, dispersion, diffusion, chemical reaction, radioactive production and decay, and sources (waste form releases). Chemical reactions accounted for include complexation, sorption, dissolution-precipitation, oxidation-reduction, and ion exchange. Radioactive production and decay in the waste form is simulated. To improve the usefulness of BLT-EC, a pre-processor, ECIN, which assists in the creation of chemistry input files, and a post-processor, BLTPLOT, which provides a visual display of the data have been developed. BLT-EC also includes an extensive database of thermodynamic data that is also accessible to ECIN. This document reviews the models implemented in BLT-EC and serves as a guide to creating input files and applying BLT-EC.

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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 simulate container performance, waste-form performance, and advective-dispersive transport in a 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, ^{3}H, ^{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) [Sullivan et al, 1996]. To address geochemical interactions, BLT-EC (Breach, Leach, and Transport - Equilibrium Chemistry) has also been developed [MacKinnon et al, 1995].

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

- Container degradation models; BLT-EC 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-EC permits simulation of multiple sets (currently dimensioned as 20) of container failure parameters. This feature permits an easy method to simulate the different failure times expected from the different containers.

- Waste-form leaching models; BLT-EC 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-EC 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.

- A transport model that considers advection, dispersion, diffusion, radioactive decay and production, chemical reactions, waste-form sources, and external sources and sinks.

- An equilibrium chemistry model that simulates complexation, sorption, dissolution-precipitation, ion-exchange, and oxidation-reduction.

- Simulation of up to 25 radionuclides and chemical components, 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.
- Seven sorption models including 1) the activity K_d model, 2) the activity Langmuir model, 3) the activity Freundlich model, 4) the ion-exchange model, 5) the constant capacitance model, 6) the triple-layer model, and 7) the diffuse-layer model.
- An input processor to assist the user in defining system chemistry.
- A thermodynamic database that is accessed automatically during simulation.

BLT-EC, 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:

- improved treatment of how the sources are placed 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 reactive transport in porous media.
- the results of a number of verification studies that demonstrate BLT-EC is capable of accurately predicting transport with chemical reaction, chain decay, and ingrowth of progeny in the waste form prior to release.
- a detailed discussion of input requirements and formatting requirements.
- an overview on how to use ECIN, a menu-driven pre-processor that is useful in creating chemistry input files used by BLT-EC.
- a discussion of the output files generated by BLT-EC.
- 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-EC.
- an overview of chemical concepts, adsorption models, and the thermodynamic database.

FOREWORD

This technical report was prepared by Brookhaven National Laboratory as part of a research project with the Waste Management Branch of the Office of Nuclear Regulatory Research (FIN A3276). This report documents the background and requirements for use of one of the research computer codes developed under this project.

NUREC/CR-6515 is not a substitute for NRC position papers or regulations, and compliance is not required. The results, approaches, and methods described in this NUREG are provided for information only. Publication of this report does not necessarily constitute NRC approval or agreement with the information contained herein.

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]. This regulation specifies license requirements and performance objectives for low-level radioactive waste (LLW) disposal facilities with the goal of protecting public health and safety and the environment. In particular, 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 potential releases do not 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." A LLW performance assessment is an essential component of the licensing process to provide reasonable assurance that these performance objectives will be met.

A LLW performance assessment integrates all of the processes and events that influence the potential for human exposure to radioactivity disposed in a LLW facility. A key component of a performance assessment is the source term. The source term is defined as the radionuclide release rate from a disposal facility. In general, release can occur in both gaseous and aqueous (ground water) phases. Often, there is confusion over the definitions of inventory and source term. Inventory is the mass of each contaminant disposed and is one component of the source term. The source term refers to a more general concept that includes the inventory as well as the physical and chemical processes that influence release and transport of contaminants out of a facility.

In this report, attention is focused on radionuclide releases to ground water. Releases to ground water from a disposal facility are controlled by water infiltrating into the facility, access of water to the waste forms, release of radionuclides to the contacting water, and subsequent migration of radionuclides out of the facility. 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.

The BLT-EC (Breach, Leach, Transport - Equilibrium Chemistry) code has been developed to simulate the major processes that control release to the ground water from LLW disposal facilities. This code can simulate container degradation, waste-form leaching, geochemical processes, radioactive production and decay in the waste form as well as during transport, and contaminant migration in unsaturated or saturated porous media. In addition, BLT-EC allows the user to specify releases of iron, calcium hydroxide, or other materials to infiltrating water resulting from the degradation of metal containers and concrete engineered barriers.

BLT-EC combines portions of three existing computer codes, BLT [Sullivan and Suen, 1989], HYDROGEOCHEM [Yeh and Tripathi, 1989], and MINTEQA2 [Allison et al., 1991]. The container and waste-form performance models (Breach and Leach) from BLT are improved and used in BLT-EC to estimate the time at which release begins and the rate of release of contaminants from waste forms. The transport model in BLT-EC is based on a modified version of the hydrologic transport module contained in the finite-element code HYDROGEOCHEM. The geochemical model used to solve the chemical equilibrium reaction equations in BLT-EC is a modified version of the geochemical computer code MINTEQA2. The fact that this geochemical computer code has a large user community was an important factor in the selection of this code for BLT-EC. In addition, the code's extensive thermodynamic data base is continually being expanded for applications in waste management. Also provided with BLT-EC is the preprocessor ECIN, an interactive program designed to help the BLT-EC user create BLT-EC's chemistry input file. Water flow is handled through tabular input, or auxiliary files created by hydrological codes. BLT-EC 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.

1.2 An Overview of BLT-EC

An objective in developing the BLT-EC 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 primary output from BLT-EC is the time evolution of contaminant concentrations resulting from the time-dependent release and transport of aqueous phase species out of a disposal facility. This information is used as input to other codes with the ultimate objective of obtaining an estimate of the dose that could potentially occur due to waste disposal. An overview of the processes considered in BLT-EC is presented in Table 1.1. BLT-EC has the following features:

- Container degradation models. BLT-EC 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-EC permits simulation of multiple sets (currently dimensioned as 20) of container failure parameters. This feature permits an easy method to simulate the different failure times expected from the different containers.

- Waste-form leaching models. BLT-EC 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-EC 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.

- Water-flow rates and moisture contents, which influence container degradation, waste-form leaching, and transport are input variables.

- A transport model that considers advection, dispersion, diffusion, radioactive decay and production, chemical reactions, waste-form sources, and external sources and sinks.

- An equilibrium chemistry model that simulates complexation, sorption, dissolution-precipitation, ion-exchange, and oxidation-reduction.

- Simulation of up to 25 radionuclides and chemical components, 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.

- Seven sorption models including 1) the activity K_d model, 2) the activity Langmuir model, 3) the activity Freundlich model, 4) the ion exchange model, 5) the constant capacitance model, 6) the triple-layer model, and 7) the diffuse-layer model

- An input processor to assist the user in defining system chemistry.

- A thermodynamic database that is accessed automatically during simulation.

Each of these features are discussed in detail in this report.

Table 1.1 Overview of Process Models Considered in BLT-MS

	CONTAINER DEGRADATION
Model:	Local failure (partial failure) General failure (time to failure)
	Output:Fraction of the container that is breached as function of time
	WASTE-FORM RELEASES
Model:	Rinse release subject to partitioning Diffusion controlled release Uniform degradation release Solubility limited release Chain decay
Output:	Waste-form mass release rate per unit volume for the transport equation.
	TRANSPORT
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 sources)
Output:	Time evolution of concentration at each spatial location in the modeled domain
	CHEMISTRY
Model:	Simultaneous solution of nonlinear mass action and linear mass balance equations to represent complexation, dissolution-precipitation, sorption, ion-exchange, and oxidation-reduction reactions
Output:	Total component concentrations in aqueous, sorbed, and solid phase, speciation of chemical components, and pH and Eh conditions

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

- water-flow rates and moisture contents are updated based on input, if necessary.
- container performance is calculated.
- radioactive production and decay in each waste form is calculated.
- if container failure has occurred, waste-form release rates are calculated for each contaminant in each container.
- the transport of each contaminant is calculated over the time step.
- chemical reactions controlling solubility and sorption during transport are calculated.

BLT-EC, in addition to the capability of simulating multiple-species transport with chemical reactions, has a number of other improvements over its predecessor, BLT. These include:

- improved treatment of how sources are placed into the transport equation,
- improved treatment of the rinse release model with partitioning, and
- improved treatment of the uniform degradation model,
- 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 Code Structure

The modular structure of the complete BLT-EC code package is illustrated in Figure 1.1. This package consists of six modules: (1) an optional preprocessor, ECIN, that assists the user in preparing chemical input data; (2) the BLT module that simulates radionuclide release and migration; (3) the EC module that simulates the chemical reactions; (4) the hydrogeologic data module that transfers data from FEMWATER's finite-element mesh to BLT-EC's finite-element mesh for use by the BLT module; (5) the thermodynamic data base that provides the EC module with the pertinent reactions and data; (6) the postprocessing module BLTPLOT that provides graphical displays of output.

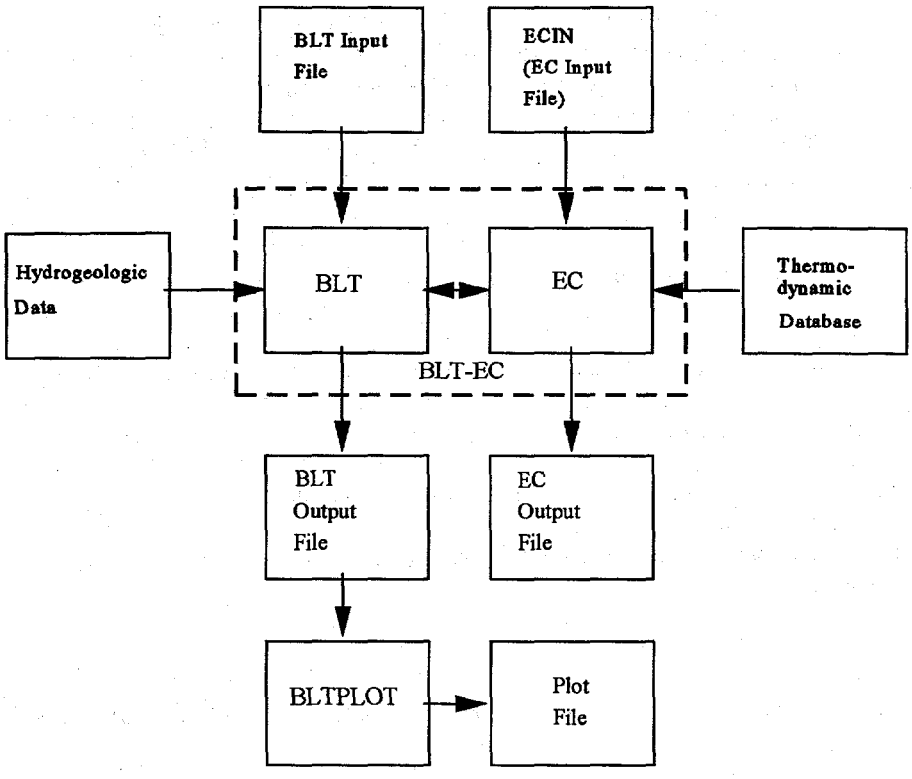


Figure 1.1 Top-Level Flow Chart of the BLT-EC Code

1.4 User Requirements

To effectively apply BLT-EC 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 are summarized in section 2 of this report and are described in detail in a companion report [MacKinnon, et al. 1995]. In addition, a basic understanding of finite-element methods is also needed. A number of references on the finite-element method exist [Finlayson, 1980; Carey and Oden, 1986] and implementation of the finite-element methods in the FEMWATER code is discussed in [Yeh, 1987].

Misuse of computer codes occurs frequently. The chances of misapplication of the code can be minimized by acquiring basic experience with BLT-EC prior to application on a field-scale problem. Basic experience can be gained through the application of test problems supplied with the code and examination of the output generated by the code.

1.5 Computer Requirements

BLT-EC and ECIN are written in standard FORTRAN 77 and can be compiled on most personal computer (PC) and work station systems with only minor alterations (i.e., changes in OPEN statements, etc.). The majority of development and testing of BLT-EC and ECIN 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-EC requires, as a minimum, a 486-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-EC. Much smaller configurations can be obtained by redimensioning the arrays in BLT-EC. ECIN requires 1 MB of memory.

1.6 Report Outline

The objective of this document is to provide the necessary information to understand and apply the BLT-EC code to problems in subsurface waste disposal. Section 2 provides the theory, governing equations, and numerical approximations 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, contaminant transport, chemical reactions, and finite-element approximations to the governing equations. 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-EC is capable of accurately predicting reactive transport with chain decay, and ingrowth of progeny in the waste form prior to release. Section 5 provides an input guide for BLT-EC's main input file which defines material properties, problem geometry, chemical components, waste forms, inventory, and initial and boundary conditions. Section 6 provides an overview on how to use ECIN, a preprocessor that creates BLT-EC's chemistry input file. The chemistry input file defines the chemical reactions and conditions that are to be included in an analysis. Section 7 discusses the output files generated by BLT-EC. In addition to the main output file, a number of auxiliary output files containing information on waste-form releases, waste-form mass balances, and detailed chemical conditions at 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-EC. Section 9 provides a summary and conclusion of the material contained in this report. Finally, appendices A, B, C, D, and E provide descriptions of program routines and arrays, output files, chemical and mathematical concepts, the thermodynamic database, and adsorption models, respectively.

2 MATHEMATICAL MODEL DESCRIPTION OF BLT-EC

2.1 Overview of Important Processes Controlling Release

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 with chemical reactions. This section of the report describes the conceptual models, major assumptions, and governing equations used to represent these processes.

A flow diagram of the major processes and events is presented in Figure 2.1. In this diagram, the centrally located components (inventory, container performance, waste-form performance, and transport) represent the primary factors that directly determine the release of contaminants. The secondary factors, represented by infiltration and chemistry, influence the primary factors and their control on release. Arrows leading from one factor to another denote coupling between the factors. Arrows that point in both directions indicate that each factor can influence the other. The dashed arrow signifies a weak coupling between infiltration and container performance. Each of the factors, and the influence they exert on the release of radionuclides, are briefly summarized in the following paragraphs.

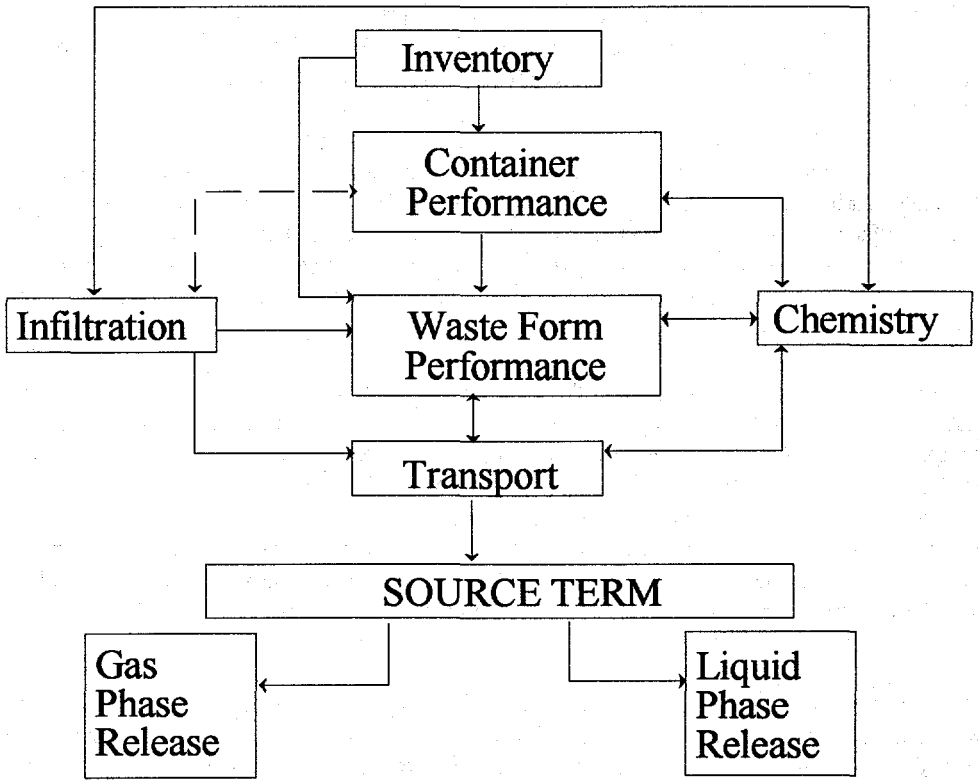


Figure 2.1 Major Processes Involved in BLT-EC Simulations of Release and Transport

The inventory represents the mass of radioactive contaminants in the system upon disposal. Ideally, the distribution of the inventory by waste container and waste form is known and this information is used in estimating releases from the

waste form. The use of this information is represented by the arrows leading from the inventory to the waste form and container performance sections, as shown in Figure 2.1. In general, the chemical form of the inventory can influence container performance through interactions that cause degradation of the container. Typically, chemical interactions between inventory and containers are not considered explicitly in source-term modeling. The physical and chemical forms of the inventory, however, directly impact waste-form performance.

Accurate representation of the source term requires knowledge of the inventory in terms of its physical and chemical form, its incorporation into specific waste forms, and its disposal in specific containers. Close to 300 different radionuclides have been disposed in LLW disposal sites. The vast majority of these do not significantly contribute to predicted dose. Almost all of the disposed activity is found in relatively short-lived (e.g., half life < 30.1 years) radionuclides including Cs-137, Co-60, Sr-90, H-3, Fe-55. These radionuclides are generally precluded from serious concern in terms of predicted dose because of their short half-lives, waste container and waste-form performance, and long travel times to the accessible environment. The major contributors to predicted dose tend to be long-lived, soluble, mobile, radionuclides. These radionuclides include I-129, Tc-99, C-14, Cl-36, and, under the proper chemical conditions, uranium isotopes and their daughter products.

Container performance is measured in terms of the ability of the container to control the access of air and water to the waste form. While the container is intact, it will provide a barrier to prevent contact of wastes with aqueous fluids. Failed containers permit communication between aqueous fluids and waste forms and this communication is represented schematically in Figure 2.1 by the arrow pointing from container performance to waste-form performance. Container performance can be influenced by chemistry and, to a lesser extent, infiltration. Electrochemical reactions are the primary means by which containers degrade, e.g., corrosion. As containers degrade, reactions can alter the local chemical environment in the disposal facility, in particular the redox and pH conditions. Although container performance is typically assumed to be independent of infiltration rate, subsidence of containers and wastes can influence the infiltration rate into the waste containing region.

LLW containers span a wide variety of sizes, shapes, and materials of construction. The majority of LLW containers are 55 gallon carbon steel drums. More active wastes, Class B and C wastes, are often disposed in high integrity containers (HICs). Material used to construct HICs include stainless steels, Ferallium, and high-density polyethylene (HDPE). To simplify the task of modeling container performance, assumptions are typically made which permit containers to be grouped into a few different categories. Within each category of container, the performance of each individual container is assumed to be identical.

The waste as generated is called a waste stream. A waste stream may be placed untreated into the container, or it may be treated with sorbents or solidification agents, compacted or incinerated to reduce volume, de-watered, or surrounded with backfill to minimize void space in the container. A waste form is defined as the final physical form of the contaminated material as placed in the waste container. Waste-form performance is measured in terms of the ability of the waste form to control release of the radionuclides to the contacting fluids. Release to contacting fluids is denoted in Figure 2.1 by the arrow pointing from waste-form performance to transport. Waste-form performance can depend on the initial physical and chemical form of the inventory, time of container failure, the local chemical environment, infiltrating water flow rate, and transport away from the waste form. Release of contaminants and other waste form constituents may also alter the local chemical environment.

A review of the compilation of data from commercial shipping manifests [Roles, 1990] indicate there are 19 categories of waste forms. Evaluating the release from different waste forms on an individual basis is impractical. Therefore, as with containers, assumptions are made to group waste forms into a few different categories. Examination of inventory data indicate that over 95% of the total activity [Cowgill and Sullivan, 1993] is contained in the following waste form groups: activated metals, cement solidified wastes, dry solids, de-watered resins, evaporator bottoms, filter sludges, and solid noncombustibles. The grouping of wastes assumes that all different waste forms within a group have the same release mechanism, although the release rates could be different.

Release from the waste form provides a source of contaminants for transport out of the disposal facility. The processes that influence transport of contaminants include advection, diffusion, dispersion, solubility, sorption, and

radioactive decay. Advection caused by infiltrating water is often the dominant transport mechanism. As radionuclides migrate away from their release point, they may encounter progressive changes in chemical conditions (e.g., pH, Eh, mineralogical constituents) and experience changes in their chemical form. These changes, if significant, may produce substantial alterations in solubilities and sorption capacities of the contaminants and ultimately their transport rates. Transport of materials released from facility components (e.g., engineered barriers, containers, and waste forms) due to chemical reactions may also alter the chemical environment.

Infiltration is the rate of water flow into the disposal facility. Infiltration into a facility is controlled by the rate and duration of precipitation at the surface, and the hydraulic properties of the cover and engineered barriers. Water that enters the top soil layer ultimately becomes separated into four fractions: (1) water that remains in storage in the soil pores; (2) water that returns to the atmosphere due to evapotranspiration; (3) water that is diverted laterally by the cover; and (4) water that percolates downward. If the duration and application of precipitation at the surface are sufficiently large, a wetting front will penetrate deep into the waste containing region. Once the application of precipitation stops, water infiltration in near-surface materials will cease, while the deeper penetrating water will continue to redistribute as it flows downward through the facility. In general, flow through shallow-land disposal facilities is three-dimensional and nonuniform due to obstructions to flow and localized effects such as cracking of engineered barriers. In performance assessment, the source region is typically treated as containing a steady and spatially uniform flow field.

The time frame for performance assessments (thousands of years) often leads to the assumption of steady-state flow. The justification for this assumption is that seasonal fluctuations will not be important, in the long term, as compared to the long-term average [Kozak et al., 1989]. Numerical studies have shown this to be true for non-reactive transport in a spatially uniform flow field [Duguid and Reeves, 1977; Weirenga, 1977]. However, sorption processes often exhibit hysteresis and transitory effects can influence long-term transport in a non-linear manner [Jones and Watson, 1990]. In addition, use of time-dependent flow rates may be required if there are localized effects that favor movement of contaminants over large distances in short periods of time due to episodic flow events. In a disposal vault, this could occur through channels that may form due to improper placement of backfill or subsidence of the wastes.

The secondary factor denoted as chemistry consists of all chemical reactions, including microbially facilitated reactions, that can alter the mobility of radionuclides. Chemical controls on transport involve solubility limits and sorption reactions. Solubility limits may restrict the amount of contaminant in solution. Excess amounts form an immobile precipitate. Chemical reactions may be reversible, or irreversible. Chemical reactions such as surface adsorption and ion exchange act to reduce solution concentrations and delay or retard the movement of radionuclides. Complexation of radionuclides with ligands and chelating agents can enhance the mobility of radionuclides by increasing their solubility and reducing their tendency to adsorb. In addition to solution reactions, colloidal particles may form. Colloids are naturally occurring suspended particles with diameters less than ten microns. Colloids have different transport properties than aqueous solution species and can serve as an important mechanism for increasing the mobility of radionuclides.

In LLW shallow land disposal facilities, the dependence of water flow parameters, such as hydraulic conductivity, on container degradation and waste form leaching should be small. Therefore, water flow is assumed to be independent of all other processes. All other processes, however, are coupled to water flow. Container degradation (breach) modeling involves the prediction of pitting and general corrosion rates. These processes are, in general, functions of the moisture content, pH, and redox conditions in the backfill adjacent to the containers. Waste-form release (leach) modeling requires information from all four other process models. This information includes the breached area as a function of time from the container degradation model; the concentration of contaminants in solution adjacent to the waste form from the transport-chemical process models; and the inlet and outlet flow rates and moisture content from the water flow model. Chemical process modeling requires, besides thermodynamic data, concentrations of all chemical components in the system; these are provided by the transport model. Transport modeling requires the release rate from the leaching models, and the water flux and moisture content distribution in the soil.

Before proceeding with the mathematical model description, a brief description of the finite-element approach is provided in the next section. This description is necessary to provide the framework for model calculations in BLT-EC.

2.2 Overview of the Finite-Element Approach to Modeling a LLW Disposal Facility

A general approach to modeling a low-level waste disposal facility begins with a definition of a conceptual model of the system and its behavior. 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.) are also defined. Based on this information, assumptions are typically made to simplify the system into a form amenable for numerical simulation. For BLT-EC, these assumptions will likely 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 collection of subregions called finite elements. An example of a finite-element grid is presented in Figure 2.2. The modeled region shown is subdivided into a number of quadrilateral regions. The size of the finite elements are selected to provide the desired level of numerical spatial accuracy in the solution. As the finite element size becomes larger, numerical dispersion can significantly degrade solution accuracy. The corner points of finite elements are called node points and each element has four node points and four quadrature or Gauss integration points. Concentrations are calculated in BLT-EC at the node points.

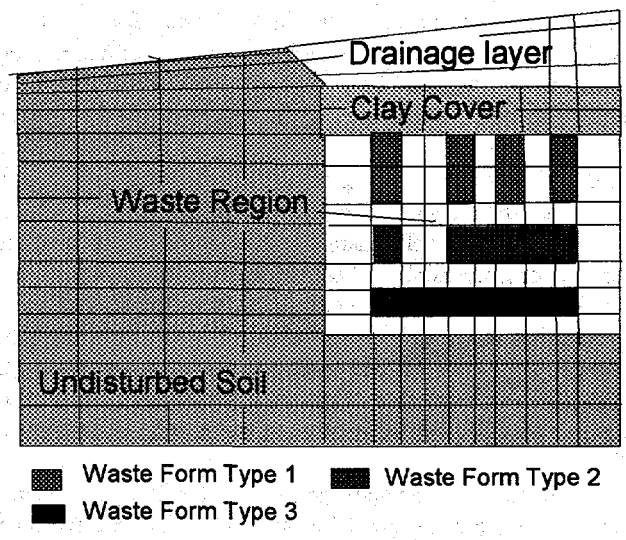


Figure 2.2 Example of a Finite-Element Grid Representation of the Model Domain

The finite-element grid represents the transport domain of the BLT-EC calculation. Waste forms are associated with an element, and mass released from a 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 described in section 2.8. However, waste-form processes are assumed to be independent of 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-release model (section 2.5.1).

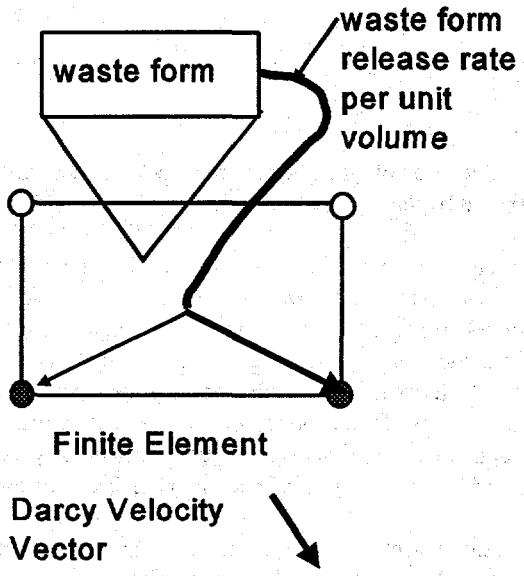


Figure 2.3 Graphical Display of Waste Form Release to Specific Nodes in a Finite Element Based on the Darcy Flux Vector

2.3 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 being analyzed. BLT-EC can accept these moisture and flow rate values from two sources: 1) they can be specified as part of the input file or b) be automatically read from an auxiliary file. The auxiliary file contains a series of velocities and moisture contents to represent the time evolution of the quantities at finite-element quadrature points.

The foundation for modeling ground-water 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 ground-water 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 is proportional to the hydraulic gradient and the cross-sectional area.

$$V_d = -K \nabla H \qquad \textbf{(2.1)}$$

where V_d is the Darcy flux (cm/s), K is the hydraulic conductivity (cm/s), and H is the total head (cm) which is the sum of the gravitational head and the pressure head. The mass balance equation obtained using Darcy's law to specify the flux is:

$$S \frac{\partial H}{\partial t} = \nabla \cdot K \cdot \nabla H \qquad \textbf{(2.2)}$$

where S is the storativity, the additional volume of water stored in the porous medium, per unit rise of hydraulic head, per unit volume of porous medium multiplied by the aquifer thickness.

Equation 2.2 is the fundamental equation for ground-water 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. As a consequence, the solution of Eqn. 2.2 is 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 certain regions of the conductivity versus head curves, 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 total head in the modeled domain. The calculated total 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 it 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.

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

Similar to hydraulic conductivity, the moisture content is a non-linear function of suction head. Knowledge of the head permits an estimation of the moisture content in the vadose zone. In the saturated zone, the moisture content is equal to 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 and concrete engineered barriers with markedly different hydrologic properties.

To overcome 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 above the watertable. With this assumption, the Darcy flux can be obtained by estimating the hydraulic conductivity. As an upper bound to flow, the flow velocity is limited in magnitude 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 that this approach leads to conservative release rates, particularly when production of progeny is a concern.

BLT-EC uses a two-dimensional finite-element representation of the subsurface system to simulate transport. The flow velocities must be provided at the nodal points that are simulated. BLT-EC is currently structured to accept flow velocity input from an auxiliary file created by the computer code FEMWATER, Version 1 [Yeh, 1987]. The interface between FEMWATER and BLT-EC is identical to that between FEMWATER and BLT. A detailed description on how to

create FEMWATER input decks 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 robust 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-EC. This can be overcome by either writing a post-processor for the FEMWATER version 2 output file, or by altering the statements in BLT-EC 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-EC.

Time-dependent flow rates can be simulated in BLT-EC through the auxiliary file created by FEMWATER. The auxiliary file can have several sets of flow velocities at various times. BLT-EC 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.

2.4 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 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 approximated through the BREACH models in the code. BLT-EC has two general categories of container degradation models: (1) general degradation models in which the container fails completely, exposing the entire waste form to water at the time of failure; and (2) local degradation models which permit only a fraction of the container to fail and thereby expose only 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 this data has been included in [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, 1992] with the conclusion that the data available to predict the long-term behavior of high density polyethylene has 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 container lifetime, it is often 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.

2.4.1 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:

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

where d is the degradation allowance thickness (cm) and g is 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. This value is often taken to be the container thickness minus a small fraction of the thickness. This small fraction of thickness accounts for mechanical failure when the container gets too thin to support the overburden.

To simulate failure at the start of the calculation, set g 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.

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

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

2.4.2 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-EC is structured to evaluate pitting corrosion of metallic containers. The data base used to generate the empirical parameters are 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 is 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-EC are not appropriate for modeling crack formation in 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

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

$$A_b = 0, \qquad h_d \le 0$$

In BLT-EC, 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 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:

$$h = k\, t^n \left[\frac{A}{372}\right]^a \qquad (2.6)$$

where k is the empirical pitting parameter cm/yr^n, t is the corrosion time in years, A is the surface area of the container in cm^2, the constant 372 cm^2 is a scaling factor and represents the size of the samples in Romanoff's study, and a is an experimentally derived empirical correlation coefficient. All of the parameters necessary for calculating the maximum pit depth can be input directly in BLT-EC, or the code will calculate values based on the following expressions.

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

$k = 0.01458\,(10 - pH)$ pH < 6.8

$k = 0.0457$ $6.8 <$ pH < 7.3

$k = 0.0256(pH - 5.13)$ 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. This pH value provides the minimum value of the pitting parameter; pH 7 is the mean value in the studies of Romanoff [Romanoff, 1957]. In the present version of BLT-EC, the pH value used for calculating the pitting parameter is a constant and must be provided by the code user in the BLT-EC input file. In theory, this pH value could be computed by BLT-EC and provided for the pitting parameter calculation.

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 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 course 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 n value 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:

$$n = n_o\, \theta\, (1 - CL)^{0.4} \qquad (2.7)$$

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

Values for the exponent "a" 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.

2.5 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-EC 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 in 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, and ion-exchange resins. 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, 1990].

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 assumed to release contaminants by dissolution of the metal and glass 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-EC. BLT-EC 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 easier to understand, but it does not always account for different interactions between release mechanisms. The second approach represents the waste form release processes numerically using a finite-difference method. 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 between the masses available for each release process. In BLT-EC, user-specified 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 sections 2.5.4.1 (partial container failure) and 2.5.6 (solubility limited release).

It is important for the analyst to realize that within the finite-element framework, the waste-form sources act to inject 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. Numerical treatment of waste forms will be discussed in section 2.8 in more detail.

2.5.1 Rinse Release with Partitioning

The conceptual model represented by the rinse-release model assumes 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 approach 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 under predict 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-EC, 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 of component k in the system is:

$$M_{kt} = M_{kwf} + M_{ka} + M_{ks} \tag{2.8}$$

where, for component k, M_{kt} is the total mass (moles) in the system (i.e., finite element), M_{kwf} is the mass on the waste form, M_{ka} is the mass in aqueous solution, and M_{ks} is the mass sorbed on the porous media. The latter two quantities are given by the following expressions:

$$M_{ka}(t) = \theta(t)\ V_e\ C_{ka}(t) \tag{2.9}$$

$$M_{ks}(t) = \rho\ S_{ks}(t)\ V_e \tag{2.10}$$

where θ is the volumetric moisture content in the system, V_e (cm^3) is the volume of the porous media and aqueous solution system, t is the time (s), C_{ka} is the concentration of component k in the aqueous solution (mole/cm^3), ρ (g/cm^3) is the bulk density of the porous media, and S_{ks} is the mass of component k adsorbed on the solid per unit mass of the solid (mole/g).

The mass contained in the waste form, M_{wfk}, 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:

$$M_{kwf}(t) = \rho_{wf}\ S_{kwf}(t)\ V_{wf} \tag{2.11}$$

where the subscript wf refers to the waste form. Notice that 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:

$$S_{kp}(t) = K_{dk} C_{ka}(t) \tag{2.12}$$

and

$$S_{kwf}(t) = K_{pk} C_{ka}(t) \tag{2.13}$$

where, for component k, K_{dk} (cm^3/g) is the soil-solution distribution coefficient and K_{pk} (cm^3/g) is the waste form-solution partition coefficient. 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.

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

$$M_{ka}(t)\, R_k + M_{kwf}(t) = M_{ka}(t+\Delta t)\, R_k' \tag{2.14}$$

where R_k is the retardation coefficient ($R_k = 1 + \rho K_k/\theta$). R_k' is the three component (soil, porous media, waste form) retardation coefficient and is given by:

$$R_k' = 1 + \frac{\rho K_{dk}}{\theta} + \frac{\rho_{wf} V_{wf} K_{kp}}{\theta V_e} \tag{2.15}$$

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

Solving Eqn. 2.1.4 for the mass in solution at time t + Δt yields:

$$M_{ka}(t+\Delta t) = \frac{M_{ka}(t)\, R_k + M_{kwf}(t)}{R_k'} \tag{2.16}$$

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

$$\Delta M_k = M_{kwf}(t) - \rho_{wf} V_{wf} K_{pk} C_{ka}(t+\Delta t) \tag{2.17}$$

The estimate for the concentration can be obtained from Eqns. 2.9 and 2.16. To ease the input burden in BLT-EC, 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:

$$\Delta M_k = \frac{R_k \left[M_{kwf}(t) - \frac{\rho_{wf} V_{ratio}}{\theta} K_{kp} M_{ka}(t) \right]}{R_k'} \qquad (2.18)$$

BLT-EC requires the mass release per unit time per unit volume, s_{wk}, as the source to the transport equation. This source is:

$$s_{wk} = \frac{\Delta M_k}{V_e \Delta t} \qquad (2.19)$$

where ΔM_k is determined from Eqn. 2.18.

Examining Eqn 2.18 the following limiting behavior can be determined. In the case of no partitioning ($K_{kp} = 0$), the entire inventory of component k is released over the first time step. In the other extreme, as the partition coefficient becomes large, the amount sorbed can become negative. That is, the waste form will act as a sink to adsorb 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_k' is approximately twice the value for R_k and the mass released at the first time step ($C_{ka}(0) = 0$) is about ½ of the total inventory. The model in BLT [Sullivan and Suen, 1989], 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 ½. 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 behavior 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 large release 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_k'. This approach has the advantage of being an implicit approach. The fact that release can be recast into a form that modifies the transport equation by R_k' 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 ensure that sorption is not excessively represented. This can be done by appropriate choice of the retardation parameters (ρ, K_{kp}, K_{kp}, V, and V_{ratio}).

2.5.1.1 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-EC through the use of an exponentially decaying value for the partition coefficient. The expression is:

$$K_{kp}(t) = K_{kp}(0)\ e^{-\lambda_{kp}t} + K_{kp}(\infty)\ (1 - e^{-\lambda_{kp}t}) \qquad (2.20)$$

where, for component k, $K_{kp}(0)$ is the initial value for the partition coefficient, $K_{kp}(\infty)$ is the value for the partition coefficient as time approaches infinity , and λ_{kp} is the partition decay coefficient. Input for BLT-EC requests $K_{kp}(0)$, $K_{kp}(\infty)$, and λ_{kp}.

Often, reliable parameters for the degradation rate constant and the final value for the partition coefficient are not available. If these are unavailable, input the degradation rate as zero and the partition coefficient will be maintained at its initial value at all times.

2.5.2 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 dominant process. Under these conditions, analytical solutions for release rates from waste forms can be obtained for a variety of geometries. However, exact analytical methods for treating ingrowth of progeny are unavailable. BLT-EC uses an approximate method. It is strongly recommended to use the finite-difference waste-form release models, section 2.5.5, when ingrowth occurs.

The BLT-EC 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 model simulates 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 in the DUST code [Sullivan, 1993].

All three models solve the diffusion equation:

$$\frac{\partial C_{kw}(x,t)}{\partial t} = D_{kwf}\,\nabla^2 C_{kw}(x,t) - \lambda_k C_{kw}(x,t) \qquad (2.21)$$

where, for component k, $C_{kw}(x,t)$ (mole/cm^3) is the concentration within the waste form, D_{kwf} (cm^2/s) is the waste form diffusion coefficient, λ_k (s^{-1}) is the radioactive decay constant, x is the spatial location vector, and t is the time since container failure. 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-EC code allows selection of a unique diffusion coefficient for each radionuclide.

The initial condition for all three models is:

$$C_{kw}(x,0) = C_{0kw} \qquad (2.22)$$

where C_{0kw} is the initial concentration of component k in the pore waters of the waste form. It is estimated from the initial inventory and waste form volume.

2.5.2.1 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 $0 \le x \le h$. 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 there releases to interact and if diffusion is appropriate for transport outside of the waste form. The boundary conditions are, symmetry in the waste form,

$$\frac{\partial C_{kw}(0,t)}{\partial x} = 0 \qquad (2.23)$$

and zero concentration as x approaches infinity.

$$C_{kw}(\infty,t) = 0 \qquad (2.24)$$

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

$$J_k = 0.5\, C_{0kw} \sqrt{\frac{D_{kwf}}{\pi t}}\; e^{-\lambda_k t} \left[\, 1 - e^{\frac{-h^2}{D_{kwf}\, t}} \,\right] \qquad (2.25)$$

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.

$$Q_{dk} = \frac{J_k A_{wf}}{V_e} \qquad (2.26)$$

This value of Q_{dk} is placed into the transport equation as the release from the waste form.

2.5.2.2 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 $-h \le x \le h$. 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:

$$\frac{\partial C_{kw}(0,t)}{\partial x} = 0 \qquad (2.27)$$

$$C_{kw}(h,t) = 0 \qquad (2.28)$$

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_k.

$$\gamma_k = \frac{h^2}{D_{kwf}\, t} \tag{2.29}$$

If $\gamma_k < 0.05$

$$J_k = 0.5\, C_{0kw} \sqrt{\frac{D_{kwf}}{\pi t}}\; e^{-\lambda_k t} \left[\, 1 - e^{\frac{-h^2}{D_{kwf}\, t}} \,\right] \tag{2.30}$$

This solution is equivalent to the solution for release into a semi-infinite medium. This result 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 $0.05 < \gamma_k < 1$

$$J_k = C_0 \sqrt{\frac{D_{kwf}}{\pi t}}\; e^{-\lambda_k t} \sum_{n=0}^{n=N} (-1)^n \left[\, e^{-n^2\gamma_k} - e^{-(n+1)^2\gamma_k} \right] \tag{2.31}$$

If $1 < \gamma_k < 20$

$$J_k = \frac{2\, D_{kwf}\, C_0\, e^{-\lambda_k t}}{h} \sum_{n=0}^{n=N} e^{\frac{-\pi^2(2n+1)^2\gamma_k}{4}} \tag{2.32}$$

If $\gamma_k > 20$

$$J_k = 0 \tag{2.33}$$

The number of terms evaluated in the series is estimated based on the value of γ_k. It is selected to ensure 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 $\gamma_k < 0.05$ is the leading order term in Eqn 2.31. For $\gamma_k > 20$ 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_k, is placed into Eqn. 2.26 to obtain the release rate per unit volume required in the transport equation.

2.5.2.3 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:

$$\frac{\partial C_{kw}(0,z,t)}{\partial r} = 0 \tag{2.34}$$

$$C_{kw}(R,z,t) = C_{kw}(r,0,t) = C_{kw}(r,H,t) = 0 \tag{2.35}$$

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

$$CFR_k = 1 - \frac{32\ S_{qk}\ S_{dk}}{\pi^2} \tag{2.36}$$

where:

$$S_{qk} = \sum_{n=1}^{n=\infty} \frac{1}{(2n-1)^2}\ e^{\frac{-(2n-1)^2\ \pi^2\ D_{kwf}\ t}{H^2}} \tag{2.37}$$

$$S_{ck} = \sum_{m=1}^{m=\infty} \frac{1}{\beta_m^2}\ e^{\frac{-\beta_m^2\ D_{kwf}\ t}{R^2}} \tag{2.38}$$

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

The American Nuclear Society (ANS) 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 recommendation 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:

$$CFR_k = \frac{2\ SA_{wf}}{V_{wf}} \sqrt{\frac{D_{kwf}\ t}{\pi}} \tag{2.39}$$

where SA_{wf} is the surface area of the waste form and V_{wf} is the volume of the waste form.

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 approximation,

$$CFR_k = 1 - \frac{32\ S_{qk,N}\ S_{ck,M}}{\pi^2} \tag{2.40}$$

where

$$S_{qk,N} = \sum_{n=1}^{n=N-1} \frac{1}{(2n-1)^2}\ e^{\frac{-(2n-1)^2\ \pi^2\ D_{kwf}\ t}{H^2}} + \frac{N}{(2N-1)^2} e^{\frac{-(2n-1)^2\pi^2 D_{kwf} t}{H^2}} - \sqrt{\frac{\pi D_{kwf} t}{2H}}\ erfc\left[(2N-1)\pi\sqrt{\frac{D_{kwf} t}{H}}\right] \tag{2.41}$$

and

$$S_{ck,M} = \sum_{m=1}^{m=M-1} \frac{1}{\beta_m^2}\ e^{\frac{-\beta_m^2\ D_{kwf}\ t}{R^2}} + \left[\frac{1}{\beta_M f_M} + \frac{1}{2\beta_M^2}\right] e^{\frac{-\beta_M^2 D_{kwf} t}{R^2}} - \frac{1}{R f_M}\sqrt{\pi D_{kwf} t}\ erfc\left[\beta_M \frac{\sqrt{D_{kwf} t}}{R}\right] \tag{2.42}$$

where

$$f_M = \pi - \frac{1}{8\pi M^2} \tag{2.43}$$

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

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

$$Q_{dk} = \frac{CFR_k(t+\Delta t) - CFR_k(t)}{V_e} M_k^o \, e^{-\lambda_k t} \qquad (2.44)$$

where M_k° is the original mass in the waste form.

2.5.2.4 Approximate Treatment of Ingrowth in the Analytical Diffusion Models

The analytical diffusion release models 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 that 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 2.5.5 should be used.

2.5.3 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-EC each radionuclide may be assigned a unique uniform release rate. In the absence of ingrowth the release rate per unit volume is estimated from:

$$Q_{uk} = \frac{u \, M_k^0}{V_e} \, e^{-\lambda_k t} \left[1 - \frac{C_{ka}}{C_{ka}^{sat}}\right] \qquad (2.45)$$

where u is the fractional release rate, C_{ka} is the solution concentration of component k, C_{ka}^{sat} is the user-specified solubility limit, and other quantities have been previously defined. If ingrowth occurs, the mass available for release, $M_k^0 e^{-\lambda kt}$, is generalized to the mass available at that time M(t) based on ingrowth as well as decay. This treatment discussed further in section 2.5.7

A further difference between BLT and BLT-EC 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, 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. If the solubility limit is exceeded, the excess mass released will precipitate according to solution of the mass action equations. The release rate is zero when the solution concentration reaches the solubility limit. The treatment of solubility is discussed further in section 2.5.6.

2.5.4 Total Waste-Form Release Rate

BLT-EC permits each waste form to release mass by any of the release mechanisms described in section 2.5.1 (rinse with partitioning), 2.5.2 (diffusion) , and 2.5.3 (uniform degradation). 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 exceeding the solubility limit. This procedure is discussed in more detail in section 2.5.6.

2.5.4.1 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 in section 2.5.2. 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 treatment 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) does 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.

2.5.5 Finite-Difference Waste-Form Release Model

BLT-EC provides an alternative approach to simulating release from the waste form as compared to the analytical models presented in section 2.5.3. 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
- method for modeling ingrowth of radionuclides in the waste form which are released by the diffusion process.

The disadvantages 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-EC 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 media with a liquid phase that permits movement by diffusion of aqueous species and a solid phase that 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, 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:

$$\theta \frac{\partial C_{kw}}{\partial t} = \nabla \cdot \theta D_{kwf} \nabla C_{kw} + \nabla \cdot V_{wf} C_{kw} - \lambda_i \theta C_{kw} + \sum_{j=1-N}^{j \neq i} f_{kj} \lambda_j C_{jw} + S_k \qquad \textbf{(2.46)}$$

where:

θ is the moisture content within the waste form. For simplicity this is taken as the moisture content within the finite element volume.
C_{kw} is the concentration of the k^{th} radionuclide (mole/cm^3),
D_{kwf} is the waste form diffusion coefficient for the k^{th} radionuclide (cm^2/s),
V_{wf} is the volumetric flow rate per unit area through the waste form (cm/s),
λ_k is the radioactive decay constant for the k^{th} radionuclide (1/s)
f_{kj} is the fraction of decays of species j that form species k, and
S_{kj} is the source/sink term within the waste form. This term could be used to represent coupling between the immobile and mobile phases in the waste form due to precipitation or sorption.

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 2.5.1.

Although Eqn 2.46 is quite general, this equation is numerically difficult to solve 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:

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

where

y is a dimensionless distance variable,
x is the dimensioned distance variable (cm),
L(t) is the 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 as shown in Figure 2.4. However, the distance variable y is now a function of time. Differentiating Eqn. 2.47 with respect to time gives:

$$\frac{dy}{dt} = -\frac{y}{L}\frac{dL}{dt} \tag{2.48}$$

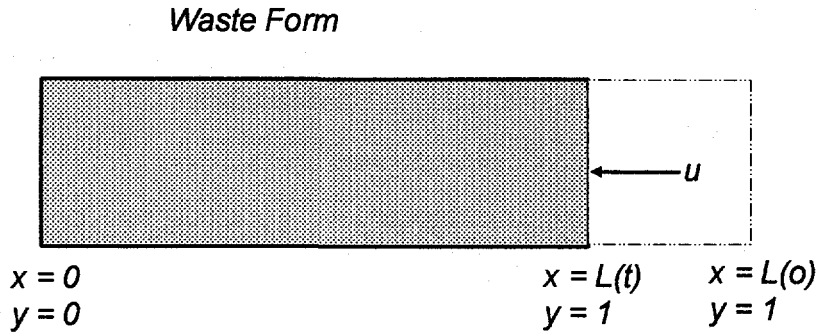


Figure 2.4 One-dimensional representation of a waste form that undergoes surface degradation at a uniform rate, u. x is the distance variable, y is the normalized distance variable such that at the surface y=1 at all times.

The time derivative of concentration in the transformed plane becomes:

$$\frac{\partial C_{kw}(y(t), t)}{\partial t} = \frac{\partial C_{kw}}{\partial t} + \frac{\partial y}{\partial t}\frac{\partial C_{kw}}{\partial y} \tag{2.49}$$

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

$$\frac{\partial C_{kw}(y,t)}{\partial t} = \frac{\partial C_{kw}}{\partial t} - \frac{u_k y}{L(t)}\frac{\partial C_{kw}}{\partial t} \tag{2.50}$$

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:

$$u_k(t) = - u_o L_o \left(1 - \frac{C_{ka}}{C_{ka}^{sat}}\right) \quad \textbf{(2.51)}$$

where u_o is the fractional degradation rate, section 2.5.3 (1/s) and L_o is the original waste form half width (radius) (cm). 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:

$$\theta \frac{\partial C_{kw}}{\partial t} = \frac{\theta D_{kwf}}{L(t)^2} \frac{\partial^2 C_{kw}}{\partial y^2} + \frac{V_{wf}}{L(t)} \frac{\partial C_{kw}}{\partial y} + \frac{\theta u_k(t) y}{L(t)} \frac{\partial C_{kw}}{\partial y}$$

$$+ C_{yL} \left(\frac{-\theta D_{kwf}}{yL^2} \frac{\partial C_{kw}}{\partial y} + \frac{V_{wf} C_{kw}}{yL} \right) + \sum_{j=i,n}^{j=i} f_{kj} \lambda_j C_{jw} - \lambda_k \theta C_{kw} + S_k \quad \textbf{(2.52)}$$

where C_{yi} takes the value of 0 for plane geometry and 1 for cylindrical geometry. 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-EC, 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:

$$(1-\eta) \frac{\partial C_{kw}}{\partial t} = \frac{(1-\eta)\, u_k(t)\, y}{L(t)} \frac{\partial C_{kw}}{\partial y} - \lambda_k \theta C_{kw} + \sum_{j=1,N}^{j \neq i} f_{kj}\, \lambda_j\, C_{jw} + S_k \quad \textbf{(2.53)}$$

where C_{kw} is the concentration of immobile species in the waste form.

Eqn 2.53 is used to calculate the immobile species concentrations in the waste form in BLT-EC. 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 ($dC_{kw}/dy = 0$ in the waste form). This condition is consistent with the assumptions used to generate the analytical model. To improve the computational efficiency of BLT-EC, solution of Eqn 2.53 could be omitted and the releases due to degradation could be accounted for using the analytical models of section 2.5.3.

The initial waste-form condition used in BLT-EC is that initially mass is homogeneously distributed within the waste form. This condition prevents the need to input detailed information on the distribution of contaminants within the waste form. The only information that is required is the waste form inventory and volume. Conceptually, non-uniform initial conditions could be handled by the finite-difference approach if 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 source as well as transport processes.

The treatment of solubility limited release is provided in section 2.5.6.

2.5.5.1 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 2.5.3. However, for a cylindrical waste form, as the waste form radius decreases due to corrosion, 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 behavior occurs because the waste-form volume dissolved per unit time in a cylinder is initially greater than for a plane form.

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, 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 2.5.6.

2.5.6 Solubility Limited Release

In BLT-EC solubility limited release is treated by 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-EC uses an explicit procedure to estimate the amount of mass that can be released without exceeding solubility limits. However, if the solubility limit is exceeded the excess mass released will precipitate according to solution of the mass action equations. 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.

- The mass released due to the diffusion release mechanism is calculated. The aqueous solution concentration, C_{ka}^{est} is estimated by dividing the released mass, ΔM_{kd}, 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_k, as follows:

$$C_{ka}^{est} = C_{ka}(t) + \frac{\Delta M_{kd}}{\theta V_e R_k} \quad \textbf{(2.54)}$$

This concentration 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_{ka}^{m}, defined as:

$$C_{ka}^{m} = C_{ka}^{sat} + \frac{V_d\,[C_{ka}^{sat} - C_{ka}]\,\Delta t}{\theta R_k L} \quad \textbf{(2.55)}$$

where V_d is the Darcy flow velocity, C_{ka} 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-EC 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 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:

$$\Delta M_k = [\,C_{ka}^{m} - C_{ka}]\;\theta\; V_e\; R_k \quad \textbf{(2.56)}$$

In this case, ΔM_k 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 treatment 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 ½ of the mass was released during the time step, the finite-difference models would release ½ 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-EC. BLT-EC 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 Chapter 7 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. However, if the finite-difference models are being used, mass transferred to the rinse release mechanism is treated as "rinse" mass. Therefore, in solubility limited problems with diffusion and degradation processes, the rinse mass will actually increase in time due to the transfer process.

2.5.7 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-EC 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-EC permits multiple decay chains and branching of decay chains. Guidance on how to simulate these processes within the BLT-EC framework is provided in Chapter 5.

The treatment of chain decay is complicated by the multiple release models permitted in BLT-EC. 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 somewhat of 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 does not exist. For this reason, it is strongly recommended that when using BLT-EC to simulate decay chains, all members of the chain should 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-EC 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 at the beginning of the time step. 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:

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

where f_{ij} is the fraction of decay of species i that produce species j, $M_i(t)$ is the mass available at time t, and ATM is the atomic mass. This 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.

2.5.8 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} cm^2/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 this data and its 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 ensure that properties are not accounted for twice. For example, if BLT-EC 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.

2.6 Contaminant Migration (Transport)

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

In BLT-EC, 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. Two governing transport equations are solved in BLT-EC; one equation describes the transport of aqueous-phase "components" and the other equation describes conservation of immobile adsorbent "components." Components are linearly independent basis entities that linearly combine to produce all chemical species in the system [Van Zeggeren and Storey, 1970]. For example, the two chemical components UO_2^{2+} and CO_3^{2-} can combine to form the chemical species UO_2CO_3. During transport, the various chemical components are distributed among the aqueous, precipitated, and sorbed phases under the assumption of local chemical equilibrium. In BLT-EC, chemical equilibrium is governed by nonlinear mass action and linear mass balance equations.

2.6.1 Transport Equation with Chemical Reactions and Radioactive Decay

The equation that describes the transport of chemical components in variably saturated media can be written as [Yeh and Tripathi, 1991; MacKinnon et al., 1995]:

$$\theta\frac{\partial T_k}{\partial t}+T_k\frac{\partial \theta}{\partial t}+\boldsymbol{V}\cdot\nabla T_k-\nabla\cdot\theta\boldsymbol{D}\cdot\nabla T_k$$

$$=C_{ka}\frac{\partial \theta}{\partial t}+\boldsymbol{V}\cdot\nabla(C_{ks}+C_{kp})-\nabla\cdot\theta\boldsymbol{D}\cdot\nabla(C_{ks}+C_{kp}) \qquad \textbf{(2.58)}$$

$$+R_k^d+S_k^w+S_k^s+Q(C_{ka}^*-C_{ka})$$

where θ is the volumetric moisture content [$cm^3 \cdot cm^{-3}$] and $\mathbf{V}$ is the Darcy flux [$cm \cdot s^{-1}$]. T_k is the total concentration of component k and can be written as:

$$T_k=C_{ka}+C_{kp}+C_{ks} \qquad \textbf{(2.59)}$$

with C_{ka}, C_{kp}, and C_{ks} defined as total concentrations of component k in moles of k per unit volume of the aqueous phase [mole/liter] in the aqueous, precipitated, and sorbed phases, respectively. These concentrations are given by:

$$C_{ka}=\sum_{i\in A}\nu_{ki}c_i \qquad \textbf{(2.60)}$$

$$C_{ks}=\sum_{i\in S}\nu_{ki}c_i \qquad \textbf{(2.61)}$$

$$C_{kp}=\sum_{i\in P}\nu_{ki}c_i \qquad \textbf{(2.62)}$$

where $\in$ is read "belonging to" and each sum ranges over the species containing component k, υ_{ki} is the stochiometric coefficient of the k-th component in chemical species i, and c_i, are species concentrations in moles of species i per unit volume of the aqueous phase [mole/liter] in the aqueous ($i \in A$), precipitated ($i \in P$), and sorbed phases ($i \in S$). $\mathbf{D}$ is the hydrodynamic dispersion tensor [$cm^2 \bullet s^{-1}$] given by [Bear, 1972]:

$$\theta\boldsymbol{D}=\theta D_m\tau\delta_{kl}+\varepsilon_T|v|\delta_{kl}+(\varepsilon_L-\varepsilon_T)\frac{v^k v^l}{|\boldsymbol{v}|} \qquad \textbf{(2.63)}$$

where $\mathbf{D}_m$ is the molecular diffusion coefficient [$cm^2 \bullet s^{-1}$], τ is a tortuosity factor [$cm \bullet cm^{-1}$], $\mathbf{V}^k$ and $\mathbf{V}^l$ are the components of the Darcy flux vector [$cm \bullet s^{-1}$], and ε_L and ε_T are longitudinal and transverse dispersivities [cm], respectively. Q ($cm^3 \bullet cm^{-3} \bullet s^{-1}$) is the source/sink term due to aqueous fluid injection and C_k^* is the concentration of component k in the injected aqueous phase. The total radioactive decay rate, R_k^d, and total source terms, S_k^w and S_k^s, for component k, are given by:

$$R_k^d = \theta \sum_{i \epsilon A} \nu_{ki} r_i^d + \theta \sum_{i \epsilon P} \nu_{ki} r_i^d + \theta \sum_{i \epsilon S} \nu_{ki} r_i^d$$

$$= -\theta [\lambda_k T_k - \sum_L f_{kL} \lambda_L T_L] \quad \textbf{(2.64)}$$

and

$$S_k^w = \sum_i \nu_{ki} s_i^w \quad \textbf{(2.65)}$$

$$S_k^s = \sum_i \nu_{ki} s_i^s \quad \textbf{(2.66)}$$

where the sum over L represents the sum over all parent species of component k, f_{kL} is the branching fraction for component k, λ_k is the decay constant [s^{-1}], s_j^w [mole• l^{-1} • s^{-1}] represents the release of radioactive and nonradioactive species from waste forms, and s_j^s represents the release of species from engineered structures and waste containers.

Equations governing conservation of adsorbent component concentrations (these concentrations are on a per unit volume of aqueous phase basis) are required to complete the system of transport equations. This equation can be written as:

$$\frac{\partial(\theta T_k)}{\partial t} = 0 \quad \textbf{(2.67)}$$

with

$$T_k = \sum_{i \epsilon S} \nu_{ki} c_i \quad \textbf{(2.68)}$$

for k ranging over the adsorbent components only.

2.6.2 Initial and Boundary Conditions

The solution of aqueous phase transport Eqn. (2.58) and sorption/ion exchange conservation Eqn. (2.67) requires that the initial total analytical concentrations of all components [mole•l^{-1}], including aqueous phase and adsorbent components and number of equivalents of ion exchange sites [mole•gm^{-1}], be specified in the flow domain Ω, that is:

$$T_k(x,y,z,0) = T_k^I(x,y,z) \quad \textbf{(2.69)}$$

and

$$A_{ms}(x,y,z,0)=A_{ms}^{I}(x,y,z) \tag{2.70}$$

where k ranges over the aqueous components, m ranges over the adsorbent components and ion-exchange sites, and the superscript I denotes initial values.

In BLT-EC, two types of boundary conditions may be specified on the boundary Γ of flow domain Ω. If a boundary condition is not specified, the default boundary condition, which is zero dispersive mass flux through the boundary, is applied.

Dirichlet conditions prescribe analytical concentrations on boundary segment Γ_D:

$$T_k(x,z,t)=T_k^D(x,z,t), \quad (x,z)\in\Gamma_D, t>0 \tag{2.71}$$

The second type of boundary condition is a variable boundary condition on boundary segment Γ_v. This boundary condition is usually applied at the air/ground surface boundary. If aqueous-phase flow is outward from the variable condition boundary, the Neumann flux of dissolved component k is set to zero, that is:

$$-\theta \boldsymbol{D}\cdot\nabla(C_{ak})\cdot\boldsymbol{n}=0, \qquad (x,z)\in\Gamma_v, t>0 \tag{2.72}$$

If flow is into the domain at the variable condition boundary, the Neumann flux is prescribed as:

$$\begin{aligned} -\theta \boldsymbol{D}\cdot\nabla(C_{ak})\cdot\boldsymbol{n} &= \boldsymbol{V}C_{ak}\cdot\boldsymbol{n}-\theta \boldsymbol{D}\cdot\nabla(C_{ak})\cdot\boldsymbol{n} \\ &- \boldsymbol{V}T_k\cdot\boldsymbol{n} + \boldsymbol{V}(C_{sk}+C_{pk})\cdot\boldsymbol{n}, \ (x,z)\in\Gamma_v, t>0 \end{aligned} \tag{2.73}$$

In the above boundary conditions (Eqns. 2.69 - 2.73), k ranges over the aqueous components and **n** is the outward unit normal vector to Γ_v. In Eqn. 2.73, the gradients in flux cancel and the flux entering the system is the advective flux, i.e., incoming concentration multiplied by velocity component normal to the surface.

2.6.3 Chemical Processes

The various chemical species of concern include radioactive and nonradioactive substances introduced into the subsurface by waste disposal and those naturally present in the subsurface. Key reactions among the various chemical species include complexation, acid-base, oxidation-reduction, precipitation-dissolution, sorption, and ion exchange. The complete system of key chemical reactions can be written in symbolic matrix form as:

$$0 \leftrightarrows \boldsymbol{N}\ \boldsymbol{B} \tag{2.74}$$

where **B** is the vector of molecular formulas B_i (e.g., $B_{1a} = H_2{}^{16}0$, $B_{2a} = {}^{238}U^{16}O_2$, etc.) and **N** is the stochiometric reaction matrix comprised of stochiometric coefficients υ_{ki} for each k^{th} component in chemical species i. Chemical species may reside in the aqueous, precipitated, and sorbed phases; any two chemical species having the same molecular formula but occupying different phases (e.g., calcium carbonate $CaCO_3$(s) in the solid phase (calcite) and $CaCO_3^\circ$ in the aqueous phase) are two

different species. It is important to note that each product species is expressed as a linear combination of the components and components cannot be expressed as linear combinations of other components.

The key reactions in (Eqn. 2.74) can be separated into three main categories of reactions: aqueous complexation, dissolution-precipitation, and sorption reactions. These reaction can be written as:

Aqueous Complexation

$$\sum_{k=1}^{M_a} \nu_{kj} B_k \leftrightarrow B_j \qquad \forall \quad \textit{product species } j \quad \in \quad \boldsymbol{A} \tag{2.75}$$

Dissolution-Precipitation

$$\sum_{k=1}^{M_a} \nu_{kj} B_k \leftrightarrow B_j \qquad \forall \quad \textit{product species } j \quad \in \quad \boldsymbol{P} \tag{2.76}$$

Sorption Reactions

$$\sum_{k=1}^{M_a} \nu_{kj} B_k + \sum_{k=1}^{M_s} \nu_{kj} B_k \leftrightarrow B_j \qquad \forall \quad \textit{product species } j \quad \in \quad \boldsymbol{S} \tag{2.77}$$

where **A**, **P**, and **S** denote the sets of species that may be present in the aqueous, precipitated, and sorbed phases, respectively, the symbol $\forall$ is read "for every," and $\in$ is read "belonging to."

Under the assumption of chemical equilibrium, the above chemical reactions are described by a system of (N_s-M) nonlinear mass action equations and a system of M mass balance equations. The (N_s-M) mass action equations can be written as:

Aqueous Complexation

$$Y_j = K_j \prod_{k=1}^{M_a} X_k^{\nu_{kj}} \qquad \forall \quad \textit{product species } j \quad \in \quad \boldsymbol{A} \tag{2.78}$$

Precipitation-Dissolution

$$1 = K_j \prod_{k=1}^{M_a} X_k^{\nu_{kj}} \qquad \forall \quad \textit{product species } j \quad \in \quad \boldsymbol{P} \tag{2.79}$$

Sorption

$$Y_j = K_j \prod_{k=1}^{M_a} X_k^{\nu_{kj}} \prod_{k=1}^{M_s} X_k^{\nu_{kj}} \qquad \forall \quad \textit{product species } j \quad \in \quad \boldsymbol{S} \tag{2.80}$$

where $\prod$ indicates the product over component species k, K_j is the equilibrium constant for the formation of species j, and X_k and Y_j are thermodynamic activities of component species and product species [mole•l^{-1}], respectively. For solid phases, the activity is assumed to equal 1 as indicated in Eqn. (2.79). The thermodynamic activities are approximated by the relations:

$$Y_j=\gamma_j c_j \tag{2.81}$$

and

$$X_k=\gamma_k c_k \tag{2.82}$$

where γ_k and γ_j are activity coefficients of the component and product species and c_k and c_j are the component and product species concentrations [mole•l^{-1}]. In general, equilibrium constants in Eqns. 2.78 - 2.80 and activity coefficients in 2.81 and 2.82 are functions of temperature and ionic strength. Often used approximations for these parameters are described in Appendix C.

The companion M mass-balance equations for the M components are given by:

$$\sum_{j\in A,P,S} \nu_{kj} c_j - T_k = 0 \qquad k=1,2,....,M \tag{2.83}$$

where T_k is the total concentration of component k. T_k is provided at each point (x,z,t) in the problem domain by the solution to the hydrologic transport equations.

2.6.4 System Summary

In general, all N_s chemical species are present at all points (x,z,t) in the spatial and temporal problem domain. Recall that the N_s chemical species are divided into M_a+M_s independent species called components and N_s-M_a-M_s dependent species called product species. Therefore, in general, at each point (x,z,t) we have M_a unknown aqueous component concentrations, M_s unknown adsorbent component concentrations and/or number of ion-exchange site equivalents, and (N_s-M_a-M_s) unknown product species concentrations. These unknowns are determined by M_a transport Eqns. 2.58, M_s conservation Eqns. 2.67, and (N_s-M_a-M_s) algebraic Eqns. 2.78 - 2.83. The unknown dependent quantities C_{ks} and C_{kp} in Eqn. 2.58 are determined from product species concentrations according to Eqns. 2.61 and 2.62. The system of equations is completed by auxiliary relations 2.81 and 2.82 and associated equations in Appendix C, the total radioactive decay rate given by 2.64, the waste-form release term given by 2.65, and the source term given by 2.66 due to injection/extraction.

2.7 Numerical Approximation to Contaminant Migration (Transport)

The transport model in the BLT-EC computer code is based on a modified version the hydrological transport module contained in the finite-element code HYDROGEOCHEM [Yeh and Tripathi, 1989]. This module approximates the governing transport Eqns. 2.58 and 2.67 with bilinear finite elements for the spatial discretization, a variable two-point finite-difference scheme for time integration, and either direct or pointwise iteration methods for solution of the matrix equations. The code user can also select the following options: (a) an upstream weighting finite-element approximation for advection-dominated flows, (b) lumping of the mass matrix, and (c) tetrahedral or quadrilateral elements (although the source term models require quadrilateral elements for their implementation).

The chemical equilibrium Eqns. 2.78 - 2.83 are solved with a modified version of the computer code MINTEQA2 referred to herein as EC-MINTEQA2. In a BLT-EC simulation, mixture compositions at each node and time step are

provided by the transport module. The pre-solution routines in MINTEQA2 have been modified extensively to interface efficiently with the transport module. The chemical concepts, mathematical structure, solution procedures, and thermodynamic data base used in EC-MINTEQA2 are described in detail in Appendix E. This appendix is taken directly from the MINTEQA2/PRODEFA2 Version 3.0 User's manual [Allison et al., 1991] and reproduced here for completeness. Minor text changes necessary to maintain consistency in notation and to distinguish differences between EC-MINTEQA2 and MINTEQA2 have been introduced when appropriate.

2.7.1 Transport Equations

The hydrologic transport equations in BLT-EC are solved using the finite-element method. The hydrologic transport module contained in HYDROGEOCHEM was used for this purpose and coupled with EC-MINTEQA2. The approximation of transport equations by the finite element method is described by several authors [Huyakorn and Pinder, 1983; Carey and Oden, 1986; Yeh and Tripathi, 1991]; therefore, only a brief development is presented here.

To obtain a discrete form of the continuum problem defined by 2.58 - 2.68, the problem domain Ω is discretized as a union Ω_h of M_e finite elements and M_{np} nodal points. Let $\{N_i\}$ be the global finite element basis approximation space $H^h \subset H^1$ on Ω_h. The approximate semi-discrete statement of transport Eqn. 2.58, after integration by parts, is: for $t > 0$ find $T_k \in H^h(\Omega)$ such that

$$\begin{aligned}
&\int_{\Omega_h} [\theta \frac{\partial T_k}{\partial t} W_h + T_k \frac{\partial \theta}{\partial t} W_h + \boldsymbol{V} \cdot \nabla T_k W_h + \theta \boldsymbol{D} \cdot \nabla T_k \cdot \nabla W_h \\
&- C_{ak} \frac{\partial \theta}{\partial t} W_h - \boldsymbol{V} \cdot \nabla (C_{sk} + C_{pk}) W_h - \theta \boldsymbol{D} \cdot \nabla (C_{sk} + C_{pk}) \cdot \nabla W_h] dx dz \\
&= \int_{\Omega_h} [R_k^d + S_k^w + S_k^s + Q(C_{ak}^* - (T_k - (C_{pk} + C_{sk})))] W_h dx dz \\
&+ \int_{\Gamma_h} \theta \boldsymbol{D} \cdot \nabla T_k \cdot \boldsymbol{n} W_h d\Gamma_h
\end{aligned} \tag{2.84}$$

where T_k and W_h have the form:

$$T_k(x,z,t) = \sum_{j=1}^{N_e} T_{kj}(t) N_j(x,z) \tag{2.85}$$

and

$$W_h = N_j(x,z) \tag{2.86}$$

Introducing Eqns. 2.85 and 2.86 into 2.84, the following set of semi-discrete matrix equations are obtained:

$$[M]\{\frac{dT_k}{dt}\} + ([A] + [K] + [E])\{T_k\} = ([A] + [K])(\{C_{ak}\} + \{C_{pk}\}) + \{Q\} + \{B\} \tag{2.87}$$

where { dT_k/dt },{ T_k },{ C_{ak} }, and { C_{pk} } are column vectors at all nodes and matrices [M], [A], [K], and [E] and load vectors {Q} and {B} are given by:

$$M_{ij} = \sum_{e \epsilon M_e} \int_{\Omega_e} N_i^e \theta N_j^e \, dxdz \tag{2.88}$$

$$A_{ij} = \sum_{e \epsilon M_e} \int_{\Omega_e} N_i^e (V \cdot \nabla N_j^e) dxdz \tag{2.89}$$

$$K_{ij} = \sum_{e \epsilon M_e} \int_{\Omega_e} [\nabla N_i^e \cdot \theta \boldsymbol{D} \cdot \nabla N_j^e + N_i^e (Q - \frac{\partial \theta}{\partial t}) N_j^e] dxdz \tag{2.90}$$

$$E_{ij} = \sum_{e \epsilon M_e} \int_{\Omega_e} N_i^e \frac{\partial \theta}{\partial t} N_j^e \, dxdz \tag{2.91}$$

$$Q_i = \sum_{e \epsilon M_e} \int_{\Omega_e} N_i^e Q C_{ka}^* dxdz \tag{2.92}$$

$$\begin{aligned} B_{ij} = \sum_{e \epsilon B_e} \int_{\Gamma_e} N_i^e \theta \boldsymbol{D} \cdot \nabla C_{ak} \cdot \boldsymbol{n} \, ds = -\sum_{e \epsilon B_e} \int_{\Gamma_e} N_i [V C_{ak} \cdot \boldsymbol{n} - \theta \boldsymbol{D} \cdot \nabla (C_{ak}) \cdot \boldsymbol{n} \\ - V T_k \cdot \boldsymbol{n} + V (C_{sk} + C_{pk}) \cdot \boldsymbol{n}] ds \end{aligned} \tag{2.93}$$

where Ω_e is the subdomain of element e , Γ_e is the length of boundary segment B_e, and N_j^e and N_i^e are finite element basis and weighting functions. Note that boundary condition Eqn. 2.73 was used in 2.93.

Quadrilateral bilinear elements are used to discretize the spatial domain. Triangular linear elements are coded in BLT-EC, however, these elements have not been tested. Also, the source-term models described in section 2.5 are implemented in quadrilateral elements only. The bilinear basis functions for the j-th node of a typical quadrilateral element are:

$$N_j^e = (1 + \xi_j \xi)(1 + \eta_j \eta), \qquad -1 \le \xi \le 1, \quad -1 \le \eta \le 1 \tag{2.94}$$

where ξ_j and η_j are the local coordinates of the four corner nodes which are numbered from j=1 to j=4 beginning with the lower left hand corner and going around the element in a counter clockwise direction. The mapping from local coordinates ξ and η to the global coordinates x znd z is defined by:

$$x = \sum_{j=1}^{4} x_j N_j^e(\xi,\eta) \quad \Lambda \quad z = \sum_{j=1}^{4} z_j N_j^e(\xi,\eta) \tag{2.95}$$

For advection dominated flows it may be necessary to upwind bias the weighting function in the advection term so that the nodal solution of total concentrations T_j will not exhibit supurious oscillations. Refer to the upwind weighting option flag, IWET, in data set 4. If this option is selected (IWET=1), the weighting function N_i is set equal to an upwind biased weighting function W_i defined as follows [Yeh and Tripathi, 1989]:

$$N_i = W_j \tag{2.96}$$

where

$$W_1 = [(2-3\alpha_1) - 2\xi + 3\alpha_1\xi^2][(2-3\beta_2) - 2\eta + 3\beta_2\eta^2]/16 \tag{2.97}$$

$$W_2 = [(2+3\alpha_1) + 2\xi - 3\alpha_1\xi^2][(2-3\beta_1) - 2\eta + 3\beta_1\eta^2]/16 \tag{2.98}$$

$$W_3 = [(2+3\alpha_2) + 2\xi - 3\alpha_2\xi^2][(2+3\beta_1) + 2\eta - 3\beta_1\eta^2]/16 \tag{2.99}$$

$$W_4 = [(2-3\alpha_2) - 2\xi - 3\alpha_2\xi^2][(2+3\beta_2) + 2\eta - 3\beta_2\eta^2]/16 \tag{2.100}$$

where α_1, α_2, β_1, and β_2 are weighting factors assigned to element sides 1-2, 4-3, 2-3, and 1-4, respectively, of a typical four-node quadrilateral element. If the optimization flag, IOPTIM = 1, these weighting factors are determined by the equation:

$$\alpha = \coth[(UL)/2D] - [(2D)/UL] \tag{2.101}$$

where α denotes α_1, α_2, β_1, and β_2, L is the length of the corresponding element side, and U and D are the average values of velocity component and dispersion along the corresponding element side. If IOPTIM = 0, first-order upwinding is invoked and these parameters are set to 1 or -1 depending on the flow direction and 0 if flow velocity along the element side is zero.

Eqn. 2.87 represents a system of ordinary differential equations for nodal concentrations $T_j(t)$. To evaluate the behavior of this system in the time domain, the variation of T_j over time step Δt is approximated with the linear function:

$$T_j(t^*) = wT_j^{n+1} + (1-w)T_j^n, \qquad 0 \le w \le 1 \tag{2.102}$$

where $t^*=t^n+w(t^{n+1}-t^n)$. The velocities are approximated in similar fashion as:

$$V_j(t^*) = w_v V_j^{n+1} + (1-w_v)V_j^n, \qquad 0 \le w_v \le 1 \tag{2.103}$$

For Eqn. 2.103 to be strictly true the velocity weighting parameter w_v must equal w. However, for added flexibility the value of w_v is permited to be different than w. The time derivative is approximated with a two-point difference approximation as:

$$\frac{dT_j(t^*)}{dt} = \frac{T_j^{n+1} - T_j^n}{\Delta t} \tag{2.104}$$

Applying Eqn. 2.87 at time t* and introducing Eqns. 2.102 and 2.104, the fully discrete system of equations is obtained:

$$[G^*][T]^{n+1} = [H^*]([C_s]^{n+1} + [C_p]^{n+1}) + [L^*] \tag{2.105}$$

where

$$[G^*] = [M^*]/\Delta t + w_v[A^*] + w([K^*] + [E^*]) - w_v[V]^{n+1} \tag{2.106}$$

$$[H^*] = w_v[A^*] + w[K^*] - w_v[V]^{n+1} \tag{2.107}$$

$$\begin{aligned}[L^*] &= [Q^*] + ([M^*]/\Delta t - (1-w)[E^*][T]^n \\ &- ((1-w_v)[A^*] + (1-w)[K^*])[C_a]^n + [q] + (1-w_v)[V]^n[C_a]^n\end{aligned} \tag{2.108}$$

where

$$q_i = -\sum_{e \in B_e} \int_{\Gamma_e} N_i(\boldsymbol{V}\cdot\boldsymbol{n})\overline{C}_a ds \tag{2.109}$$

$$V_i = -\sum_{e \epsilon B_e} \int_{\Gamma_e} N_i (\boldsymbol{V} \cdot \boldsymbol{n}) ds \qquad \textbf{(2.110)}$$

and the asterisk denotes evaluation at time t^*. The values of w and w_v control the implicitness of the time integration scheme. If w=0 and w_v=0 ($t^*=t^n$) the integration scheme is explicit. If w=0.5 and w_v=0.5 ($t^*=(t^n+ t^{n+1})/2$) the scheme is an implicit Crank-Nicolson scheme. If w=1 and w_v=1 ($t^*=t^{n+1}$) the scheme is a fully implicit Backward-Euler scheme.

2.7.2 Chemical EquilibriumEquations

The solution method used EC-MINTEQA2 to solve the multi-component chemical equilibrium problem is outlined in this section. The primary unknowns of the chemical equilibrium problem are the activities of the components. To begin, the algebraic system Eqns. 2.78 - 2.80 can be represented by the single mass action expression:

$$c_j = K_j^* \prod_{k=1} X_k^{\nu_{kj}} \qquad \textbf{(2.111)}$$

with K_j^*, using Eqn. 2.81, defined as

$$K_j^* = \frac{K_j}{\gamma_j} \qquad \textbf{(2.112)}$$

where $\prod$ indicates the product over all components in species j. To reduce the nonlinearitites, Eqn. 2.111 is solved in logarithmic form:

$$\log \boldsymbol{c} = \log \boldsymbol{K}^* + \boldsymbol{N} \log \boldsymbol{X} \qquad \textbf{(2.113)}$$

where the vector **c** of length N_s contains the concentrations of all species, vector **K*** is the vector of modified equilibrium constants of length N_s, the matrix **N** of dimension (M x N_s) contains the stoichiometric coefficients ν_{kj}, and the vector **X** of length M contains the component activities.

The iteration begins by solving for the concentrations of each species, according to Eqn. 2.113, based on an initial guess for each component activity. The total mass of each component is then calculated from the concentrations of every species containing that component using Eqn. 2.83, written here in matrix form as:

$$\boldsymbol{T}' = \boldsymbol{N}^T \boldsymbol{c} \qquad \textbf{(2.114)}$$

where matrix $\mathbf{N}^T$ is the transpose of matrix **N** and **T'** is the vector of calculated total component concentrations of length N_s. The calculated total concentration for each component is then compared with the known input total component concentration (provided by the solution to the component transport Eqn. 2.105, that is:

$$|T_k' - T_k| \leq TOL, \qquad k=1,2,...N_s \tag{2.115}$$

where TOL is preset in EC-MINTEQA2 to be 10^{-4} times T_k. If TOL is exceeded by any component k, a new estimate of the component activity is made and the entire process is repeated. The Newton-Raphson approximation method is used to estimate **X** at each iteration (see Appendix C).

After the the aqueous phase is equilibrated, EC-MINTEQA2 computes the saturation index (SI) for each possible solid with respect to the aqueous solution. The solid with the largest SI is allowed to precipitate by reducing the dissolved concentrations of those components comprising the solid species according to stoichiometry. Once mass is removed from the aqueous phase, the aqueous phase solution is re-equilibrated as described above with one less degree of freedom. The reverse process (dissolution) occurs if a solid is found to be undersaturated with respect to the aqueous solution. In this case an additional degree of freedom is added and the aqueous phase is re-equilibrated.

2.7.3 Solution Scheme

Since C_{si} and C_{pi} are functions of T_i, matrix Eqn. 2.105 is nonlinear and therefore requires an iterative solution technique. This solution scheme is as follows:

1. At current time level t^n, obtain an initial estimate of $[T]^{n+1}$ using $[C_s]^n$ and $[C_p]^n$ in Eqn. 2.114 in place of $[C_s]^{n+1}$ and $[C_p]^{n+1}$.

2. The new estimate $[T]^{n+1,k}$ is computed from a weighted average of the initial estimate and the previous time step solution; $[T]^{n+1,k} = \omega [T]^{n+1} + (1-\omega)[T]^n$.

3. Using $[T]^{n+1,k}$, the sorbed and precipitated concentrations $[C_s]^{n+1,k}$ and $[C_p]^{n+1,k}$ are computed using the equilibrium chemical reaction equations.

4. Substitute $[C_s]^{n+1,k}$ and $[C_p]^{n+1,k}$ into 2.114 and resolve for $[T]^{n+1}$.

5. If $|[T]^{n+1} - [T]^{n+1,k}| \leq$ specified tolerance then stop iteration, otherwise continue.

6. The new iterate value is calculated from $[T]^{n+1,k+1} = \omega [T]^{n+1} + (1-\omega)[T]^{n+1,k}$

7. Repeat steps 3-6 until convergence is achieved or until the maximum number of iterations is achieved.

In the above iteration, iteration parameter ω can range from 0 to 2. When iteration parameter ω satisfies $0 \leq \omega < 1$, the solution iteration is under relaxed. If $\omega=1$, there is no relaxation and if $1<\omega \leq 2$ the iteration is over relaxed.

The solution to the linearized matrix equation inside the iteration loop can be obtained by either direct elimination or pointwise iteration methods [Yeh and Tripathi, 1989]. The pointwise iteration method offers three options for solution: successive under relaxation (SUR), successive over relaxation (SOR), and Gauss-Seidel (G-S) iteration. The user selects the solution option in Data Set 11 (Chapter 5).

Finally, the solution to the conservation equation for adsorbent components is determined using the following implicit scheme:

$$[\theta + \Delta t \frac{\partial \theta}{\partial t}][T_k]^{n+1} = [\theta T_k]^n \tag{2.116}$$

where k ranges over the adsorbent components.

2.8 Numerical 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-EC 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, if the mass release rate per unit volume was one, the four corners would all have a concentration of 1/4. While this is a consistent finite element approach, it is felt that this approach may underestimate peak concentrations that could occur.

In BLT-EC 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-EC approach the concentrations in the two downstream nodes (i.e., the two bottom nodes) would be ½ 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-EC depends on the flow velocity. 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 upstream 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 Figure 2.5 and the direction of flow. As drawn in Figure 2.5, nodes 2 and 3 are the upstream nodes.

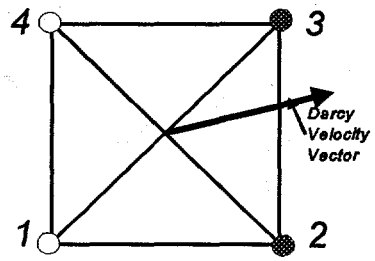


Figure 2.5 General procedure to select upstream nodes based on the Darcy flux vector.

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 Figure 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 ½ 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.

2.9 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; National Research Council, 1990]. These parameters are often critical to transport and care should be exercised to insure that the Darcy velocities 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 subsurface systems is dominated by advective transport. Typical values for diffusion coefficients (including the effects of tortuosity) in soil are of the magnitude 10^{-6} cm^2/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 Darcy flux, which represents an average flow rate. The cause for the variation around the average flow rate is the different transport paths experienced by individual fluid particles as they flow through pores and around soil particles. 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 this 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.

2.10 Limitations in the BLT-EC Computer Code

BLT-EC is capable of simulating a wide range of container, waste form, and material behaviors that will impact the release and subsurface transport of radionuclides from LLW disposal facilites. However, a number of assumptions have been made in the development of BLT-EC. Under certain conditions these assumptions may lead to limitations in the applicability of BLT-EC. The potential limitations are:

- BLT-EC approximates only two spatial dimensions in rectangular coordinates.
- BLT-EC is structured as a deterministic computer code. The range of uncertainties in many transport parameters may require multiple simulations using BLT-EC. However, BLT-EC 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 is non-existent.
- 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 affect release.
- Chemical reactions are computed under the assumption of local chemical equilibrium. Some important reactions such as precipitation and adsorption may be kinetically limited and far from equilibrium. In such cases, BLT-EC may under estimate contaminant migration if the analyst does not take care in introducing off-setting assumptions.
- BLT-EC can model closed systems only. Mass transfer between the aqueous and gaseous phases is not accounted for, nor is transport in the gaseous phase. In some applications, dynamic changes in CO_2 concentrations in the gaseous phase may impact contaminant mobility.
- Although quite extensive, the thermodynamic database provided with BLT-EC does not include data for a number of important radionuclides such as Pu and Th.
- BLT-EC does permit transport calculations that involve sorption only. This capability is useful in applications where standard K_d type calculations are adequate or when there is a lack of thermodynamic data for contaminants of concern. However, in such applications, the transport equations do not limit concentrations based on solubility. This limitation may cause a problem for species produced due to radioactive decay during transport. For example, consider a two member decay chain at secular equilibrium. Further, the solubility of the first member of the chain is several orders of magnitude greater than that of the second member. Also, 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-EC. They must be supplied by input. Time dependent velocities can be accommodated through input files containing this 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-EC SOLUTION PROCEDURE

The first step towards using BLT-EC 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.) must 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, for example, may assume that the water flow rate 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 additional chemical processes, 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.

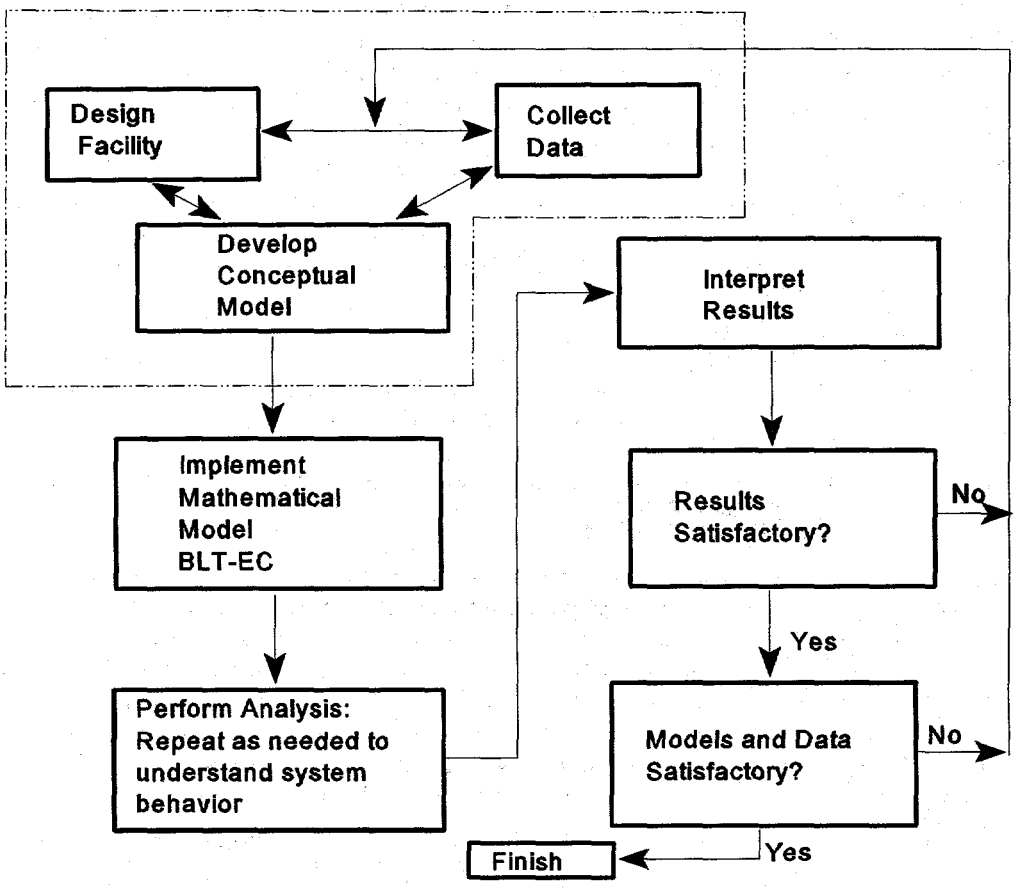


Figure 3.1 Flow chart of the procedure to examine releases from a subsurface disposal facility using BLT-EC.

Typically, five 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,
- transport,
- and chemical processes.

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

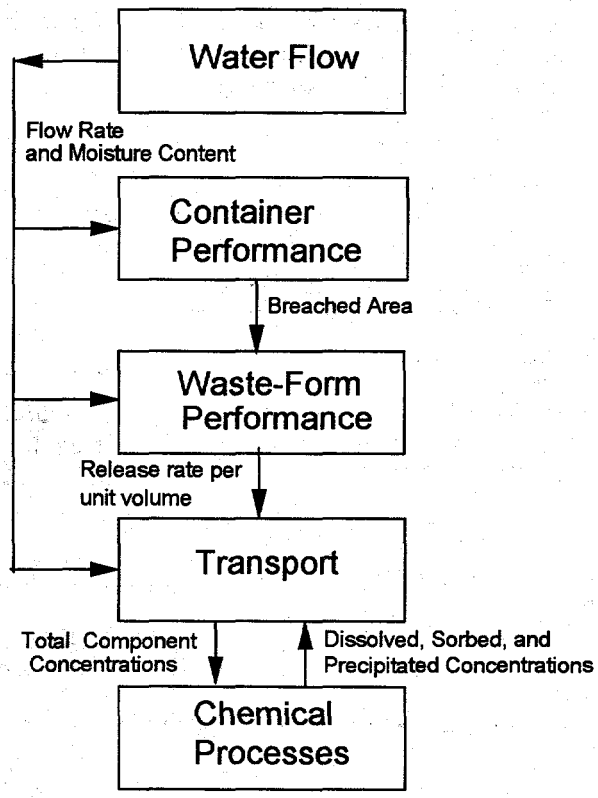


Figure 3.2 Coupling between major processes simulated in BLT-EC.

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 approach 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-EC 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-EC 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-EC. 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 key physical processes affecting transport are advection and diffusion/dispersion.

Several chemical processes potentially play a role in determining the sorption and solubility properties and, hence, mobilities of radionuclides during transport. These processes include complexation, dissolution-precipitation, reduction-oxidation, sorption, and ion exchange. Chemical process modeling requires, besides thermodynamic data, concentrations of all chemical components in the system; these are provided by the transport model. The equilibrium chemistry model provides the transport model, in return, with the data describing how the radionuclides and other chemical components in the system are distributed among the solid, dissolved, and adsorbed phases present in the pore space.

The BLT-EC 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 and provide chemistry model with total concentrations of each component.
- calculate the chemical reactions among the various chemical components and provide transport with sorbed, dissolved, and precipitated concentrations.

The last two calculational steps are repeated a user-specified number of times or until a convergent solution is obtained. If convergence is not obtained after the user specified the number of iterations, a warning message containing the degree of non-convergence, an identifier specifying the chemical component that is not converging, and the spatial location where convergence is not achieved is printed. The calculation proceeds using the latest estimate of concentration.

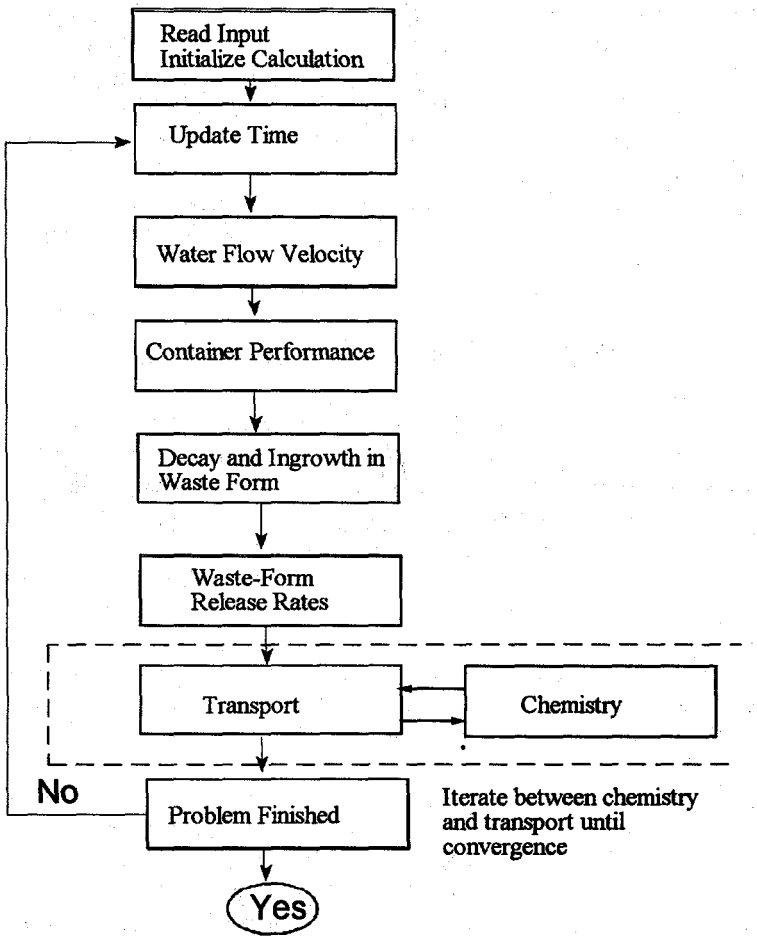


Figure 3.3 Flow chart of BLT-EC solution procedure

4 VERIFICATION PROBLEMS

It is important to verify that BLT-EC 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-EC 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 that the code is properly implemented (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-EC, in all likelihood, will not be able to reproduce the actual release rates that will eventually occur with a high degree of accuracy. The primary causes for potential 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 containers, and lack of understanding of the physical and chemical processes that control release and transport. These limitations apply to all models. BLT-EC provides an excellent method for evaluating the interaction between several processes that are believed to control release from a disposal site.

BLT-EC incorporates the waste-form leaching and container degradation models of the BLT code [Sullivan and Suen, 1989]. These models have undergone extensive verification studies previously [Sullivan and Suen, 1989, Sullivan and Suen, 1991]. Verification test cases have been performed to demonstrate that in the absence of chain decay the BLT-EC model can 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 capabilities which permit solution of reactive transport and chain decay problems. Three major classes of problem were investigated: (1) multi-species transport with chain decay; (2) release of contaminants from the waste form when ingrowth occurs due to radioactive decay; and (3) reactive transport. The results of the first two classes of problem are presented in section 4.1 through 4.3.

In section 4.4 through 4.7 we present four example problems which partially verify and demonstrate the reactive chemistry capabilities of BLT-EC. All problems make comparisons between solutions computed with HYDROGEOCHEM and BLT-EC. The first three of these problems focus on testing the equilibrium chemistry module at a single node point; complexation, redox, acid-base, and precipitation reactions are considered. The fourth problem considers both transport and reaction in a one-dimensional column. These four problems were used previously as HYDROGEOCHEM verification problems in the earlier work by Yeh and Tripathi [1990]. The final example problem is more representative of a performance assessment application and simulates the release of uranium from a hypothetical two-dimensional shallow land burial trench. This example is non-site specific and is designed to demonstrate BLT-EC's ability to couple transport, chemical reaction, container degradation, and waste-form release.

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

To demonstrate that BLT-EC 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 concentration of the radionuclide of interest is specified. 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 concentration values at specified times, Table 4.1. Linear interpolation was used for times not in the table. 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 of 273 years, essentially no material reached the right boundary. For comparison purposes, the contaminant and material specific transport

parameters for this test problem were chosen to correspond 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 contaminant 1 always decays to contaminant 2 which always decays to contaminant 3. Branching of the decay chain is not considered. The values of 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 half-life of the first member of the chain was selected 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 contaminant 1, 2, and 3 to emphasize that this problem does not represent a real decay chain.

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

Concentrations versus time at the boundary. Concentration values are in g/cm^3.				
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

	Radionuclide Dependent Properties	
Contaminant	T ½ (years)	Distribution Coefficient (K_d)
1	433	0
2	15	0
3	6540	0

Transport Properties for all Contaminants	
Moisture Content	0.1
Darcy Flux	2.47 10^{-8} 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. A constant time step of one year was used 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 BLT-MS [Sullivan, et. al., 1996] shows excellent agreement [Table 4.3]. Previously, BLT-MS was compared to VAM2D on a similar problem [Huyakorn, et al., 1989]. In that problem, the advective flux was specified at the boundary instead of the concentration, the ground water flow rate was much higher, and sorption was modeled. Agreement between BLT-MS and VAM2D was within a few percent at locations up to the first 50 meters after 273 years. In this problem, differences between the BLT-MS and BLT-EC concentrations were generally less than a few percent in the regions where the concentration is within two orders of magnitude of the maximum incoming concentration (unity). For the first contaminant, the codes gave identical results. For the second and third contaminants slight differences were observed. This is due to the treatment of ingrowth due to decay. BLT-MS calculates the transport of contaminants sequentially and uses the most recently calculated concentrations to estimate ingrowth. BLT-EC uses the values available at the beginning of the time step to estimate ingrowth. Both approximations are accurate to order Δt. Comparisons at other times during the simulation showed similar differences in predicted results. The largest differences occurred for contaminant three as shown in Table 4.5.

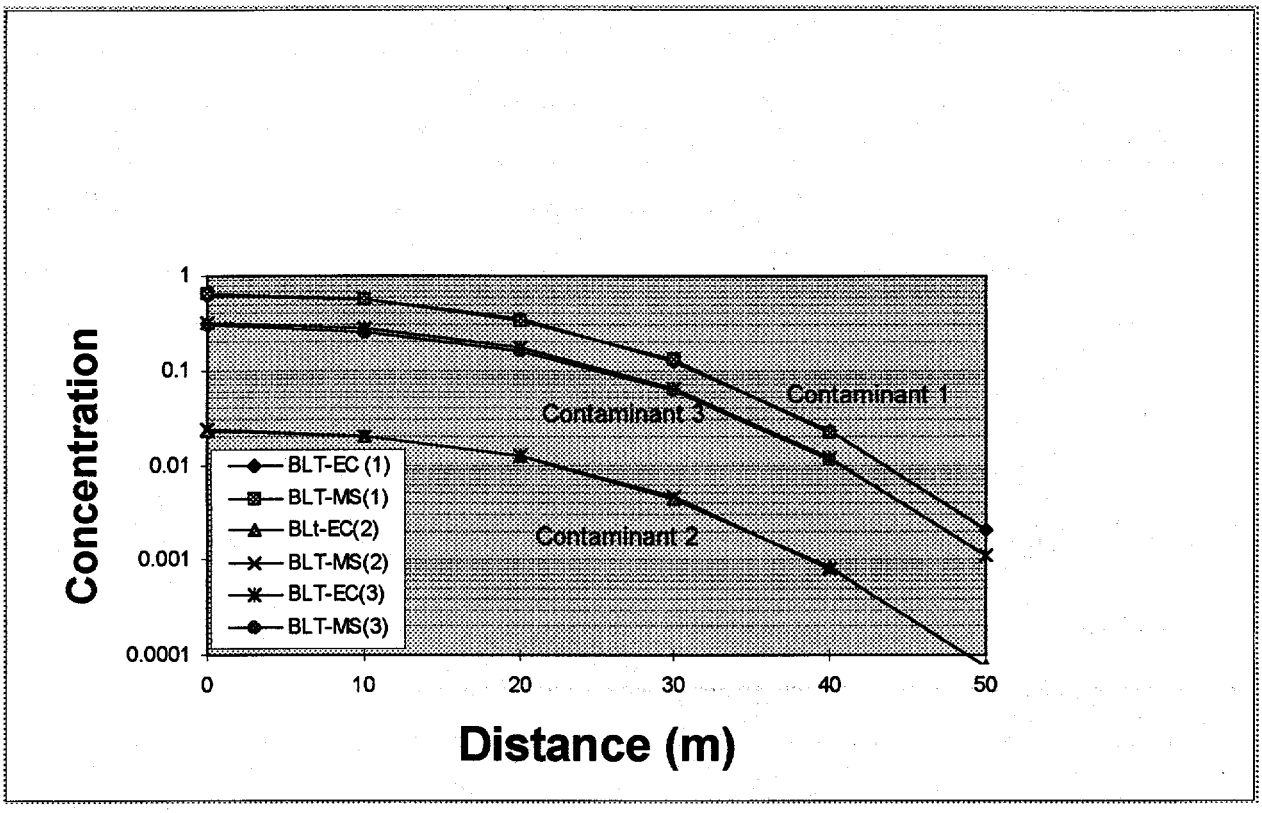


Figure 4.1 Comparison of BLT-EC and BLT-MS Predicted Concentrations at 273 Years for a Three Member Decay Chain

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

Contaminant 1	Distance (m)					
	0	10	20	30	40	50
BLT-MS	0.6476	0.5977	0.4179	0.16805	0.0359	0.00366
BLT-EC	0.6476	0.5977	0.4179	0.16805	0.0359	0.00366
Contaminant 2	Distance (m)					
	0	10	20	30	40	50
BLT-MS	0.0231	0.02144	0.0148	0.00603	0.00127	1.33E-4
BLT-EC	0.0231	0.02145	0.0148	0.00598	0.00125	1.28E-4
Difference	0	-0.00001	0.0000	0.00005	0.00002	5.0E-6
% Difference	0	-0.005	0.0	0.8	1.6	3.8
Contaminant 3	Distance (m)					
	0	10	20	30	40	50
BLT-MS	0.3244	0.3005	0.2079	0.0856	0.01834	0.00196
BLT-EC	0.3244	0.3003	0.2065	0.0839	0.01761	0.00184
Difference	0.0	0.0002	0.0014	0.0017	0.00073	0.00012
% Difference	0.0	0.1	0.7	2.0	3.9	6.1

4.2 One-dimensional Transport with Two Decay Chains

To demonstrate the ability of BLT-EC 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, contaminant 1 decays to contaminant 2 one-half the time and it decays to contaminant 3 one-half of the time. Contaminant 2 always decays to contaminant 3. The change in decay chain causes a change in the boundary conditions for the second and third contaminants. 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 contaminant 2 by a factor of one-half. This reduction in source is reflected in the boundary concentrations specified in Table 4.4. Therefore, predicted concentrations for contaminant 2 should be one-half the value of the previous test case. The situation is more complex for contaminant 3. One-half of the decay from contaminant one goes directly to contaminant 3 while the other half goes to contaminant 2 before decaying to contaminant 3. The decay directly to contaminant 3 would indicate that the predicted concentrations should be higher than in the previous case when all of contaminant 1 decayed to contaminant 2 prior to becoming contaminant 3. Due to the short-half life of contaminant 2 (15 years), this effect is not large. If the half-life of contaminant 2 were much larger (hundreds or thousands of years), the effect of branching on contaminant 3 would be much more pronounced.

Table 4.4 Incoming Concentrations at the Boundary for the Two Decay Chain Problem

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 results from BLT-MS and the previous results from BLT-EC. The results are as expected. Contaminant 1 concentrations remain unchanged, contaminant 2 concentrations have decreased by ½, and contaminant 3 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-EC 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-EC Results at 273 Years for Chain Decay and Chain Decay with Branching

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

Contaminant 1	Distance (m)					
	0	10	20	30	40	50
Single Chain	0.6476	0.5977	0.4179	0.16805	0.0359	0.00366
Branched Chain						
BLT-EC	0.6476	0.5978	0.4129	0.1681	0.0353	0.00366
BLT-MS	0.6476	0.5978	0.4129	0.1681	0.0353	0.00366
Contaminant 2	Distance (m)					
	0	10	20	30	40	50
Single chain	0.0231	0.02144	0.0148	0.00603	0.00127	1.33E-4
Branched chain						
BLT-EC	0.0115	0.01072	0.0074	0.003	0.000623	6.44E-5
BLT-MS	0.0115	0.01072	0.0074	0.003	0.000635	6.64E-5
Contaminant 3	Distance (m)					
	0	10	20	30	40	50
Single chain	0.343	0.3002	0.2064	0.0839	0.0176	0.00184
Branched chain						
BLT-EC	0.336	0.3111	0.2143	0.0873	0.0184	0.00192
BLT-MS	0.336	0.3112	0.2154	0.0886	0.0189	0.00201

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-EC 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. For the analytical release models in BLT-EC, 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-EC 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 contaminant 1 was selected to be unity while the initial inventories of contaminant 2 and 3 were zero. Therefore, any inventories of contaminant 2 and 3 are 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, contaminant 1 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-EC Predicted Rinse Release Compared to Analytical Rinse Release (Analyt)

Container	Contaminant 1		Contaminant 2		Contaminant 3	
Failure Time (yrs)	BLT-EC	Analyt	BLT-EC	Analyt	BLT-EC	Analyt
0	1.0	1.0	0	0	0	0
99	0.853	0.852	0.0309	0.0309	0.115	0.116

4.3.2 Diffusion Model

BLT-EC 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 sections 2.32. 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 parent 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 contaminant. 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 contaminants. The initial inventory of contaminant 1 was unity while the initial inventory of the second and third contaminants were zero. In the first test problem, the diffusion coefficient of each contaminant was 10^{-8} cm^2/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 contaminants. For the first contaminant, the results of the two models are essentially identical. This agreement indicates that the finite-difference model can accurately reproduce the analytical solution when ingrowth is not a concern. For the second contaminant the available mass in the two models is almost identical. This agreement is due to the short-half life of the second contaminant 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 contaminant 2 released is substantially higher for the finite-difference model as compared to the approximate analytical model. Similarly for contaminant 3, the amount released is higher for the finite-difference model. For both contaminants 2 and 3, the difference between the two models is greatest for the container that failed at t = 0. This behavior 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 Contaminant Having Identical Diffusion Coefficients

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

	Contaminant 1		Contaminant 2		Contaminant 3		Container Failure time
Model	Avl	Rel	Avl	Rel	Avl	Rel	
FD	0.376	0.359	0.0135	9.57E-3	0.1892	0.0448	0
AAM	0.375	0.365	0.0136	1.74E-3	0.2051	0.0345	0
FD	0.430	0.255	0.0154	9.10E-3	0.216	0.0634	99
AAM	0.429	0.261	0.0156	4.64E-3	0.224	0.0594	99

Assuming negligible decay of the third contaminant (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 contaminant and the mass released for each contaminant. 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 contaminant from a cylindrical waste form. The releases of the first contaminant are much higher in this case. This result is due to the waste-form 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 contaminant. For the second and third contaminants, the results were similar to those found for plane geometry. The finite-difference model predicts higher releases of each contaminant 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 Contaminant Having Identical Diffusion Coefficients

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

	Contaminant 1		Contaminant 2		Contaminant 3		Container Failure time
Model	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 procedures 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-EC, the test problem described in the previous section was modified slightly. The problem again considers three contaminants with the initial condition that contaminant one has a unit inventory while contaminant two and three are initially absent. The fractional degradation rate was set to 0.001 for all three contaminant. 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 contaminant and the mass released for each contaminant. 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 Cylindrical Waste Form with Each Contaminant Having Identical Diffusion Coefficients

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

	Contaminant 1		Contaminant 2		Contaminant 3		Container Failure time
Model	Avl	Rel	Avl	Rel	Avl	Rel	
PFD	0.470	0.221	0.0168	7.5E-3	0.24	0.048	0
AM	0.469	0.221	0.0165	7.38E-3	0.239	0.0438	0
CFD	0.342	0.387	0.0123	0.0129	0.224	0.073	0
PFD	0.534	0.129	0.0191	4.84E-3	0.271	0.039	99
AM	0.533	0.129	0.0187	4.91E-3	0.272	0.03886	99
CFD	0.441	0.238	0.0158	8.95E-3	0.1745	0.071	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.

$$Q = \int_0^t u\, L_0\, M_o\, e^{(-\lambda t)}\, \frac{A(t)}{V_0} \qquad \textbf{(4.1)}$$

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

$$Q_p = \frac{uM_o}{\lambda}\,[1 - e^{(-\lambda t)}] \qquad \textbf{(4.2)}$$

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-EC analytical model and plane finite-difference model. For the container that fails at 0.99 years, M_o 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-EC model predictions. The above relationship could be generalized by replacing $M_o\ e^{(-\lambda t)}$ by the expression for the mass as a function of time as determined from the Bateman equations.

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

Using these expressions,

$$L_0 A(t)/V_0 = 2(1 - ut) \tag{4.4}$$

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

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

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.

4.4 Aqueous Complexation

This problem considers aqueous complexation of the following components, Na^+, Pb^{2+}, H^+, and Cl^- in a solution having a fixed hydrogen activity of pH=7.10535. The initial analytical concentrations (mole/liter) of these components are $1.0x10^{-1}$, $2.9x10^{-4}$, $1.0x10^{-1}$, and $2.9x10^{-4}$, respectively. Two BLT-EC simulations were performed; (1) reactions are specified a priori and correspond with the reactions considered in the HYDROGEOCHEM simulation, and (2) reactions are not predefined and are automatically selected by the equilibrium module and thermodynamic database. The HYDROGEOCHEM solution was obtained from Yeh and Tripathi [1990]. Species concentrations at equilibrium, along with equilibrium constants, are presented in Table 4.10. Slight differences in computed equilibrium concentrations between simulations are apparent. By comparing the tabulated results we see that BLT-EC concentration results, $C^{(2)}$, agree closely with the HYDROGEOCHEM results, the exception being hydrogen concentration. It is stated in the HYDROGEOCHEM problem description [Yeh and Tripathi, 1990] that hydrogen *activity* is fixed at pH=7.10535, yet the negative log of the computed equilibrium hydrogen *concentration* is given as 7.11 (7.10535 rounded up). However, activity and concentration values are equal only in solutions of very low ionic strength. Note that the negative log of the BLT-EC hydrogen concentration, which corresponds to pH = 7.10535, is 6.99.

BLT-EC results, $C^{(3)}$, are computed by allowing BLT-EC to select, from its database, the relevant reactions. These results are significantly different than the HYDROGEOCHEM results because a significant quantity of $Pb(OH)_2$ precipitates. As a result, the concentrations of free Pb^{2+} differ substantially. This latter simulation illustrates the advantage of having the computational capability to automatically access a thermodynamic database. This capability eases the burden of having to predefine the reactions, which may lead to errors or misleading results if important reactions are neglected. Moreover, an automatically accessible database eliminates the cumbersome and error prone task of organizing and inputting the required stoichiometric and thermodynamic constants.

For further verification, this problem was also examined using MINTEQA2. The results of BLT-EC, concentrations $C^{(3)}$, and MINTEQA2 were in exact agreement with each other.

4.5 Acid-Base and Redox Reactions

This problem considers acid-base and redox reactions involving Fe^{3+}, SO_4^{2-}, H^+, and e^-. The initial concentrations (mole/liter) of these components are, respectively, $2.0x10^{-1}$, $3.0x10^{-1}$, $1.0x10^{-2}$, and $1.3x10^{-8}$. Equilibrium concentrations of these components, associated dependent species, and equilibrium constants are given in Table 4.11. In this problem, the reactions that are automatically selected by BLT-EC correspond with the reactions considered in the HYDROGEOCHEM simulation. Disagreements in concentrations are significant for several species, particularly for Fe^{3+}, $Fe(OH)_2^+$, and HSO_4^-. These differences are likely do in part to differences between equilibrium constants for Fe species. Comparisons between MINTEQA2 and BLT-EC showed exact agreement with each other.

4.6 Precipitation -Dissolution Reactions

This problem considers complexation and precipitation-dissolution reactions involving Na^+, UO_2^{2+}, H^+, CO_3^{2-}, SO_4^{2-}, and Cl^-. The equilibrium results are presented in Table 4.12. The HYDROGEOCHEM concentrations are denoted by $C^{(1)}$. Two BLT-EC simulations were performed. In the first simulation, BLT-EC was allowed to select, from its database, the relevant reactions; the resulting concentrations are denoted by $C^{(2)}$. Moreover, several of the equilibrium constants differ from those used in the HYDROGEOCHEM simulation. In the second BLT-EC simulation, the database was modified so that the reactions and equilibrium constants matched those in the HYDROGEOCHEM calculations. Reasonable agreement between the HYDROGEOCHEM and BLT-EC results is obtained with very slight differences occurring between the two BLT-EC simulations. In addition, results computed using BLT-EC (i.e., $C^{(2)}$) and MINTEQA2 were in exact agreement.

4.7 Reactive Transport

This application compares BLT-EC and HYDROGEOCHEM simulation results for a problem involving transport with reaction in a one-dimensional column. The reactions involve components Ca^{2+}, Mg^{2+}, CO_3^{2-}, SO_4^{2-}, and H^+ in water. Twelve aqueous species and eight minerals were considered as shown in Table 4.13.

The column is 100 dm long with a porosity of 0.3, a bulk density of 1.2 g/cc, and dispersivity of 5 dm. Water flow is from right to left at a velocity of 0.5 dm/day. For each simulation the column was partitioned into one hundred finite elements of size 1 dm x 1 dm. Simulations were conducted for 100 days using a constant time step of 0.5 days. Two iterations between transport and reaction calculations were allowed.

Initial conditions in the column were the following. The pH varied linearly from 7.7 at the left end to 8.0 at the right end (the pH is held fixed during the simulation). The initial Ca^{2+} concentration was uniform at 10^{-4} mole/liter. The concentration of Mg^{2+} decreased linearly from $5x10^{-3}$ mole/liter at the left end to 10^{-3} mole/liter at the right end. The SO_4^{2-} concentration also decreased linearly from left to right, ranging from $2x10^{-3}$ to 10^{-4} mole/liter. The CO_3^{2-} concentration increased linearly from $2x10^{-4}$ mole/liter at the left end to $8x10^{-3}$ mole/liter at 85 dm and then finally to $8.6x10^{-3}$ mole/liter at the right end.

At the right end of the column the boundary conditions describing the composition of the incoming water were as follows: the pH was held fixed at 8.0; the CO_3^{2-}, Mg^{2+}, and SO_4^{2-} concentrations were constant at $2x10^{-3}$, 10^{-3}, and $2x10^{-3}$ mole/liter, respectively; and the concentration of Ca^{2+} was fixed at 10^{-4} mole/liter between 0.0 and 1.0 days, $9x10^{-3}$ mole/liter between 1.0 and 9.5 days, and 10^{-4} mole/liter thereafter.

Simulation results showing calcium carbonate and magnesium carbonate at 50 and 100 days are presented in Figures 4.2 - 4.5. HYDROGEOCHEM results are represented by a solid line and BLT-EC results are represented by triangle symbols. As shown, excellent agreement between the simulations was obtained. Initially magnesium carbonate precipitation existed throughout most of the column. Near the right end of the column, competition for carbonate by the injected calcium pulse, see Figure 4.2, caused gradual dissolution of magnesium carbonate as shown in Figure 4.4. Note that the concentration scales in the figures at 50 and 100 days are different to accommodate the substantial increase in magnesium

carbonate precipitation and decrease in calcium carbonate precipitation at the right end after the passing of the injected calcium pulse.

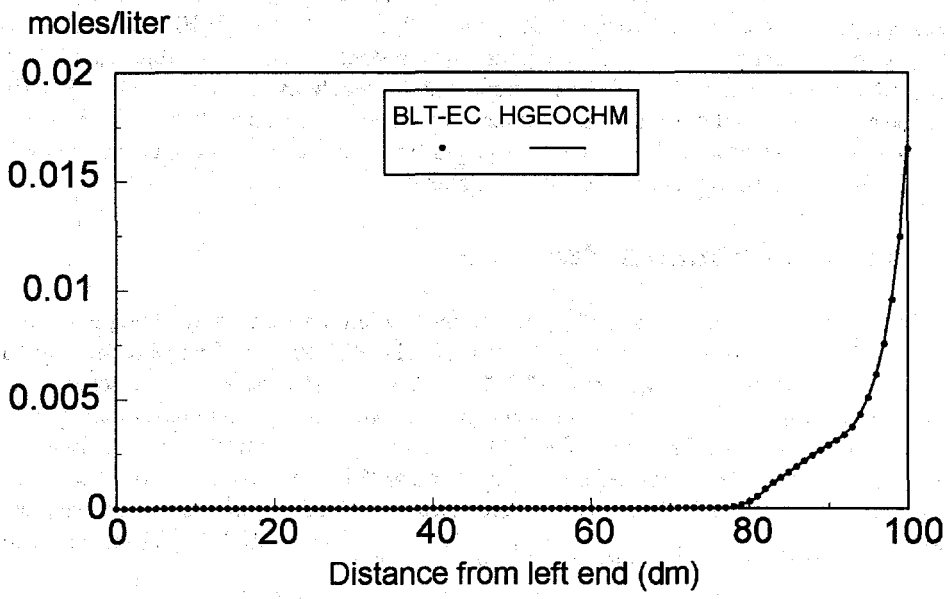


Figure 4.2 Distribution of Calcium Carbonate at 50 Days.

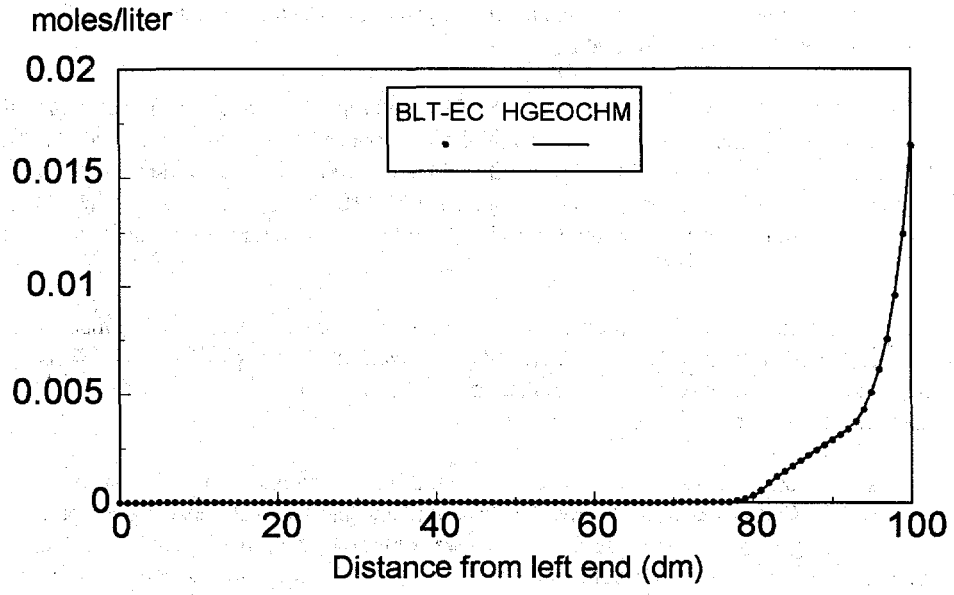


Figure 4.3 Distribution of Calcium Carbonate at 100 days.

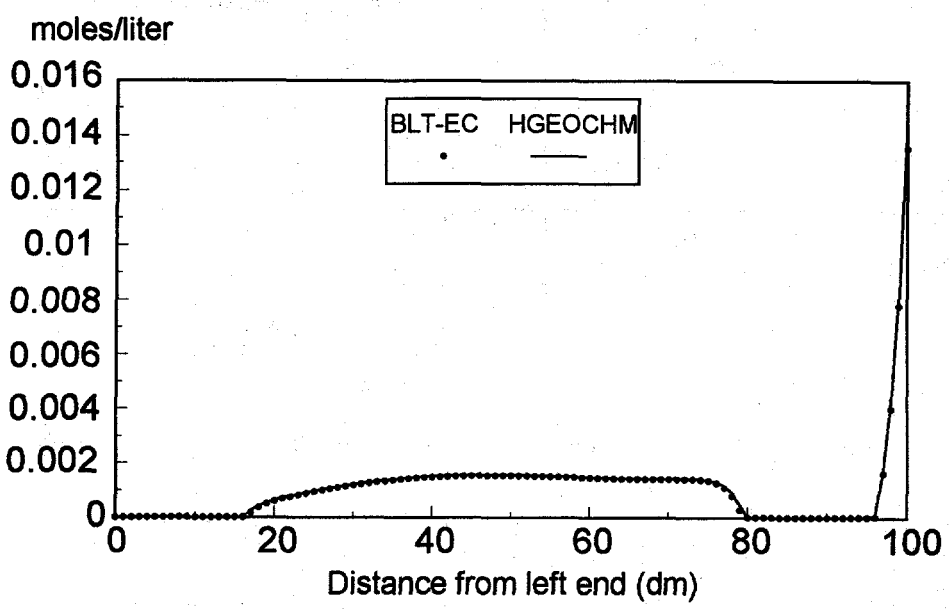


Figure 4.4 Distribution of Magnesium Carbonate at 50 Days.

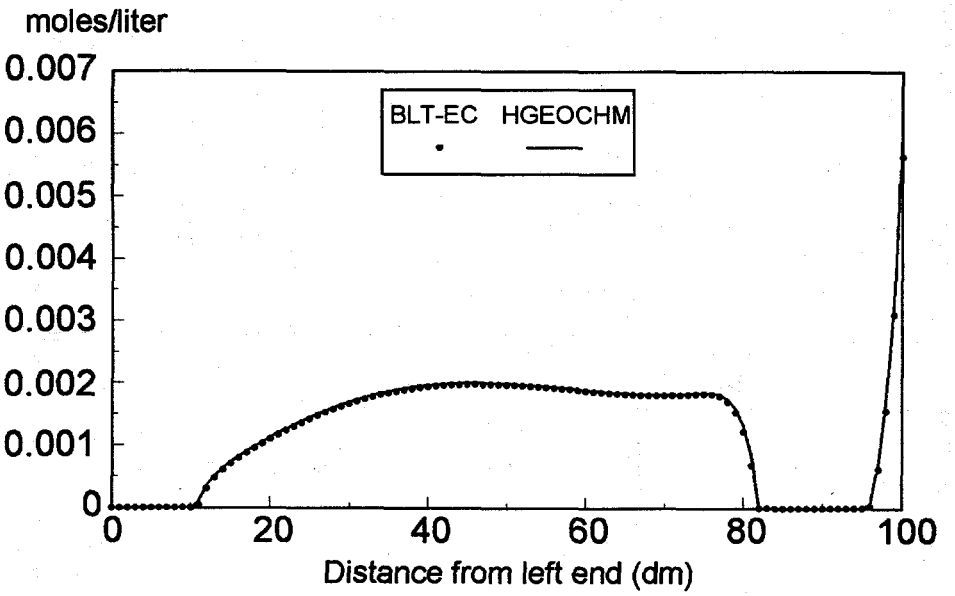


Figure 4.5 Distribution of Magnesium Carbonate at 100 Days.

Table 4.10 Species Concentrations at Equilibrium for the Complexation Problem

Species	Log K[1]	C[1]	Log K[2]	C[2]	Log K[3]	C[3]	Components and Stoichiometry			
							Na^+	Pb^{2+}	H^+	Cl^-
Na^+	0.00	1.000E-1	0.00	1.000E-1	0.00	1.000E-1	1	0	0	0
Pb^{2+}	0.00	2.570E-4	0.00	2.600E-4	0.00	2.421E-6	0	1	0	0
H^+	0.00	7.845E-8	0.00	1.012E-7	0.00	1.012E-7	0	0	1	0
Cl^-	0.00	1.000E-1	0.00	1.000E-1	0.00	1.000E-1	0	0	0	1
OH^-	-13.99	1.660E-7	-13.99	1.647E-7	-13.99	1.646E-7	0	0	-1	0
$Pb(OH)^+$	-7.71	3.090E-5	-7.71	2.999E-5	-7.71	2.796E-7	0	1	-1	0
Other species from database:										
$Pb_3(OH)_4^{2+}$	---	---		---	-23.88	6.369E-14	0	3	-4	0
$Pb(OH)_4^{2-}$	---	---		---	-39.69	1.261E-17	0	1	-4	0
$PbCl^+$	---	---		---	1.60	3.485E-6	0	1	0	1
$PbCl_2$	---	---		---	1.80	3.245E-7	0	1	0	2
$PbCl_3^-$	---	---		---	1.69	2.631E-8	0	1	0	3
$PbCl_4^{2-}$	---	---		---	1.38	2.099E-9	0	1	0	4
$Pb(OH)_2$	---	---		---	-17.12	1.047E-9	0	1	-2	0
$Pb(OH)_3^-$	---	---		---	-28.06	2.016E-13	0	1	-3	0
Pb_2OH^{3+}	---	---		---	-6.36	4.193E-11	0	2	-1	0
Precipitated solids from database:										
$Pb(OH)_2$	---	---		---	-8.15	2.835E-4	0	1	-2	0

C[1]HYDROGEOCHEM solution
C[2]BLT-EC solution
C[3]BLT-EC solution involving additional reactions provided by MINTEQA2 database

Table 4.11 Species Concentrations at Equilibrium for the Acid-Base and Redox Reactions Problem

Species	Log K[1]	C[1]	Log K[2]	C[2]	Components and Stoichiometry			
					Fe^{3+}	SO_4^{2-}	H^+	e^-
Fe^{3+}	0.00	6.516E-4	0.00	1.398E-2	1	0	0	0
SO_4^{2-}	0.00	2.148E-2	0.00	5.598E-2	0	1	0	0
H^+	0.00	1.633E-3	0.00	8.528E-3	0	0	1	0
e^-	0.00	4.426E-19	0.00	2.772E-19	0	0	0	1
OH^-	-13.99	6.266E-12	-13.99	2.273E-12	0	0	-1	0
$FeSO_4^+$	3.92	1.167E-1	3.92	1.198E-1	1	1	0	0
$Fe(SO_4)_2^-$	5.42	7.925E-2	5.42	5.599E-2	1	2	0	0
$FeOH^{2+}$	-2.19	2.576E-3	-2.19	2.771E-3	1	0	-1	0
$Fe(OH)_2^+$	-5.67	5.236E-4	-5.67	5.481E-5	1	0	-2	0
$Fe(OH)_3$	-13.60	3.767E-9	-13.60	6.972E-11	1	0	-3	0
$Fe(OH)_4^-$	-21.60	2.307E-14	-21.60	1.694E-16	1	0	-4	0
$Fe_2(OH)_2^{4+}$	-2.95	1.791E-4	-2.95	2.965E-3	2	0	-2	0
$Fe_3(OH)_4^{5+}$	-6.31	1.914E-5	-6.31	4.871E-4	3	0	-4	0
$FeSO_4$	15.21	1.005E-8	2.25	5.103E-9	1	1	0	1
$FeOH^+$	3.51	5.715E-16	-9.50	1.492E-16	1	0	-1	1
$Fe(OH)_2$	-7.56	2.979E-24	-20.61	1.375E-25	1	0	-2	1
$Fe(OH)_3^-$	-17.99	6.776E-32	-31.01	1.241E-33	1	0	-3	1
HSO_4^-	1.99	3.428E-3	1.99	1.223E-2	0	1	1	0
Fe^{2+}	13.01	2.951E-9	13.03	7.897E-9	1	0	0	1

C[1] HYDROGEOCHEM solution
C[2] BLT-EC solution

Table 4.12 Species Concentrations at Equilibrium for the Precipitation-Dissolution Problem

Species	Log K	$C^{(1)}$	$C^{(2)}$	$C^{(2*)}$	Components and Stoichiometry					
					Na^+	UO_2^{2+}	H^+	CO_3^{2-}	SO_4^{2-}	Cl^-
Na^+	0.00	3.532E-1	3.567E-1	3.531E-1	1	0	0	0	0	0
UO_2^{2+}	0.00	2.512E-9	1.053E-8	2.649E-9	0	1	0	0	0	0
H^+	0.00	1.000E-7	1.412E-7	1.000E-7	0	0	1	0	0	0
CO_3^{2-}	0.00	1.194E-6	2.289E-6	1.187E-6	0	0	0	1	0	0
SO_4^{2-}	0.00	3.614E-3	6.896E-3	3.611E-3	0	0	0	0	1	0
Cl^-	0.00	4.797E-1	4.800E-1	4.800E-1	0	0	0	0	0	1
$NaCO_3^-$	1.27	7.834E-6	3.809E-6	7.767E-6	1	0	0	1	0	0
$NaHCO_3$	10.08	5.047E-4	1.581E-4	5.038E-4	1	0	1	1	0	0
$NaSO_4^-$	0.70	6.383E-3	3.103E-3	6.389E-3	1	0	0	0	1	0
$UO_2(OH)^+$	-5.30	1.259E-7	1.847E-7	1.308E-7	0	1	-1	0	0	0
$(UO_2)_2(OH)_2^{2+}$	-5.68	1.318E-9	5.658E-9	1.424E-9	0	2	-2	0	0	0
$(UO_2)_3(OH)_4^{2+}$	-11.88	2.089E-10	9.184E-10	2.312E-10	0	3	-4	0	0	0
$(UO_2)_3(OH)_5^+$	-15.82	2.399E-7	3.692E-7	2.615E-7	0	3	-5	0	0	0
$(UO_2)_4(OH)_7^+$	-21.90	5.012E-8	7.901E-8	5.596E-8	0	4	-7	0	0	0
$(UO_2)_3(OH)_7^-$	-28.34	7.244E-6	1.083E-5	7.669E-6	0	3	-7	0	0	0
UO_2CO_3	9.65	1.337E-5	1.736E-5	3.958E-5	0	1	0	1	0	0
$UO_2(CO_3)_2^{2-}$	17.08	4.295E-4	3.513E-4	3.752E-4	0	1	0	2	0	0
$UO_2(CO_3)_4^{4-}$	21.70	2.138E-5	6.327E-4	2.220E-5	0	1	0	3	0	0
$(UO_2)_2CO_3(OH)_3$	-1.18	4.977E-4	2.310E-4	5.266E-4	0	2	-3	1	0	0
UO_2Cl^+	-0.21	7.430E-10	7.841E-10	7.841E-10	0	1	0	0	0	1

Table 4.12 Continued

Species	Log K	$C^{(1)}$	$C^{(2)}$	$C^{(2*)}$	Components and Stoichiometry					
					Na^+	UO_2^{2+}	H^+	CO_3^{2-}	SO_4^{2-}	Cl^-
UO_2SO_4	2.95	8.091E-9	2.186E-9	5.031E-9	0	1	0	0	1	0
$UO_2(SO_4)_2^{2-}$	4.00	3.273E-10	5.037E-10	5.485E-10	0	1	0	0	2	0
HCO_3^-	10.32	2.495E-3	1.737E-3	2.535E-3	0	0	1	1	0	0
H_2CO_3	16.67	5.585E-4	2.497E-4	5.693E-4	0	0	2	1	0	0
HSO_4^-	1.99	3.532E-8	2.379E-8	3.505E-8	0	0	1	0	1	0
$UO_2(OH)_2^+$ (Schoepite)	-5.40	1.517E-3	1.502E-3	1.486E-3	0	1	-2	0	0	0
UO_2CO_3 (Rutherfordin)	13.03	---	---	---	0	1	0	1	0	0

$C^{(1)}$HYDROGEOCHEM solution
$C^{(2)}$BLT-EC solution
$C^{(2*)}$BLT-EC solution (activity coefficients = 1)

Table 4.13 Chemical Species for the Reactive Transport Problem

Species	Log K	Components and Stoichiometry				
		H^+	CO_3^{2-}	Ca^{2+}	Mg^{2+}	SO_4^{2-}
		Aqueous Species				
H^+	0.0	1	0	0	0	0
CO_3^{2-}	0.0	0	1	0	0	0
Ca^{2+}	0.0	0	0	1	0	0
Mg^{2+}	0.0	0	0	0	1	0
SO_4^{2-}	0.0	0	0	0	0	1
OH^-	-13.99	-1	0	0	0	0
$CaCO_3$	3.22	0	1	1	0	0
$CaHCO_3^+$	11.43	1	1	1	0	0
$CaSO_4$	2.31	0	0	1	0	1
$CaOH^+$	-12.85	-1	0	1	0	0
$MgCO_3$	2.98	0	1	0	1	0
$MgHCO_3^+$	11.40	1	1	0	1	0
$MgSO_4$	2.25	0	0	0	1	1
$MgOH^+$	-11.44	-1	0	0	1	0
HCO_3^-	10.32	1	1	0	0	0
H_2CO_3	16.67	2	1	0	0	0
HSO_4^-	1.99	1	0	0	0	1
Minerals allowed to precipitate						
Calcite	8.48	0	1	1	0	0
$MgCO_3$	8.20	0	1	0	1	0
Gypsum	4.62	0	0	1	0	1
Calcium Hydroxide	-21.90	-1	0	1	0	0
$Mg_2(OH)_2CO_3$	-9.65	-2	1	0	2	0
$Mg_5(OH)_2(CO_3)_4$	9.72	-2	4	0	5	0
$Mg(OH)_2$	-16.80	-2	0	0	1	0
$MgSO_4$	2.14	0	0	0	1	1

5 BLT-EC DATA INPUT GUIDE

This section gives the input requirements for BLT-EC's main input file. BLT-EC handles up to 25 different contaminants in a single run and can simulate multiple decay chains and chemical reactions. In many respects, the input variables of BLT-EC 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-EC input formats, there are also substantial differences. The BLT-EC code uses an annotated input deck 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-EC 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.

A BLT-EC input file is divided into 24 data sets, Table 5.1. Each data set is a unique grouping of input variables which perform a specific function within BLT-EC. In the BLT-EC input file, 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. The remainder of this section proceeds through all 24 data sets providing definition of each variable in BLT-EC and the FORTRAN read statements and the logic used when deciding which input to read.

When using BLT-EC, the code asks for the name of the input file for this problem. This file is designated as unit 7. BLT-EC creates a file called ECHO.DAT. This file echos the input as it is read. It is extremely useful in determining the cause of an error in the input deck. In BLT-EC ECHO.DAT is designated as unit 60. These unit designations can be seen in the FORTRAN programming found in BLT-EC's subroutine GM2DXZ.

In addition to the main input file described in this chapter, BLT-EC may use two additional input files. If requested by input read in the main file, water flow rates, moisture content, and geometry definition may be read from an auxiliary file. This auxiliary file may be created by the code FEMWATER or constructed on an ad hoc basis following the input format required for this file. Instructions for creating a FEMWATER input file can be found in Sullivan and Suen, 1989. An example FEMWATER input file is presented in Appendix B. The other input file that may be required defines the chemical reactions that are simulated. A complete discussion of the chemistry input is provided in Chapter 6.

5.1 Input File

All data sets must be preceded by an input line containing the data set name. Data Set 1 is one of the few areas where formatted input is required.

5.1.1 Data Set 1: Title

Formatted input for the problem number and description are read on one line.

Definitions:

NPROB = Problem number.

TITLE = Alpha-numeric description of the problem. It may contain up to 70 characters from column 6 to column 75.

Table 5.1 BLT-EC Data Sets

Data Set	Title	Types of Values Defined
1	Problem Identification	Title and problem identifier
2	Integer Velocity, Storage, and Restart Control	Selection of source for velocities and storage and restart control
3	Container and Waste Parameters	Number of contaminants, containers and waste types
4	Integer Integration Parameters	Numerical solution control factors
5	Integer Solution 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 Integration Control Parameters	Time step size, maximum simulation time
11	Parameters for Nonlinear Solve	Iteration, relaxation, tolerance, and upstream weighting factors
12	Facility Width and Grid Generation Data	X and Z locations, element definitions, automatic mesh generation if selected
13	Porous Media Properties	Diffusion, dispersion, coefficients, porosity
14	Material Type Correction	Redefine material index
15	Initial/Pre-Initial Conditions	Initial concentrations for all components
16	Variable Boundary Conditions	Flux at the specified boundaries
17	Dirichlet Boundary Conditions	Concentration at the specified boundaries
18	Element Source/Sink Data	Element source strength versus time and their location
19	Well (POINT) Source/Sink Data	Point source strength versus time and their location
20	Element Source/Sink(LEACHING) Data	Element source strength versus time and their location (For corrosion and barrier degradation)
21	Waste Container Parameters	Container performance parameters, container locations
22	Waste Form And Leaching Info	Waste form performance parameters, inventory
23	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.

Format:

Subroutine	Statement	
GM2DXZ		
		READ(7,6) LABEL
	100	READ(7,40) NPROB, (TITLE(I),I=1,7)
	40	FORMAT(I5,7A10,3I1,I2)
	6	FORMAT(A79)

5.1.2 Data Set 2: Integer Velocity, Storage, and Restart Control Parameters

Free formatted input contains 4 integers. Four lines of input are required between the data in data sets 1 and 2. The first line is typically blank, indicating the end of the data set. The next three lines define the data set and variables (examples of BLT-EC input files are provided in Appendix B).

Definitions:

KVI = Velocity input control,
- 1 = input for velocity and moisture content read in Data Set 23,
1 = steady state velocity and moisture content input via logical unit 1,
2 = transient velocity and moisture content input via auxiliary storage logical unit 1.

KSTR = Auxiliary storage output control;
0 = no storage,
1 = output stored in logical unit 2.

NSTR = Number of logical records to be read via Logical Unit 3 for restarting calculation;
0 = no restart.

KSS = Steady-state simulation control;
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.

Format:

Subroutine	Statement	
DATAHT		
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,*) KVI,KSTR,NSTR,KSS
	6	FORMAT(A79)

5.1.3 Data Set 3: Integer Parameters For Containers and Waste

Free formatted input contains 5 integers.

Definitions:

NCON = Number of containers.

NCTYPE = Number of container types.

NWTYPE = Number of waste types.

IDIFF = Used to select the waste-form diffusion controlled release model. In all cases, the analytical 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. Waste form is treated as a plane with half-length POREL(I), defined in Data Set 21, and diffusion occurs into a semi-infinite medium. The boundary condition is the concentration approaches zero as X approaches infinity.

1 = plane geometry, finite medium model. 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, or 1 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, Data Set 22). 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 input with units of moles.

1 = waste form inventory, initial conditions, and boundary conditions input with units of curies (presently not an option). For typical geochemical calculations, may of the components will not be radioactive. Therefore, this option is not allowed.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) NCON,NCTYPE,NWTYPE,IDIFF,IACT
6	FORMAT(A79)

5.1.4 Data Set 4: Integration Integer Parameters

Free formatted input contains 4 integers.

Definitions:

ILUMP = Mass matrix lumping control,
0 = no lump,
1 = lump. Lumping leads to a more diagonally dominant matrix representation of the system which tends to be more stable but less accurate.

IMID = Mid difference control,
0 = no mid-difference,
1 = mid-difference and W in DATA SET 10 should be 1.

IWET = Weighting function control,
0 = Galerkin weighting,
1 = upstream weighting.

IOPTIM = Optimization factor computing indicator,
1 = optimization factor is to be computed,
0 = optimization factor is set to 1.0, 0.0, or -1.0.

Format:

Subroutine	Statement	
DATAHT		
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,*) ILUMP,IMID,IWET,IOPTIM
	6	FORMAT(A79)

5.1.5 Data Set 5: Integer Solution Control Parameters

Free formatted input contains 5 integers.

Definitions:

NTI = Number of time steps or time increments.

NITER = Number of iterations allowed between transport and chemical equilibrium solutions. Typically less than 10.

NDTCHG = Number of times the time step size 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.

NPITER = Number of iterations allowed for solving the linear transport matrix equation with pointwise iteration. Not used if IPNTS=0. In this case, the matrix equation for transport is solved by direct conversion

IPNTS = Is pointwise iteration method to be used to solve the matrix equations?
0 = no,
1 = yes.

NOTE: NTI can be computed by NTI = I1 + 1 + I2 + 1, where
I1 = largest integer not exceeding Log(DELMAX/DELT)/LOG(1+CHNG),
I2 = largest integer not exceeding (RTIME-DELT*((1+CHNG)**(I1+1)-1)/CHNG)/DELMAX,RTIME = real simulation time, DELMAX, DELT, and CHNG are defined in DATA SET 10.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) NTI,NITER,NDTCHG,NPITER,IPNTS
6	FORMAT(A79)

5.1.6 Data Set 6: Grid and Element Parameters

Free formatted input contains 5 integers.

Definitions:

NNP = Number of nodal points.

NEL = Number of elements.

NMAT = Number of material types.

NCM = Number of elements with material property correction. 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.

KMESH = Mesh generator flag,
0 = do not use mesh generator, specify all locations in data set 12.
1 = use mesh generator, specify mesh in data set 12..

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) NNP,NEL,NMAT,NCM,KMESH
	6 FORMAT(A79)

5.1.7 Data Set 7: Integer Parameters For Boundary Conditions

A) DIRICHLET BOUNDARY CONDITIONS DATA

Free formatted input contains 3 integers. The specified values apply to all components in the simulation.

Definitions:

NDNP	=	Number of Dirichlet nodes.
NDPR	=	Number of Dirichlet profiles, should be greater than or equal to 1.
NDDP	=	Number of data points in each of the NDPR profiles, should be greater than or equal to 2.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) NDNP,NDPR,NDDP
	6 FORMAT(A79)

B) VARIABLE BOUNDARY CONDITIONS DATA

Free formatted input contains 4 integers. The specified values apply to all components.

Definitions:

NVNP	=	Number of variable-boundary nodes.
NVES	=	Number of variable-boundary sides.
NVPR	=	Number of incoming fluid concentration profiles to be applied to variable-boundary element sides.
NVDP	=	Number of data points in each of the NVPR profiles.

Format:

Subroutine	Statement	
DATAHT		
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,*) NVNP,NVES,NVPR,NVDP
	6	FORMAT(A79)

5.1.8 Data Set 8: Integer Parameters For Sources

A) ELEMENT SOURCE/SINK DATA

Free formatted input contains 3 integers. The specified values apply to all components in the simulation.

Definitions:

NSEL	=	Number of source/sink elements.
NSPR	=	Number of source/sink profiles.
NSDP	=	Number of records in each source/sink profile.

Format:

Subroutine	Statement	
DATAHT		
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,*) NSEL,NSPR,NSDP
	6	FORMAT(A79)

B) POINT SOURCE/SINK DATA

Free formatted input contains 3 integers. The specified values apply to all components in the simulation.

NWNP	=	Number of well or point source/sink nodes.
NWPR	=	Number of well or point source/sink strength profiles.
NWDP	=	Number of data points in each of the NWPR profiles.

Format:

Subroutine	Statement	
DATAHT		
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,*) NWNP,NWPR,NWDP
	6	FORMAT(A79)

C) ELEMENT SOURCE/SINK DATA (LEACHING)

Free formatted input contains 3 integers. The specified values apply to all components in the simulation.

Definitions:

NLEL	=	Number of leaching source elements.
NLPR	=	Number of leaching source profiles.
NLDP	=	Number of data pairs in each leaching source profile.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) NLEL,NLPR,NLDP
	6 FORMAT(A79)

5.1.9 Data Set 9: Chemical Component Information

Line 1: Free formatted input contains 3 integers.

Definitions:

NON	=	Number of components.
NONC	=	Number of non-conservative components
LNH	=	The number K corresponding to the hydrogen component. Hydrogen component is signified by CNAM = Hydrogen. If hydrogen is not modeled, set LNH to a value greater than NON.
LNE	=	The number K corresponding to the electron component. If electrons are not modeled, set LNE to a value greater than NON.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) NON,NONC,LNH,LNE
	6 FORMAT(A79)

Line 2 through Line (NON + 1): Free formatted input contains 9 variables.

Definitions:

CNAM(J)	=	Component name of the J^{th} component.
IDN(J)	=	Identification number of the J^{th} component.
INDC(J)	=	Indicator of the J^{th} component, 0 = conservative component, i.e., does not undergo chemical reaction. 1 = nonconservative mobile component. 2 = immobile component, 3 = component whose activity is fixed.
CSAT(J)	=	Solubility limit for contaminant J (mole/liter). This value cannot be input with mass units of curies.
DCAY(J)	=	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-EC.
JDOTER1	=	Component number of progeny number 1 of the J^{th} component.
DFRAC1	=	Branching fraction for decay of component J to daughter product number 1.
JDOTER2	=	Component number of progeny number 2 of the J^{th} component.
DFRAC2	=	Branching fraction for decay of component J to daughter product number 2.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*)CNAM(J),IDN(J),INDC(J),CSAT(J),DCAY(J),JDOTER1
	1,DFRAC1,JDOTER2,DFRAC2
6	FORMAT(A79)

5.1.10 Data Set 10: Time Integration Control Parameters

Free formatted input contains 6 real numbers, followed by NDTCHG (specified in data set 5) real numbers. Note two label cards are required, between the end of the first set of variables and the time when the time step is changed.

Definitions:

DELT	=	Initial time-step size, (yr).
CHNG	=	Percentage of change in time step size in each of the subsequent time increment, (dimensionless in decimal point).
DELMAX	=	Maximum value of DELT, (yr).

TMAX = Maximum simulation time, (yr).

W = Time derivative weighting factor for all terms except for the velocity terms;
0.5 = Crank-Nicolson central difference schemes,
1.0 = backward difference scheme.

WV = Time integration factor for the velocity terms,
0.0 = forward difference (explicit),
0.5 = central difference,
1.0 = backward difference (complete implicit).

TDTCH (1) = Time when the first time to reset time-step size (yr),

TDTCH(2) = Time when the second time to reset time-step size (yr),

TDTCH(N) = Time when the N^{th} time to reset time-step size (yr).

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) DELT,CHNG,DELMAX,TMAX,W,WV
	DELT0=DELT
	IF(TMAX.LE.0.0) TMAX=1.0D38
	IF(NDTCHG.GT.0) THEN
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) (TDTCH(I)I=1,NDTCHG)
	ELSE
	NDTCHG=1
	TDTCH(1)=TMAX+1.0
	ENDIF
6	FORMAT(A79)

5.1.11 Data Set 11: Real Parameters for Nonlinear Solve

Free formatted input contains 4 real numbers.

Definitions:

OME = Iteration parameter for solving nonlinear equation;
0.0 - 1.0 = under-relaxation,
1.0 = exact relaxation,
1.0 - 2.0 = over-relaxation.

OMI = Relaxation parameter for pointwise solution of the matrix equation;
0.0 - 1.0 = under-relaxation,
1.0 = exact relaxation,
1.0-2.0 = over-relaxation.

TOLA = Error tolerance for solving the nonlinear chemistry equations. Half of its value is used as the tolerance for solving the linearized matrix equation for transport with pointwise iteration, IPNTS=1 in Data Set 5.

APHAG = Upstream weighting factor if IOPTIM = 0, (Data Set 4). Values are between 0.0 and 1.50 when the advection form of the equation is used. If APHAG .GE. 1.34D0, the program will choose appropriate values of weighting factor. When the conservative form of the equation is used or when IOPTIM = 1, this value is not used by the program.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) OME,OMI,TOLA,APHAG
	6 FORMAT(A79)

5.1.12 Data Set 12: Facility Width And Grid Generation Data

Data set 12 is composed of three sets of information, to be used according to conditions being met. Facility width data comprise data set 12A, and is required input. Nodal coordinate data and node connectivity comprise data set 12B, and is required when KVI is less than or equal to zero and when KMESH is less than or equal to zero. Automatic grid generation data comprise data set 12C. Data set 12C is required when KVI is less than or equal to zero and when KMESH is greater than zero. For KVI greater than zero, data are read via an auxiliary file and labels are required (see data set 12B, Part 1).

5.1.12.1 Data Set 12A: Facility Width

Definitions:

WIDFAC = Facility width (cm). Used to calculate concentrations. Often, the total inventory of the facility is known. Because BLT-EC models two-dimensions, a value for the third dimension is needed to properly estimate concentrations. For example, consider a trench that is 100 m long, 25 m wide, and 10 m deep with an initial inventory of 100 Moles. Typically, BLT-EC 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 Moles and the concentrations will be calculated correctly.

Format:

Subroutine	Statement
DATAHT	
	C READ A BLANK LINE, TITLE OF DATA SET, SUBTITLE,
	C AND WIDTH OF WASTE CONTAINING REGION
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) WIDFAC
	6 FORMAT(A79)

5.1.12.2 Data Set 12B: Nodal Coordinate Data And Node Connectivity

Data set 12B is composed of two parts: Nodal coordinate data and node connectivity. Data set 12B is required when KVI is less than or equal to zero and when KMESH is less than or equal to zero.

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:

KVI (Data Set 2)	KMSH (Data Set 6)	Option
> 0	N.A.	a
≤ 0	0	b
≤ 0	1	c

PART 1: NODAL COORDINATE DATA SET 12B1, OPTION B

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. All other values must be input on this final ine due to the use of free-format input statements.

Usually a total of 2*NNP lines are required, NNP lines for the x-coordinate and NNP lines for the z-coordinate. However, if a group of cards appears in regular pattern, automatic generation may be made.

Line 1 to Line NNP: Each line is free formatted input of 6 variables.

Definitions:

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.

Format:

Subroutine	Statement
DATAHT	
	IF(KVI.LE.0) GO TO 110
	C READ A BLANK LINE, TITLE OF DATA SET 12 AND
	C NOTE THAT DATA SETS 12B AND C ARE NOT USED
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	C READ NODAL AND ELEMENT DATA FROM LOGICAL
	C UNIT 1 IF KVI.GT.0
	REWIND 1
	110 CONTINUE
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	IF(KMESH .GT. 0) THEN
	CALL RNODE(X,Z,IE,MAXEL,MAXNP)
	ELSE
	CALL READR(X,MAXNP,NNP)
	READ(7,6) LABEL
	READ(7,6) LABEL
	CALL READR(Z,MAXNP,NNP)
	ENDIF
	6 FORMAT(A79)
READR	
	150 READ(7,*) NI,NSEQ,NAD,XNI,XAD,XRD

Line (NNP+1) to Line 2*NNP: Input similarly but for the z-coordinate.

PART 2: NODE CONNECTIVITY DATA SET 12B2

Usually a total of NEL lines are needed, one for each element. However, if a group of elements appears in regular pattern, automatic generation is made.

Input of 8 variables is free formatted.

Definitions:

MI	=	Global element number.
IE(MI,1)	=	Global node number of the first node of element MI.
IE(MI,2)	=	Global node number of the second node of element MI.
IE(MI,3)	=	Global node number of the third node of element MI.
IE(MI,4)	=	Global node number of the fourth node of element MI.
IE(MI,5)	=	Material type to applied to be element MI.
MODL	=	Number of elements in the direction of most rapidly numbered nodes.
NLAY	=	Number of elements in the direction of least rapidly numbered nodes.

IE(MI,1) - IE(MI,4) are numbered beginning with the lower left corner and progressing around the element in a counterclockwise direction. For a rectangular block of elements, it is only necessary to specify the first element, the width MODL and the length NLAY, where MODL and NLAY are measured in elements. Element numbering proceeds most rapidly along MODL dimension and least rapidly along the NLAY dimension. The following figure provides an example. The object is considered to be rectangular, since it has width MODL = 5 on two opposite sides and length NLAY = 10 on the other two opposite sides. To generate definitions of elements 2 through 50 automatically, including both the indices and material type, only one card is necessary:

```
-----------------------------------------------
 1  1  5  6  2  1  5  10
-----------------------------------------------
```

Although all elements of this example will be assumed to contain the same material type, MTYP = 1, this situation can easily be changed by using material-correction facility, Data Set 14.

Format:

Subroutine	Statement	
DATAHT		
		READ(7,6) LABEL
		READ(7,6) LABEL
		READ(7,6) LABEL
		IF (KMESH.GT.0) THEN
		READ(7,6) LABEL
		GO TO 210
		ENDIF
	120	READ(7,*) MI, (IE(MI,I),I=1,5)
		READ(7,6) LABEL

```
      READ(7,6) LABEL
      READ(7,*) MODL, NLAY
      IF (MODL.LE.0) GO TO 120
      DO 200 I=1, NLAY
      LL=2
      DO 200 J=1,MODL
      IF(MJ.EQ.MI) GO TO 190
      DO 180 KQ=1,4
180   IE(MJ,KQ)=IE(MJ-1,KQ) + LL
      IE(MJ,5)=IE(MJ-1,5)
190   LL=1
200   MJ=MJ+1
      MJ=MJ-1
      IF (MJ.LT.NEL) GO TO 120
210   CONTINUE
6     FORMAT(A79)
```

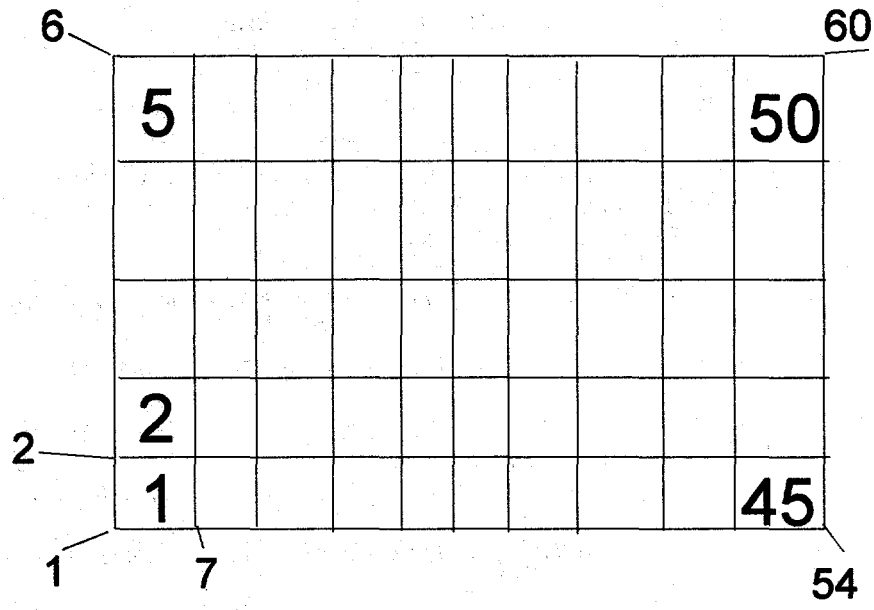


Figure 5.1 Example finite element grid that is 5 elements high by 10 elements wide. Element numbers are listed inside the grid, node numbers are listed outside the grid.

5.1.12.3 Data Set 12C: Automatic Grid Generation Data

Data set 12C is required when KVI is less than or equal to zero and when KMESH is greater than zero.

Usually a total of 1 plus (2 times NREG) lines are required.

Input is free formatted for each line.

Definitions:

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.

For each region, input with the following six variables is required.

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.

X1(I) = X coordinate of node I (cm).

X2(I) = Z coordinate of node I (cm).

Note four ordered co-ordinate paris are required to define the four corners of the region.

In this input structure, the x and z-direction nodes are numbered independently. Coordinate pairs are ordered from the lower left hand corner, counter clockwise. That is, the (X,Z) coordinates of the (IMIN, JMIN) node, the (X,Z) coordinates of the (IMAX, JMIN) node, the (X,Z) coordinates of the (IMAX,JMAX) node, and the (X,Z) coordinates of the (IMIN,JMAX) node.

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 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.

Format:

Subroutine	Statement
DATAHT	
	IF(KVI.LE.0) GO TO 110
	C READ A BLANK LINE, TITLE OF DATA SET 12 AND
	C NOTE THAT DATA SETS 12B AND C ARE NOT USED
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	C READ NODAL AND ELEMENT DATA FROM LOGICAL
	C UNIT 1 IF KVI.GT.0
	REWIND 1
	110 CONTINUE
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	IF(KMESH .GT. 0) THEN
	CALL RNODE(X,Z,IE,MAXEL,MAXNP)
	ELSE
	CALL READR(X,MAXNP,NNP)
	READ(7,6) LABEL
	READ(7,6) LABEL
	CALL READR(Z,MAXNP,NNP)
	ENDIF
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	IF (KMESH.GT.0) THEN
	READ(7,6) LABEL
	GO TO 210
	ENDIF
	210 CONTINUE
	6 FORMAT(A79)
RNODE	
	C READ THE NUMBER OF DATA RECORDS
	READ(7,*) NELX,NELZ,NREG

```
      DO 101 IREC=1,NREG
      READ (7,3) LABEL
      READ (7,3) LABEL
      READ(7,*) IMIN,JMIN,IMAX,JMAX
      READ (7,3) LABEL
      READ (7,3) LABEL
      READ(7,*) (X1(I),X2(I),I=1,KIND2)
101   CONTINUE
      CALL RELEM(X,Z,IE,IXREF,IXMAX,MAXEL,MAXNP,NELX
     1,NELZ)
3     FORMAT(A79)
```

5.1.13 Data Set 13: Porous Media Properties

A total of NMAT lines are required for this data set.

Each line is free formatted input of NMPPM=4 variables.

Definitions:

PROP(1,I)	=	Longitudinal dispersivity, (cm).
PROP(2,I)	=	Lateral dispersivity, (cm).
PROP(3,I)	=	Effective molecular diffusion coefficient of the I^{th} medium, (cm^2/s).
PROP(4,I)	=	Bulk density of medium I, (g/cm^3).

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) (PROP(J,I),J=1,NMPPM)
	6 FORMAT(A79)

5.1.14 Data Set 14: Material Type Correction

This data set is required only if NCM .GT. 0. Normally NCM lines are required. However, if the elements to be corrected with different material properties appear in regular patterns, automatic generation may be made.

Each line is free formatted input of 5 variables.

Definitions:

MI	=	Global element number of the first element in the sequence.
NSEQ	=	NSEQ subsequent elements will be generated automatically.

MAD	=	Increment of element number for each of the NSEQ subsequent elements.
MITYP	=	Type of material made up of element MI.
MTYPAD	=	Increment of the type of material for each of the end of this data set.

NOTE: A line containing five zeros must be used to signal the end of the data set.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	IF (NCM.LE.0) THEN
	READ(7,6) LABEL
	GO TO 270
	ENDIF
	CALL READN(IE(1,5),MAXEL,NCM)
	C WRITE ELEMENT INFORMATION
	270 LINE=0
	6 FORMAT(A79)
READN	
	110 READ (7,*) MI,NSEQ,MAD,MITYP,MTYPAD

5.1.15 Data Set 15: Initial or Pre-Initial Conditions

This data set is needed only if NSTR .EQ. 0. When this data set is needed, normally a total of NNP lines are required for each chemical component, one each for a node. However, if the initial or pre-initial conditions appear in a regular pattern, automatic generation may be made. The following set of lines should be repeated for each of the NON components.

Each line is free formatted input containing 6 variables.

Definitions:

NI	=	Global node number of the first node in the sequence.
NSEQ	=	NSEQ subsequent nodes will be generated automatically.
NAD	=	Increment of node number for each of the NSEQ subsequent nodes.
RNI	=	Initial or pre-initial total concentration at node NI, (mole/liter).
RAD	=	Increment of initial or pre-initial total concentration for each of the NSEQ subsequent nodes, (mole/liter).
RRD	=	Fractional increase in the concentration to be added, normally = 0.

NOTE: A line with five zeros must be used to signal end of this data set for each chemical component.

NOTE: For any chemical component, if its INDC is equal to 3, then the Log_{10} of its activity should be the input for initial values or pre-initial values.

NOTE ON INITIAL CONDITIONS: The initial conditions for a transient calculation may be obtained in three different ways: from batch input, auxiliary storage input, or steady-state calculation using time-invariant boundary conditions. In the latter case a batch input of the pre-initial conditions is required as the zeroth order iterate of the steady state solution. Auxiliary storage input is necessary whenever the restarting facility is being used. That is, concentration distribution for NSTR different times have been generated and written on a file. If NSTR .GT. 0, these distributions will be read from Logical Unit 3, and NSTRth distribution will be used as the initial condition for current calculation. If KSTR is greater than zero, the concentration values will be written on a different device as they are read out form Logical Unit 3 so that a complete record of calculations may be kept on one device, Logical Unit 2. If either the first (card input) or the last (steady-state) options are used, then NSTR = 0.

NOTE ON AUXILIARY UNITS: Logical Unit 1 is used to input hydrodynamic variables to BLT-EC if KVI .GT. 0. Logical Unit 2 is used to store output of BLT-EC if KSTR .GT. 0. Logical Unit 3 is used to input initial condition if NSTR .GT. 0. Proper identification of these three units must be made in the JCL if either of these options are used. It can be seen that the DSAME for Logical Unit 3 of the current job should be the same as that for Logical Unit 2 of the previous job.

NOTE ON STEADY-STATE INPUT: A steady-state option may be used to provide either the final state of a system under study or the initial conditions for a transient state calculation. In former case KSS = 0 and NTI = 0 and in the latter case KSS = 0 and NTI .GT. 0. If KSS .GT. 0, there will be no steady-state calculation.

Format:

Subroutine	Statement
DATAHT	
	IF (NSTR.EQ.0) GO TO 320
	C READ INITIAL OR PRE-INITIAL CONDITIONS VIA CARD IF
	C NSTR .EQ. 0
	320 CONTINUE
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	DO 330 K=1,NON
	READ(7,6) LABEL
	330 CALL READR(TP(1,K),MAXNP,NNP)
	6 FORMAT(A79)
READR	
	150 READ(7,*) NI,NSEQ,NAD,RNI,RAD,RRD

5.1.16 Data Set 16: Variable Boundary Conditions

Four groups of cards are required for this data set if and only if NVES .GT. 0. The first group is used to specify the incoming concentration profiles, the second group is used to assign the type of incoming concentration profile to each of the NVES boundary sides, the third group is used to read the global nodal number of NVNP flowing-in and flowing-out nodes, and the fourth group is used to specify the information of the NVES element sides. The first group and the second group should be repeated once for each of the NON chemical components.

A) INCOMING CONCENTRATION PROFILES

Free formatted input of 2 variables has the following profiles:

First profile:

TCVBF(1,1,K)	CVBF(1,1,K)	TCVBF(2,1,K)	CVBF(2,1,K) ...

.

.

... TCVBF(NVDP,1,K)	CVBF(NVDP,1,K)

Second profile:

TCVBF(1,2,K)	CVBF(1,2,K)	TCVBF(2,2,K)	CVBF(2,2,K) ...

.

.

... TCVBF(NVDP,2,K)	CVBF(NVDP,2,K)

.

.

.

I^{th} profile:

TCVBF(1,I,K)	CVBF(1,I,K)	TCVBF(2,I,K)	CVBF(2,I,K) ...

.

.

... TCVBF(NVDP,I,K)	CVBF(NVDP,I,K)

.

.

.

$NVPR^{th}$ profile:

TCVBF(1,NVPR,K)	CVBF(1,NVPR,K)	TCVBF(2,NVPR,K)	CVBF(2,NVPR,K) ...

.

.

...TCVBF(NVDP,NVPR,K)	CVBF(NVDP,NVPR,K)

Definitions:

TCVBF(J,I,K) = Time of the J^{th} data point on I^{th} incoming-concentration vs time profile for K^{th} component, years.

CVBF(J,I,K) = Concentration of the J^{th} data point on I^{th} incoming-concentration vs time profile for K^{th} component, (mole/liter).

Format:

Subroutine	Statement
DATAHT	
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	IF (NVES.LE.0) THEN
	READ(7,6) LABEL
	READ(7,6) LABEL
	ELSE
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	DO 360 K=1,NON
	READ(7,6) LABEL
	READ(7,6) LABEL
	DO 350 I=1,NVPR
	READ(7,*) (TCVBF(J,I,K),CVBF(J,I,K),J=1,NVDP)
	350 CONTINUE
	6 FORMAT(A79)

B) INCOMING CONCENTRATION TYPE ASSIGNED TO VARIABLE-BOUNDARY SIDES

Each line is free formatted input containing 5 variables.

Definitions:

MI = Compressed variable-boundary element side number of the first side in a sequence.

NSEQ = NSEQ subsequent sides will be generated automatically.

MIAD = Increment of the compressed variable-boundary element side number for each of the NSEQ subsequent sides.

MITYP = Type of incoming concentration profile assigned to side MI.

MTYPAD = Increment of the type of incoming concentration profile for each of the NSEQ subsequent sides.

NOTE: A line containing five zeros is used to end the input of this subdata set.

Format:

Subroutine	Statement
DATAHT	

```
                    C READ INCOMING CONCENTRATION TYPE ASSIGNED
                    C TO EACH OF VB SIDES
                    C THE FOLLOWING LABEL IS A BLANK
                          READ(7,6) LABEL
                          READ(7,6) LABEL
                          CALL READN(IVTYP(1,K),MXVES,NVES)
                    C THE FOLLOWING LABEL IS A BLANK
                          READ(7,6) LABEL
                    360   CONTINUE
                    6     FORMAT(A79)
READN
                    110   READ (7,*) MI,NSEQ,MAD,MITYP,MTYPAD
```

C) GLOBAL NODAL NUMBER OF NVNP VARIABLE-BOUNDARY CONDITION NODES

Normally NVNP lines are needed. However, automatic generation can be made.

Each line is free formatted input containing 5 variables.

Definitions:

NI	=	Compressed variable-boundary node number of the first node in a sequence.
NSEQ	=	NSEQ subsequent nodes will be generated automatically.
NIAD	=	Increment of the compressed variable-boundary node number for each of the NSEQ subsequent sides.
NODE	=	Global node of the compressed node NI.
NODEAD	=	Increment of NODE for each of the NSEQ subsequent nodes.

NOTE: A line containing five zeros is used to end the input of this subdata set.

Format:

Subroutine Statement

```
DATAHT
                    C READ GLOBAL NODE NUMBER OF VB NODES
                          READ(7,6) LABEL
                          READ(7,6) LABEL
                          CALL READN(NPVB,MXVNP,NVNP)
                    6     FORMAT(A79)
READN
                    110   READ (7,*) NI,NSEQ,NIAD,NODE,NODEAD
```

D) SPECIFICATION OF VARIABLE-BOUNDARY SIDES

Each line is free formatted input containing 9 variables.

Definitions:

Normally, NVES lines are required, one each for a variable-boundary element side. However, if a group of variable-boundary element sides appears in a regular pattern, automatic generation may be made.

Each line is free formatted input containing 9 variables.

Definitions:

MI	=	Compressed variable boundary element-side number of the first element side in a sequence.
NSEQ	=	NSEQ subsequent variable-boundary element sides will be generated automatically.
M	=	Global element number to which MIth element-side belong to.
IS1	=	Compressed variable-boundary nodal number of the first node of element side MI.
IS2	=	Compressed variable-boundary nodal number of the second node of element side MI.
MIAD	=	Increment of MI for each of the NSEQ subsequent variable-boundary element sides.
MAD	=	Increment of M for each of the NSEQ subsequent variable-boundary element sides.
IS1AD	=	Increment of IS1 for each of the NSEQ subsequent variable-boundary element sides.
IS2AD	=	Increment of IS2 for each of the NSEQ subsequent variable-boundary element sides.

NOTE: A line with 9 zeros is used to end the input of this subdata set.

Format:

Subroutine DATAHT — Statement

```
C READ VARIABLE BOUNDARY ELEMENT SIDES
      MPI=0
C THE FOLLOWING LABEL IS A BLANK
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
370   READ(7,*) MI,NSEQ,M,IS1,IS2,MIAD,MAD,IS1AD,IS2AD
      IF(MI.EQ.0) GO TO 390
      MJ=MI+NSEQ
      DO 380 MP=MI,MJ
      I=MI+(MP-MI)*MIAD
      MVES(I)=M+(MP-MI)*MAD
      ISV(1,I)=IS1+(MP-MI)*IS1AD
      ISV(2,I)=IS2+(MP-MI)*IS2AD
      MPI=MPI+1
380   CONTINUE
      GO TO 370
390   IF(MPI.EQ.NVES) GO TO 400
      STOP
```

```
C THE FOLLOWING LABEL IS A BLANK
400   CONTINUE
      READ (7,6) LABEL
6     FORMAT(A79)
```

5.1.17 Data Set 17: Dirichlet Boundary Conditions

This data set is required if and only NDNP .GT. 0. Subdata sets A) and B) should be repeated NON times, one for each of the NON components.

A) DIRICHLET CONCENTRATION PROFILE

Free formatted input of 2 variables has the following profiles:

First Profile:

```
-------------------------------------------------------------------------
TCDBF(1,1,K) CDBF(1,1,K)  TCDBF(2,1,K) CDBF(2,1,K) ...
-------------------------------------------------------------------------

                    .
                    .
-----------------------------------------------------
... TCDBF(NDDP,1,K)  CDBF(NDDP,1,K)
-----------------------------------------------------
```

Second profile:

```
-------------------------------------------------------------------------
TCDBF(1,2,K) CDBF(1,2,K)   TCDBF(2,2,K) CDBF(2,2,K) ...
-------------------------------------------------------------------------

                    .
                    .
-----------------------------------------------------
... TCDBF(NDDP,2,K)    CDBF(NDDP,2,K)
-----------------------------------------------------
```

```
                  .
                  .
                  .
```

I^{th} profile:

```
-------------------------------------------------------------------------
TCDBF(1,I,K) CDBF(1,I,K)   TCDBF(2,I,K) CDBF(2,I,K) ...
-------------------------------------------------------------------------

                    .
                    .
-----------------------------------------------------
... TCDBF(NDDP,I,K)    CDBF(NDDP,I,K)
-----------------------------------------------------
```

```
                  .
                  .
                  .
```

NDPRth profile:

TCDBF(1,NDPR,K)	CDBF(1,NDPR,K)	TCDBF(2,NDPR,K)	CDBF(2,NDPR,K) ...

.

.

... TCDBF(NDDP,NDPR,K)	CDBF(NDDP,NDPR,K)

Definitions:

TCDBF(J,I,K) = Time of Jth data point in Ith Dirichlet-concentration profile for Kth component, (years).

CDBF(J,I,K) = Dirichlet concentration of Jth data point in Ith Dirichlet concentration vs time profile for Kth component, (mole/liter).

Format:

Subroutine DATAHT

Statement

```
C READ DIRICHLET CONCENTRATION PROFILE
480   IF(NDNP.EQ.0) THEN
      READ(7,6) LABEL
      READ(7,6) LABEL
      ELSE
C READ DATA SET TITLE
      READ(7,6) LABEL
      DO 500 K=1,NON
      READ(7,6) LABEL
      READ(7,6) LABEL
      DO 490 I=1,NDPR
      READ(7,*) (TCDBF(J,I,K),CDBF(J,I,K),J=1,NDDP)
490   CONTINUE
6     FORMAT(A79)
```

B) TYPE OF DIRICHLET NODE

This subdata set is read in similarly to DATA SET 16 B).

Each line is free formatted input containing 5 integers.

Definitions:

NI	=	Compressed Dirichlet node number of the first node in the sequence.
NSEQ	=	NSEQ subsequent Dirichlet nodes will be generated automatically.
NAD	=	Increment of compressed Dirichlet node number for each of the NSEQ subsequent nodes.
NITYP	=	Type of Dirichlet concentration profile for node NI and the NSEQ subsequent nodes.
NTYPAD	=	Increment of NITYP for each of the NSEQ subsequent nodes.

NOTE: A line with 5 zeros must be used to signal the end of this subdata set.

Format:

Subroutine	Statement
DATAHT	
	C READ TYPE OF DIRICHLET CONCENTRATION PROFILE ASSIGNED
	C TO DIRICHLET NODES
	C READ BLANK
	READ(7,6) LABEL
	READ(7,6) LABEL
	CALL READN(IDTYP(1,K),MXDNP,NDNP)
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	500 CONTINUE
	6 FORMAT(A79)
READN	
	110 READ (7,*) NI,NSEQ,NAD,NITYP,NTYPAD

C) DIRICHLET NODES

This subdata set is read in similar to DATA SET 16 C).

Each line is free formatted input containing 5 integers.

Definitions:

NI	=	Compressed Dirichlet boundary node number of the first node in a sequence.
NSEQ	=	NSEQ subsequent nodes will be generated automatically.
NIAD	=	Increment of the compressed Dirichlet boundary node number for each of the NSEQ subsequent sides.

NODE = Global node of the compressed node NI.

NODEAD = Increment of NODE for each of the NSEQ subsequent nodes.

NOTE: A line containing five zeros is used to end the input of this subdata set.

Format:

Subroutine	Statement
DATAHT	
	C READ GLOBAL NODE NUMBER OF DIRICHLET NODES
	READ(7,6) LABEL
	READ(7,6) LABEL
	CALL READN(NPDB,MXDNP,NDNP)
	ENDIF
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	6 FORMAT(A79)
READN	
	110 READ (7,*) NI,NSEQ,NIAD,NODE,NODEAD

5.1.18 Data Set 18: Element Source/Sink Data

Subdata sets A) through C) are needed if and only if NSEL .GT. 0. When NSEL .GT. 0, subdata sets B) and C) should be repeated for NON + 1 times.

A) GLOBAL ELEMENT NUMBER OF COMPRESSED SOURCE/SINK ELEMENT NUMBER

Free formatted input containing element numbers.

Definitions:

LES(1) = Global element number of the first distributed source/sink element.

LES(2) = Global element number of the second distributed source/sink element.

.

.

.

LES(N) = Global element number of the N^{th} distributed source/sink element.

Format:

Subroutine	Statement
DATAHT	
	IF(NSEL.EQ.0) THEN
	READ(7,6) LABEL
	READ(7,6) LABEL
	GO TO 540
	ENDIF
	C READ SOURCE ELEMENTS
	READ(7,6) LABEL

```
      READ(7,6) LABEL
      READ(7,*) (LES(MP),MP=1,NSEL)
6     FORMAT(A79)
```

B) ELEMENT SOURCE/SINK PROFILE

Number of lines depends on NSPR, NSDP, and NON (K=1,NON + 1). Each line contains a number of data points. Each line is free formatted input.

First profile:

TSOSF(1,1,K) SOSF(1,1,K) TSOSF(2,1,K) SOSF(2,1,K) ...

.

.

... TSOSF(NSDP,1,K) SOSF(NSDP,1,K)

Second profile:

TSOSF(1,2,K) SOSF(1,2,K) TSOSF(2,2,K) SOSF(2,2,K) ...

.

.

... TSOSF(NSDP,2,K) SOS(NSDP,2,K)

.

.

.

I^{th} profile:

TSOSF(1,I,K) SOSF(1,I,K) TSOSF(2,I,K) SOSF(2,I,K) ...

.

.

... TSOSF(NSDP,I,K) SOSF(NSDP,I,K)

.

.

.

NSPRth profile:

TSOSF(1,NSPR,K) SOSF(1,NSPR,K) TSOSF(2,NSPR,K) SOSF(2,NSPR,K) ...

... TSOSF(NSDP,NSPR,K) SOSF(NSDP,NSPR,K)

Definitions:

TSOSF(J,I,K) = Time of Jth data point in Ith profile for Kth component, (years).

SOSF(J,I,K) = Source/sink value of Jth data point in Ith profile for Kth component;
(mole/s/cm^3) if K .LE. NON,
(cm^3/s/cm^3) if K .EQ. (NON+1).

Format:

Subroutine Statement
DATAHT

```
C READ ELEMENTAL SOURCE PROFILES
      NON1=NON+1
      DO 530 K=1,NON1
C THE FOLLOWING LABEL IS A BLANK
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
      DO 520 I=1,NSPR
      READ(7,*) (TSOSF(J,I,K),SOSF(J,I,K),J=1,NSDP)
520   CONTINUE
6     FORMAT(A79)
```

C) SOURCE/SINK TYPE IN EACH SOURCE/SINK ELEMENT

Usually one line per element. However, automatic generation can be made.

Each line is free formatted input containing 5 variables.

Definitions:

MI = Compressed source/sink element number of first element in the sequence.

NSEQ = NSEQ subsequent source/sink elements will have type MITYP.

MAD = Increment of MI for each of the NSEQ subsequent elements.

MITYP = Source/sink type for element MI.

MTYPAD = Increment of source type in each of the NSEQ subsequent elements.

NOTE: A line containing 5 zeros must be used to end this data set.

Format:

Subroutine	Statement
DATAHT	
	C READ SOURCE TYPE ASSIGNED TO EACH SOURCE
	C ELEMENT
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	READ(7,6) LABEL
	CALL READN(ISTYP(1,K),MXSEL,NSEL)
	530 CONTINUE
	540 CONTINUE
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	6 FORMAT(A79)
READN	
	110 READ (7,*) MI,NSEQ,MAD,MITYP,MTYPAD

5.1.19 Data Set 19: Well (Point) Source/Sink Data

Subdata sets A) through C) are needed if and only if NWNP .GT. 0. When NWNP .GT. 0, subdata sets B) and C) should be repeated for (NON + 1) times.

A) GLOBAL NODE NUMBER OF COMPRESSED POINT SOURCE/SINK NUMBER

Unformatted input contains node numbers.

NPW(1) = Global node number of the first source/sink node.

NPW(2) = Global node number of the second source/sink node.

NPW(N) = Global node number of the N^{th} source/sink node.

Format:

Subroutine	Statement
DATAHT	
	C READ WELL SOURCE/SINK NODES
	IF(NWNP.EQ.0) THEN
	READ(7,6) LABEL
	READ(7,6) LABEL
	GO TO 565
	ENDIF
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) (NPW(NP),NP=1,NWNP)
	6 FORMAT(A79)

B) POINT SOURCE/SINK PROFILE

Number of lines depends on NWPR, NWDP, and NON (K=1,NON + 1). Each card contains a number of data points.

First profile:

TWSSF(1,1,K) WSSF(1,1,K) TWSSF(2,1,K) WSSF(2,1,K) ...

... TWSSF(NWDP,1,K) WSSF(NWDP,1,K)

Second profile:

TWSSF(1,2,K) WSSF(1,2,K) TWSSF(2,2,K) WSSF(2,2,K) ...

... TWSSF(NWDP,2,K) WSSF(NWDP,2,K)

I^{th} profile:

TWSSF(1,I,K) WSSF(1,I,K) TWSSF(2,I,K) WSSF(2,I,K) ...

... TWSSF(NWDP,I,K) WSSF(NWDP,I,K)

NWPRth profile:

TWSSF(1,NWPR,K) WSSF(1,NWPR,K) TWSSF(2,NWPR,K) WSSF(2,NWPR,K) ...

... TWSSF(NWDP,NWPR,K) WSSF(NWDP,NWPR,K)

Definitions:

TWSSF(J,I,K)	=	Time of Jth data point in Ith profile for Kth component, (years).
WSSF(J,I,K)	=	Source/sink value of Jth data point in Ith profile for Kth component; (moles/s/cm^3) if K .LE. NON, (cm^3/s) if K .EQ. (NON+1).

Format:

Subroutine DATAHT

Statement

```
C READ WELL SOURCE/SINK PROFILES
      NON1=NON+1
      DO 560 K=1,NON1
C THE FOLLOWING LABEL IS A BLANK
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
      DO 550 I=1,,NWPR
      READ(7,*) (TWSSF(J,I,K),WSSF(J,I,K),J=1,NWDP)
550   CONTINUE
6     FORMAT(A79)
```

C) TYPE OF POINT SOURCE/SINK NODES

Normally one line per well node. However, automatic generation may be made.

Each line is free formatted input containing 5 variables.

Definitions:

NI	=	Compressed well node number of the first node in a sequence.
NSEQ	=	NSEQ subsequent well nodes will be generated automatically for the source type.
NIAD	=	Increment of compressed well node number for each of the NSEQ subsequent nodes.
NITYP	=	Type of well source/sink profile assigned to NIth well node.

NITYPA = Increment of NITYP for each of the NSEQ subsequent nodes.

NOTE: A line containing five zeros must be used to signal the end of this subdata set.

Format:

Subroutine	Statement
DATAHT	
	C READ WELL SOURCE/SINK TYPE ASSIGNED TO EACH OF
	C NWNP NODES
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	READ(7,6) LABEL
	CALL READN(IWTYP(1,K),MXWNP,NWNP)
	560 CONTINUE
	565 CONTINUE
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	6 FORMAT(A79)
READN	
	110 READ (7,*) NI,NSEQ,NIAD,NITYP,NTYPA

5.1.20 Data Set 20: Element Source/Sink (Leaching) Data

A) LEACHING SOURCE ELEMENTS

Free formatted input contains one variable.

Definitions:

LEA(1) = Global element number of the first leaching source element.

LEA(2) = Global element number of the second leaching source element.

LEA(MP) = Global element number of the MP^{th} leaching source element.

Format:

Subroutine	Statement
DATAHT	
	IF(NLEL.EQ.0) THEN
	READ(7,6) LABEL
	READ(7,6) LABEL
	C THE FOLLOWING LABEL IS A BLANK
	READ(7,6) LABEL
	GO TO 570
	ENDIF
	C READ LEACHING SOURCE ELEMENTS
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) (LEA(MP),MP=1,NLEL)

```
6     FORMAT(A79)
```

B) ELEMENTAL SOURCE PROFILES

Profiles are input similarly to data set 18. Free formatted input contains 2 variables.

Definitions:

TSLEA(J,I,K)	=	Time of J^{th} data point in I^{th} profile for K^{th} component, (years).
SLEA(J,I,K)	=	Source value of J^{th} data point in I^{th} profile for K^{th} component; (mole/s/liter).

Format:

Subroutine	Statement
DATAHT	

```
C READ ELEMENTAL SOURCE PROFILES
      NON1=NON + 1
      DO 567 K=1,NON
C THE FOLLOWING LABEL IS BLANK
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
      DO 566 I=1,NLPR
      READ(7,*) (TSLEA(J,I,K), SLEA(J,I,K),J=1,NLDP)
566   CONTINUE
6     FORMAT(A79)
```

C) SOURCE TYPE ASSIGNED TO EACH SOURCE ELEMENT

Free formatted input contains 5 variables.

Definitions:

NI	=	Compressed element number of the first node in a sequence.
NSEQ	=	NSEQ subsequent element will be generated automatically for the source type.
NIAD	=	Increment of compressed element number for each of the NSEQ subsequent nodes.
NITYP	=	Type of well source/sink profile assigned to NI^{th} element.
NITYPA	=	Increment of NITYP for each of the NSEQ subsequent elements.

NOTE: A line containing five zeros must be used to signal the end of this subdata set.

Format:

Subroutine	Statement
DATAHT	
	C READ SOURCE TYPE ASSIGNED TO EACH SOURCE
	C ELEMENT
	READ(7,6) LABEL
	READ(7,6) LABEL
	CALL READN(ILTYP(1,K),MXLEL,NLEL)
	567 CONTINUE
	6 FORMAT(A79)
READN	
	110 READ (7,*) NI,NSEQ,NIAD,NITYP,NTYPA

5.1.21 Data Set 21: Waste Container Parameters

NOTE: The following set of cards cannot be included if the waste containers are not simulated: i.e., NCON = 0.

A) CONTAINER DEGRADATION PARAMETERS

Requires 2*NCTYPE cards in free format.

CARD 1:

THICK(1)	PITN(1)	PITK(1)	AREA(1)	ASCALE(1)	PITS(1)

CARD 2:

GRATE(1)	CLAY(1)	SPH(1)	IAER(1)

.
.
.

CARD 2*NCTYPE - 1:

THICK(NCTYPE)	PITN(NCTYPE)	PITK(NCTYPE)	AREA(NCTYPE) ...

.
.

... ASCALE(NCTYPE)	PITS(NCTYPE)

CARD 2*NCTYPE:

GRATE(NCTYPE)	CLAY(NCTYPE)	SPH(NCTYPE)	IAER(NCTYPE)

Definitions:

THICK(I) = Thickness of the I^{th} container (cm). 55 gallon drums are generally 0.127 - 0.152 cm thick.

PITN(I) = Pitting parameter n in the I^{th} container (dimensioness). The equation for calculating pit depth is $h=k(t^n)*(A^m)$

where
h is the maximum pit depth,
k,n, and m are the parameters PITK, PITN, AND ASCALE,
A is the area of the container, AREA, normalized to the area of the NBS test samples, and
t is the simulation time in years.

If PITN(I) is zero, a value is calculated by the code based on input parameters for clay content (CLAY0, soil aeration (IAER), and the calculated moisture content.

PITK(I) = Pitting parameters k in the I^{th} container (cm/yr^n). If PITK(I) is zero, a value is calculated based on soil pH (SPH). Measured values [Romanoff, 1957] range from 0.03 - 0.15 cm/yr^n. If PITK and soil pH (SPH) are input as zero, the default value for PITK is 0.0737, the average value for all soils.

AREA(I) = Area of the waste container in cm^2. Used to calculate the area scaling factor in the equation for maximum pit depth. The area of the 55 gallon drum is 21,000 cm^2. It is also used to calculate the fraction of the container that has been breached due to pitting. This fraction is used in determining releases from partially failed containers.

ASCALE(I) = Area scaling exponent (dimensionless). Values have been measured by Logan [Logan, 1939] for wrought iron pipes buried in 47 different soils. Values ranged from 0.08 - 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 in the code.

PITS(I) = The number of penetrating pits in the container (dimensionless). The total area breached is linearly proportional to the number of pits that penetrate the container, PTIS(I). Measurement of the total number of pits on Fe samples ranged from 14 - 80 pits/cm^2 [Isaacs, 1987]. Of these, only a small fraction (less than 1%) will grow large enough to penetrate the container. Based on the carbon steel pitting data obtained by Marsh [Marsh, et al., 1986] an estimate of 0.05 penetrating pits/cm^2 has been made. For a 55 gallon drum with a surface area of 21,000 cm^2 , this implies a total of 1,000 penetrating pits. The default value is 1,000.

GRATE(I) = The general corrosion rate (L/T). Values measured in the NBS study reported by Romanoff [Romanoff, 1957] for the corrosion rate of carbon steel ranged from 2.7E-ll - 6E-10 cm/s. For a wall thickness of 0.127 cm, theses corrosion rates correspond to penetrating in 6.7 - 150 years. If the input value of GRATE(I) is xero, then the default value of 3E-10 cm/s is used.

CLAY(I) = Fraction of clay in the soil, 0 .LT. CLAY(I) .LE. 1. If PITN is input as zero, PITN is calculated as function of clay and moisture content as well as degree of soil aeration. If CLAY(I) is also zero, PITN is calculated only as function of aeration.

SPH(I) = Soil pH. If PITK is input as zero, PITK is calcualted as a function of pH. If SPH(I) is input as zero, a default value of 7.0 is used. This leads to a low value for PITK, however, it is consistent with the average value for soil pH.

IAER(I) = Aeration index of the soil. 1=good, 2=fair, 3=poor and 4 = very poor. Used in calculating PITN. If PITN and clay 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 fair or good aeration.

Format:

Subroutine DATAHT

Statement

```
570   IF(NCON.EQ.0) THEN
C IF DATA SET 21 IS NOT BEING USED
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
C IF DATA SET 22A IS NOT BEING USED
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
C IF DATA SET 22B IS NOT BEING USED
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
C IF DATA SET 22C IS NOT BEING USED
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,6) LABEL
      ENDIF
      IF(NCON.NE.0) THE
      READ(7,6) LABEL
      READ(7,6) LABEL
C READ FROM INPUT FILE THE PARAMETERS OF EACH
C CONTAINER
C TYPE
      DO 580 J=1,NCTYPE
      READ(7,6) LABEL
      READ(7,*)THICK(J),PITN(J),PITK(J),AREA(J),ASCALE(J)
     1,PITS(J)
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,*) GRATE(J),CLAY(J),SPH(J),IAER(J)
      READ(7,6) LABEL
580   CONTINUE
6     FORMAT(A79)
```

B) CONTAINER/FINITE ELEMENT LINK

Requires 1 card for each 16 values in free format as follows:

```
-------------------------------------------------------------------------
NELCON(1) NELCON(2)  NELCON(I)  NELCON(NCON)
-------------------------------------------------------------------------
```

Definitions:

NELCON(I)	=	Global element number for the I^{th} container. NELCON is the compressed element index for the elements with containers.

Format:

Subroutine	Statement
DATAHT	

```
C READ GLOBAL ELEMENT NO. AND THE CONT. TYPE
C ASSIGNMENT
      READ(7,6) LABEL
      READ(7,*) (NELCON(I),I=1,NCON)
6     FORMAT(A79)
```

C) CONTAINER TYPE

Waste container type for each element that has a waste container is given in the array ICTYPE(I). This requires at most one card for each container, however, often, automatic generation can be used. Input of 5 variables in free format is used to calculate the variables in the array ICTYPE:

Definitions:

MI	=	Compressed element number of the first element in the sequence.
NSEQ	=	The container type is calculated for NSEQ+1 elements.
MAD	=	Increment of compressed element number for each of the NSEQ + 1 elements.
MITYP	=	Container type in compressed element MI.
MTYPAD	=	Increment of container type in each of the NSEQ + 1 elements.

The values in the array ICTYPE are calculated from the following expression:

$$ICTYPE(MI+N*MAD) = MITYP + N*MTYPAD$$

where N is an index that ranges from 0 to NSEQ.

For example, to specify that the first five containers are all type 1 would require the following input:

```
1 4 1 1 0
```

To specify that the first five containers were sequentially numbered from 1 to 5 could be achieved with following:

14111

NOTE: A blank card must be used to signal the end of this data set.

Format:

Subroutine	Statement	
DATAHT		
		READ(7,6) LABEL
		READ(7,6) LABEL
		CALL READN(ICTYPE,MXCON,NCON)
	6	FORMAT(A79)
READN		
	110	READ (7,*) MI,NSEQ,MAD,MITYP,MTYPAD

5.1.22 Data Set 22A: Wasteform and Leaching Information

NOTE: The following set of cards can not be included if there are no waste forms, i.e., NCON = 0.

Required are 2*NWTYPE cards in free format.

CARD 1:

SFRACT(1,ISO) PFRACT(1,ISO) BFRACT(1,ISO) DEFF(1,ISO) ...

... DISOL(1,ISO) PARTK0(1,ISO) PARTKI(1,ISO) PARTKD(1,ISO)

CARD 2:

POREL(1) VOLWF(1) VRATIO(1)

CARD 2*NWTYPE - 1:

SFRACT(NWTYPE,ISO) PFRACT(NWTYPE,ISO) BFRACT(NWTYPE,ISO) ...

... DEFF(NWTYPE,ISO) DISOL(NWTYPE,ISO) PARTK0(NWTYPE,ISO) ...

... PARTKI(NWTYPE,ISO) PARTKD(NWTYPE,ISO)

CARD 2*NWTYPE:

POREL(NWTYPE) VOLWF(NWTYPE) VRATIO(NWTYPE)

Definitions:

SFRACT(J,ISO) = Fraction of the mass of the ISOth contaminant in the Jth waste form that is immediately available for surface wash-off in the rinse model. Useful for surface contaminated waste forms such as lab trash. 0 .LE. SFRACT(J,ISO) .LE. 1.0.

PFRACT(J,ISO) = Fraction of the mass of the ISOth contaminant in the Jth waste form that is available for release due to diffusion. Useful for diffusion controlled releases such as from cement solidified waste forms. 0 .LE. PFRACT(J,ISO) .LE. 1.0.

BFRACT(J,ISO) = Fraction of the mass of the ISOth contaminant in the Jth waste form that is available for release due to dissolution. Useful for dissolution controlled releases such as from activated metals. 0 .LE. BFRACT(J,ISO) .LE. 1.0.

DEFF(J,ISO) = Jth waste form effective diffusion coefficient for contaminant iso (cm^3/s). Used only if PFRACT(J,ISO) > 0.

DISOL(J,ISO) = Jth waste form fractional release rate (1/year) for contaminant iso. Used only if BFRACT(J,ISO) > 0.

PARTK0(J,ISO) = Jth waste form partition coefficient for contaminant iso (L^3/MASS) at time zero.

PARTKI(J,ISO) = Jth waste form partition coefficient for contaminant iso (L^3/MASS) at time t = infinity.

PARTKD(J,ISO) = Jth waste form partition coefficient degradation rate constant for contaminant iso (1/s). PARTKD(J,ISO) must be greater than or equal to 0.

POREL(J) = Effective diffusion length within the waste form (cm). For plane geometry (IDIFF = 0, 1, or 3), POREL(J) should be selected as a value that is the 1/2 the thickness of the simulated waste form. For cylindrical geometry, IDIFF = 2 or 4, POREL(J) is the radius of the waste form. Not used if PFRACT(J) = 0.

VOLWF(J) = Volume of the waste form (cm^3). Used to calculate the height of a cylindrical waste form when IDIFF = 3.

VRATIO(J) = Ratio of the volume of non-waste-form material to waste-form material in the finite element. Used when partition controlled release occurs (PARTKD > 0).

NOTE: SFRACT(J,ISO) + PFRACT(J,ISO) + BFRACT(J,ISO) = 1.0

Format:

Subroutine	Statement
DATAHT	
	C READ FROM INPUT FILE THE PARAMETERS OF EACH
	C WASTE TYPE
	READ(7,6) LABEL
	DO 610 J=1,NWTYPE
	READ(7,6) LABEL
	DO 600 ISO = 1,NON
	C READ RADIOISOTOPIC DEPENDENT QUANTITIES
	READ(7,6) LABEL
	READ(7,*) SFRACT(J,ISO),PFRACT(J,ISO),BFRACT(J,ISO)
	1,DEFF(J,ISO),DISOL(J,ISO)
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) PARTK0(J,ISO),PARTKI(J,ISO),PARTKD(J,ISO)
	READ(7,6) LABEL
	600 CONTINUE
	READ(7,6) LABEL
	READ(7,*) POREL(J),VOLWF(J),VRATIO(J)
	610 CONTINUE
	6 FORMAT(A79)

5.1.22.1 Data Set 22B: Read Initial Masses at Each Waste Element

A value is required for each waste container.

WTINIT(1,ISO) WTINIT(2,ISO) WTINIT(3,ISO) .... WTINIT(NCON,ISO)

NOTE: Additional cards required if input exceeds 80 characters.

Definitions:

WTINIT(I,ISO) = Initial mass contained in waste form I. If the input value of IACT is zero, WTINIT(I,ISO) is in moles. If IACT is not zero, WTINIT should be input in curies (presently not an option).

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	DO 650 ISO = 1,NON
	READ(7,6) LABEL
	READ(7,6) LABEL

```
      READ(7,*) (WTINIT(I,ISO),I=1,NCON)
650   CONTINUE
6     FORMAT(A79)
```

5.1.22.2 Data Set 22C: Read Waste Type Assignments

Waste form type for each element that has a waste form is given in the array IWTYPE. Required is at most one card for each waste form, however, automatic generation can be used. Free formated input of 5 variables used to calculate the variables in the array IWTYPE type.

Definitions:

MI	=	Compressed element number of the first in the sequence.
NSEQ	=	The waste form type is calculated for NSEQ + 1 elements.
MAD	=	Increment of compressed element number for each of the NSEQ + 1 elements.
MITYP	=	Waste form type in compressed element MI.
MTYPAD	=	Increment of waste form type in each of the NSEQ + 1 elements.

The values in the array IWTYPE are calculated from the following expression:

$$IWTYPE(MI+N*MAD) = MITYP + N*MTYPAD$$

where N is an index that ranges from 0 to NSEQ.

For example, to specify that the first five waste forms are all type 1 and waste forms 6, 7 and 8 are type 2 would require the following input:

```
1 4 1 1 0
6 2 1 2 0
0 0 0 0 0
```

NOTE: The input file must contain five values. The final line of input is indicated by having the first value equal 0.

NOTE: In data set 18 and 19 the Source/sink definitions, and data sets 16 and 17 the boundary condition definitions, the input structure is similar. Each of these processes are simulated through tabular input of the appropriate value as a function of time. At time intermediate to those in the tables, linear interpolation between the two times is used.

Format:

```
Subroutine   Statement
DATAHT
             READ(7,6) LABEL
             READ(7,6) LABEL
             READ(7,6) LABEL
             CALL READN(IWTYPE,MXWTYP,NCON)
          6  FORMAT(A79)
READN
          110 READ (7,*) MI,NSEQ,MAD,MITYP,MTYPAD
```

5.1.23 Data Set 23A: Printer and Auxiliary Storage Control

The number of lines is [(NTI/80+1)*2], (NTI/80+1) lines for printer output control and (NTI/80+1 lines for storage control.

Line 1 is free formatted.

Line 2 to Line [(NTI/80+1)] - FORMAT(80I1):

KPR0	KPR(1)	KPR(2) ...	KPR(I) ...	KPR(NTI)
1	2	3		80

Line [(NTI/80+1)+1] to Line [(NTI/80+1)*2] - FORMAT(80I1):

KDSK0	KDSK(1)	KDSK(2) ...	KDSK(I) ...	KDSK(NTI)
1	2	3		80

Definitions:

IITR = Integer indicating if iteration table of convergence information to be printed?
0 = no,
1 = transport iteration table be printed,
2 = both transport and chemical iteration tables printed.

INTER = Integer indicating if concentration field to be printed for each hydrological-chemical interaction?
0 = no,
1 = yes

ICOND = Integer indicating if the condition number of the Jacobian matrix in chemical equilibrium computation to be printed?
0 = no,
1 = yes.

NHGCI = Integer indicating if chemical equilibrium information to be printed?
0 = no,
>0 = every NHGC inter-hydro-geochem iterations print once.

KPR0 = Printer control for steady-state and initial conditions;
0 = print nothing,
1 = print FLOW, FRATE, and TFLOW,
2 = print above (1) plus concentration,
3 = print above (2) plus material flux.

KPR(I) = Printer control for I^{th} time-step similar to KPR0.

KDSK0 = Auxiliary storage control for steady-state and initial condition;
0 = no storage,
1 = store on logical unit 2.

KDSK(I) = Auxiliary storage control for I^{th} time-step similar to KDSK0.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,*) IITR,INTER, ICOND, NHGCI
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,30) KPR0,(KPR(I),I=1,NTI)
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,30) KDSK0,(KDSK(I),I=1,NTI)
30	FORMAT(80I1)
6	FORMAT(A79)

5.1.23.1 Data Set 23B: Nodes Where Detailed Chemical Printout Is Needed and Chemical Property (Sorption) Type Assigned to Each Node

Two groups of data are needed. The first group reads the chemical printout indicator and the second group reads type of chemical property (sorption) assigned to each node.

GROUP 1:

The number of lines depends NCPRT. Normally, two lines should be sufficient.

Line 1 input is unformatted with one integer. Line 2 input is unformatted with NCPRT integers.

Definitions:

NCPRT = Number of nodes where detailed chemical equilibrium information will be printed.

NODEP(1,2) = Global node number of the first node where detailed chemical equilibrium information will be printed.

NODEP(2,2) = Global node number of the second node where detailed chemical equilibrium information will be printed.

NODEP(N,2) = Global node number of the N^{th} node where detailed chemical equilibrium information will be printed.

Format:

Subroutine	Statement
DATAHT	
	READ(7,6) LABEL
	READ(7,6) LABEL

```
      READ(7,6) LABEL
      READ(7,*) NCPRT
      IF(NCPRT.EQ.0) THEN
      READ(7,6) LABEL
      ELSE
      DO 700 NP=1,NNP
      NODEP(NP,1)=0
      NODEP(NP,2)=0
700   CONTINUE
      READ(7,6) LABEL
      READ(7,6) LABEL
      READ(7,*) (NODEP(I,2),I=1,NCPRT)
      DO 710 I=1,NCPRT
      NP=NODEP(I,2)
      NODEP(I,2)=0
      NODEP(NP,1)=1
710   CONTINUE
      READ(7,6) LABEL
      READ(7,6) LABEL
6     FORMAT(A79)
```

GROUP 2: Sorption materal.

Up to five different sorption materials may be modeled in BLT-EC, Appendix D. This input specifies the sorption material at each node point.

The number of lines required is in general equal to NNP. However, automatic generation may be made.

Each of Lines 1 to NNP is an unformatted input of 5 variables.

Definitions:

NI	=	Node number of the first node in the sequence.
NSEQ	=	NSEQ subsequent nodes will be automatically generated.
NAD	=	Increment of node number for each of the NSEQ subsequent nodes.
NITYP	=	Type of chemical property assigned to node NI.
NTYPAD	=	Increment of NITYP for each of the NSEQ subsequent nodes.

NOTE: A line containing 5 zeros must be used to signal the end of this data set.

Format:

```
Subroutine      Statement
DATAHT
                CALL READN(NODEP(1,2),MAXNP,NNP)
READN
110             READ (7,*) NI,NSEQ,NAD,NITYP,NTYPAD
```

5.1.24 Data Set 24: Hydrological Data - Velocity and Moisture Control

If KVI .GT. 0, this data set is not needed because these will be read via Logical Unit 1.

A) VELOCITY FIELD

Normally, one line per node is needed. However, automatic generation can be made.

Each line is free formatted input containing 7 variables.

Definitions:

NI	=	Node number of the first node in the sequence.
NSEQ	=	NSEQ sebsequent nodes will be automatically generated.
NAD	=	Increment of node number in each of the NSEQ subsequent nodes.
VXNI	=	X-velocity component of node NI, (cm/s).
VZNI	=	Z-velocity component of node NI, (cm/s).
VXAD	=	Increment of x-velocity for each of the NSEQ subsequent nodes, (cm/s).
VZAD	=	Increment of z-velocity for each of the NSEQ subsequent nodes, (cm/s).

NOTE: A line with 7 zeros is used to signal the end of this subdata set.

Format:

Subroutine	Statement
GM2DXZ	
	IF(KVI.GT.0) THEN
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	ELSE
	C READ VELOCITY CARD IF KVI.LE.0
	NODES=0
	READ(7,6) LABEL
	READ(7,6) LABEL
	READ(7,6) LABEL
	110 READ(7,*) NI,NSEQ,NAD,VXNI,VZNI,VXAD,VZAD
	IF(NI.EQ.0) GO TO 120
	NJ=NI+NSEQ
	DO 115 NP=NI,NJ
	NODES=NODES+1
	I=NNI+(NP-NI)*NAD
	VX(I)=VXNI+VXAD*DFLOAT(NP-NI
	VZ(I)=VZNI+VZAD*DFLOAT(NP-NI)
	115 CONTINUE
	GO TO 110

```
120   IF(NODES.EQ.NNP) GO TO 125
      STOP
125   IF(NODES.LE.MAXNP) GO TO 130
      STOP
130   CONTINUE
6     FORMAT(A79)
```

B) MOISTURE CONTENT FIELD

Normally, one line per element. However, automatic generation can be made.

Each line is a free formatted input containing five variables.

Definitions:

NI	=	Element number of the first element in the sequence.
NSEQ	=	NSEQ subsequent elements will have the moisture content automatically generated.
NAD	=	Increment of element number for each of the NSEQ subsequent elements.
THNI	=	Moisture content of node element NI, (dimensionless, $0 \leq THNI \leq 1$).
THNIAD	=	Increment of moisture content for each of the NSEQ subsequent elements, (dimensionless).

NOTE: A line with 5 zeros signals the end of this subdata set.

Format:

Subroutine GM2DXZ

Statement

```
C READ MOISTURE CONTENT VIA CARD IF KVI.LE.0
      NODES=0
      READ(7,6) LABEL
      READ(7,6) LABEL
160   READ(7,*) NI,NSEQ,NAD,THNI,THNIAD
      IF(NI.EQ.0) GO TO 170
      NJ=NI+NSEQ
      DO 165 NP=NI,NJ
      NODES=NODES+1
      I=NI+(NP-NI)*NAD
      DO 165 IQ=1,4
      TH(IQ,I)=THNI+THNIAD*DFLOAT(NP-NI)
165   CONTINUE
      GO TO 160
170   IF(NODES.EQ.NEL) GO TO 175
      STOP
175   IF(NODES.LE.MAXEL) GO TO 180
      STOP
180   CONTINUE
6     FORMAT(A79)
```

6 ECIN: A PRE-PROCESSOR FOR CREATING CHEMISTRY INPUT FILES FOR BLT-EC

ECIN is a FORTRAN program designed to assist the BLT-EC code user in creating the chemistry input file. ECIN is an interactive code that works by supplying a series of menu's that direct the user through the steps necessary to create a chemistry input file. It is capable of creating a new chemistry input file, or modifying an existing file. ECIN also creates two auxilliary output files, LAST.DAT and SAMPLE.QUE. LAST.DAT provides a back-up listing of the chemistry input file created by the user and SAMPLE.QUE provides a listing of commands entered by the user during the course of using ECIN to create a chemistry input file. Because BLT-EC has its own database, the primary information that must be conveyed through the chemistry input file is the identification of each chemical component in the disposal system being modeled. Components are selected from the pre-defined set by specifying either the first letter of the component name or the 3-digit component ID number. In general, it is not necessary to identify the species that are reaction products of the selected components. BLT-EC will search the database to find the species that can be formed from the specified components. Exceptions are specifying that a particular species is to be excluded, specifying the disposition of a particular solid with regards to oversaturation (explained below), or for any database species, specifying a different equilibrium constant than that provided in the thermodynamic database. When it is necessary to do so, aqueous species that are reaction products are identified by specifying the components that represent the major cation and major anion. Solids are identified to ECIN by specifying the component that represents the major cation and the main mineral group to which the solid belongs (e.g. carbonate, sulfide). Alternatively, one may specify the 7-digit ID number for any aqueous or solid species if it is known. Menus and prompts within ECIN allow all of these things to be done with relative ease.

ECIN has the following features:

- New components may be defined by editing the component database file, COMP.DBS. Of course, new components are of little use unless reactions incorporating them as reactants are also provided. New reactions between new or existing components may be permanently added to the database files (see Appendix A) or may be added for a particular execution by including them in the input file. ECIN will prompt for the information needed to do this.

- BLT-EC solves the equilibrium problem iteratively by computing mole balances from estimates of component activities, that is, activities of the free species represented by the components. Hence, it is necessary to provide an initial estimate or guess for the activity of each component. ECIN makes this guess automatically for every component as equal to the component total dissolved concentration but also provides the means for the user to change the guess.

- It is possible for the user to insist that certain conditions prevail at equilibrium. For example, it may be desired to equilibrate the solution to a specified pH. This is done by specifying that the activity of H+ is fixed as dictated by the selected pH. The pe may be fixed in a similar manner. It is also possible to insist that a given solid is present at equilibrium. This is done by specifying it as an INFINITE solid in ECIN.

- The user has four options with regard to allowing oversaturated solids to precipitate (not including the infinite solids option above). 1) No solids are allowed to precipitate, 2) No solids are allowed except for those explicitly specified in the input file, 3) All oversaturated solids are allowed, or 4) All oversaturated solids are allowed except for those explicitly excluded in the input file.

- At start-up, ECIN asks for the name of the chemistry input file to be created. It also asks for the name of an existing chemistry input file to use as a seed file or "template". If the user does not wish to use a seed file, program defaults are used for all system variables and program flags and the single component H^+ is entered automatically. If a seed file is used, all system variables, program flags, and species definitions become identical to those of the seed file. Note that the seed file itself is not modified by this procedure unless the filename selected for the chemistry file to be created and the seed file's name are the same.

- ECIN is divided into four distinct sections called *edit levels*. After inquiring for file names, ECIN goes

automatically to EDIT LEVEL I to display the settings and parameters of the default problem or the seed problem represented by a seed file if one has been specified. Upon the users acceptance of the EDIT LEVEL I settings, a main menu screen is displayed from which the user may choose to enter any of the four edit levels, to use the current problem as a seed for another similar problem to be included in the same chemistry input file, or to exit the program. Upon returning from any edit level, this MAIN MENU is always displayed.

6.1 Running ECIN for the First Time

The following pages provide a basic introduction to ECIN by "walking-through" a short session where only the problem title is changed. After that session, each edit level is explored separately in greater detail.

In order to execute ECIN, you must type ECIN at the prompt. ECIN will begin by prompting you for the name of the chemistry input file you will create during this session. ECIN allows you to create an input file by beginning with the standard default values or by using an existing input file as a seed file. The following is a sample listing of the opening dialogue with ECIN. Lines that are indented and appear smaller characters represent what actually appears on your computer screen. Items that are underlined are examples of entries made by the program user.

ECIN

Version 1.00 08-21-96

ECIN is an interactive program used to build
chemistry input files for BLT-EC v1.00.

If you encounter errors, please print the file named SAMPLE.QUE or copy it to a diskette and send along with a description of the problem you were attempting to model to :

Robert J. MacKinnon
45 Caballo de Fuerza Rd SE
Albuquerque, NM 87123

or

Terry M. Sullivan
PO Box 5000
Brookhaven National Laboratory
Upton, NY 11973

In responding to prompts, use: Y or y = Yes, N or n = No,
R or r = Return to previous prompt (where applicable).
[D]=default choice obtained by pressing ENTER

Enter the name of the chemistry input file to be created. Use up to 8 characters PLUS from 0 to 3 characters for an extension.

ENTER FILENAME (enter "X" to exit ECIN) > TESTA.INP

If you want to use an existing chemistry input file as a "seed" file to be copied into ECIN and modified, enter the filename. Otherwise:
- - Enter an R to return to the previous question, or
- - Simply press ENTER to start a new file from scratch.

ENTER filename, R, or press ENTER >

The chemistry input file to be created is called TESTA.INP. No seed file is specified, so ECIN's default values will be used for all system parameters and program flags and the component H+ will be entered automatically with a log activity guess of -7.0. Had an existing filename been entered at the second prompt, the parameters, flags, and species entries of that file would be entered automatically. Note that in the VAX environment, the name of the existing file must be different from the name of the file to be created. When the two names are identical in a PC environment, the existing file is overwritten by the one being created. An accessory file called LAST.DAT is periodically updated throughout the ECIN session so that if an abnormal termination occurs, some portion of the work will be recoverable.

As previously mentioned, ECIN has four sections called edit levels. By default, you will automatically be placed in EDIT LEVEL I after responding to the filename prompts.

EDIT LEVEL I PROB # 1

1 Title 1:
2 Title 2:
3 Temperature (Celsius): 25.00
4 Units of concentration: MOLAL
5 Ionic strength: TO BE COMPUTED
6 Inorganic carbon is not specified.
7 Terminate if charge imbalance exceeds 30% ? NO
8 Oversaturated solids ARE NOT ALLOWED to precipitate. EXCEPTIONS: Solids listed in this file as TYPE-III (Infinite), -IV (Finite) or -V (Possible).
9 The maximum number of iterations is: 40
10 The method used to compute activity coefficients is: Davies equation
11 Level of output: INTERMEDIATE
12 The pH is: TO BE COMPUTED
13 The Eh is undefined.
99 Choose a different file to modify OR return to output filename prompt.

To change any of the above entries or to explore other possible values, enter the number to the left of the entry. Enter zero when you are finished. ENTER CHOICE >

In EDIT LEVEL I, a screen of information is displayed on your computer, as shown above. In this example, ECIN's default settings for system parameters, and program flags are displayed. If you had selected a previously existing input file as the starting point, its values would be displayed instead. In order to change any of the entries on this screen, enter the number to the left of the entry and respond to the questions presented. For example, to change the first line of title information for the run, enter a "1" as shown below. The program will then prompt you to enter the first line of the title for this problem.

ENTER CHOICE > 1

Enter problem title (1 of 2 lines),
OR press ENTER to omit title,
OR enter "R" to return to previous prompt:
This exercise illustrates ECIN's "default problem".

After any option is selected and changes are specified, the EDIT LEVEL I screen is updated to reflect the changes. The remainder of the EDIT LEVEL I options are discussed in a subsequent section. To exit EDIT LEVEL I enter a "0" at the "ENTER CHOICE >" prompt in the EDIT LEVEL I menu.

After exiting from EDIT LEVEL I, the MAIN MENU is displayed. From the MAIN MENU the user may choose to enter any of the four edit levels, to use the current problem as a seed for another similar problem to be included in the same chemistry input file, or the exit the program. Upon returning from any edit level, the MAIN MENU is always displayed. The

options presented in each edit level will be the subject of the remainder of this chapter. For the moment, let us exit ECIN.

```
_____MAIN MENU: SELECT OPTION____ PROB # 1_____
1 =  EDIT LEVEL I  (Change ionic strength, pH, Eh, temperature, adsorption parameters, number of iterations,
precipitation options, etc.)

2 = EDIT LEVEL II (Specify components, gas, redox, aqueous, and mineral species, adsorption sites and reactions, add
new species of all types)

3 = EDIT LEVEL III (Check, individually edit all entries)

X = EXIT (Write the current problem to the new Chemistry input file and EXIT PROGRAM)

                ENTER CHOICE > X
```

This causes the file "testa.inp" to be written to the directory that you are currently connected to and ECIN reminds you of the filename as you exit the program.

```
A Problem File Named TESTA.INP Has Now Been Generated.
It Can Be Modified By This Same Program By Recalling It As The Old File.
```

The contents of the file TESTA.INP are shown below.

```
This exercise illusrates ECIN's "default problem".

  25.00    MOLAL    0.000    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
0 0 1 0 0 0 0 0 1 1 0 0 0
0    0    0
    330   1.000E+00     -7.00  y                    /H+1
    0        0.000E+00
    0
```

6.2 Detailed Explanation of ECIN Options

The primary options available in ECIN are explained and illustrated below. The specific settings associated with each option are not necessarily default values; most were chosen for illustration only. Default values in program start-up are discussed above. Others are mentioned where appropriate.

6.2.1 Main Menu Option 1: Edit Level I

EDIT LEVEL I displays the current settings of system parameters such as temperature as well as program flag settings such as the number of iterations allowed. The user may change any of these settings by selecting the option number and responding to the resulting prompts.

This section contains a more detailed explanation of EDIT LEVEL I options and suggestions for using them. For most options, the explanation provided by ECIN will prove adequate. You are encouraged to experiment with all of the options available to become familiar with the capabilities of the program. Below is a sample of the display that appears when you enter EDIT LEVEL I.

```
_____EDIT LEVEL I _____PROB # 1____
```

1 Title 1:
2 Title 2:
3 Temperature (Celsius): 25.00
4 Units of concentration: MOLAR
5 Ionic strength: TO BE COMPUTED
6 Inorganic carbon is not specified.
7 Terminate if charge imbalance exceeds 30% ? NO
8 Oversaturated solids ARE NOT ALLOWED to precipitate. EXCEPTIONS: Solids listed in this file as TYPE-III (Infinite), -IV (Finite) or -V (Possible).
9 The maximum number of iterations is: 40
10 The method used to compute ac tivity coefficients is: Davies equation
11 Level of output: INTERMEDIATE
12 The pH is: TO BE COMPUTED
13 The pE and Eh are undefined.
99 Choose a different file to modify OR return to output filename prompt.

To change any of the above entries or to explore other possible values, enter the number to the levt of the entry. Enter zero when you are finished. ENTER CHOICE >

6.2.2 Edit Level I Options 1 and 2: Titles

These two entries allow you to enter a two line title for the BLT-EC run. The titles will appear in PART 1 of the chemistry output file and serve as a reminder of the purpose of the run.

6.2.3 Edit Level I Option 3: Temperature

Many of the parameters used in BLT-EC are temperature dependent and we recommend that you set this value to the actual conditions. BLT-EC will automatically correct as many values as possible to the temperature that you specify. See Appendix C for a description of temperature corrections to eq2uilibrium constants.

6.2.4 Edit Level I Option 4: Units of Concentration

The user does not have the option of selecting units of concentration. Option 4 is printed to the screen to remind the user that units of concentration are molar.

6.2.5 Edit Level I Option 5: Ionic Strength

Two choices are available, the ionic strength can either be computed by BLT-EC from the solution chemistry or it can be fixed at a molal value specified by the user. Fixing the ionic strength will generally improve convergence times since changes in ionic strength also change the activity coefficients and hence the solution composition. When the ionic strength is fixed, it becomes independent of the solution chemistry. Fixing the ionic strength implies that there are inert ions present in large enough concentration for their impact on ionic strength, and hence on activity coefficients, to be important. However, because these ions are not very reactive they need not be included as actual components. Examples are $Na^+$and Cl^- in many surface water problems (though it is not true that they should always be represented solely by fixing the ionic strength). An example of the dialogue when Option 5 is selected is shown below.

Should the ionic strength be fixed? (Y< N< [D] = N) > Y

Enter fixed ionic strength (molal) > .01

6.2.6 Edit Level I Option 6: Inorganic Carbon

BLT-EC needs the total dissolved concentration of each component for use in the mole balance equations. Frequently, the dissolved total for carbonate (CO_3^{2-}) is not available but alkalinity is. ECIN allows you to enter the alkalinity

in your choice of several commonly used units. The alkalinity value is stored in the data location ordinarily used for total dissolved carbonate and a special program flag is set in the input file so that BLT-EC will know to treat this value as alkalinity. BLT-EC computes the total dissolved carbonate concentration from the alkalinity value by the method described in Appendix C. You should read that portion of Appendix C carefully before using this option. When the alkalinity option is not used, total dissolved carbonate concentration may be entered just as any other concentration. Alternatively, you may set the total dissolved carbonate concentration to zero and specify that carbonate is in equilibrium with a fixed partial lpressure of $CO_2(g)$ in EDIT LEVEL II. The ECIN dialogue for entering alkalinity is shown below.

Do you want to specify dissolved inorganic carbon in this problem? (Y, N) > Y

When alkalinity is specified, no solids are allowed. (Set EDIT LEVEL I Option 8 to zero and specify the no TYPE III, IV, or V solids.)
Also, the titration used to determine alkalinity is assumed to be to the pH that is the equivalence point of the solution). Otherwise the alkalinity , factors in the database will not be applicable.

You have the option of specifying alkalinity as a measure of dissolved inorganic carbon. Alternatively, you may specify dissolved inorganic carbon explicitly. Your choice will generally depend upon the way carbonate concentration is expressed in the chemical analysis of the sample you are modeling.

Do you want to specify alkalinity? (Y, N) > Y

Select alkalinity units:
0 = Return to previous question
1 = mg/1 CO3-2
2 = mg/1 CaCO3
3 = eq/1
ENTER CHOICE > 2

Enter alkalinity in mg/1 CaCO3 > 0.500E+02

Alternatively, if you choose to entered total dissolved carbonate directly, the dialogue is:

Do you want to specify alkalininty? (Y, N)> N

Do you want to enter total inorganic carbon as total dissolved concentration of the EC component for inorganic carbon CO3-2? (Y, N) > Y

Enter total inorganic carbon as total dissolved concentration of CO3-2 in MOLAL > 0.3500E-03

The same result could have been achieved by entering total carbonate as you would any other componenent in EDIT LEVEL II.

6.2.7 Edit Level I Option 7: Termination of Charge Imbalance

Generally, it is not important for BLT-EC to terminate if the charge balance exceeds 30%. There are some cases when a large charge imbalance would indicate improper data, however. When a large charge imbalance occurs, the user should consider whether it results from omitting a relatively inert species such as Na^+ or from omitting a more reactive species such as SO_4^{2-}. In the former case the equilibrium composition will be affected very little (provided the effect on ionic strength is accounted for by fixing it as if Na+were present), but in the latter, the omission might be important.

6.2.8 Edit Level I Option 8: Precipitation

This entry allows you to turn precipitation on or off for the solids in the database except those which you explicitly specify as "POSSIBLE" or "EXCLUDED." These special designations for solids can be made in EDIT LEVEL II.

Sometimes, it is better to not allow any precipitation for the first run of a complex system and then to incoraporate p;recipitation into a second run. When precipitation is not allowed, BLT-EC will still compute the saturation indices for all the solids. Indices greater that zero indicate oversaturation with respect to the solution and indices are printed in the output file and may be used to decide which of the solids may be important in your problem.

In a model run with solid precipitation not permitted, many solids may be listed as oversaturated at equilibrium. It is important to realize that if a solid is listed as oversaturated, it may not actually precipitate when precipitation is permitted in a subsequent run. For a given cation, the most oversaturated solid will precipitate first. After it does so, others that were also oversaturated with respect to the pre-precipitation solution may not be oversaturated. When precipitation is allowed, it is generally best to also set the number of iterations to a large number (100 or 200) depending on the number of solids you expect to precipitate. BLT-EC allows you to obtain the saturation indices each time the solution is provisionally equilibrated during the program execution by specifying the solids print option as shown below. (Here, the term "provisional equilibration" means the solution is equilibrated but not with the complete or correct set of solids.) Generally, print option 1 is sufficient. With print option 1, provisional equilibration results are not written to the chemistry output file. Print option 2 causes provisional as well as final equilibrated results to be written to the output files.

```
Are all oversaturated solids to be allowed to precipitate? (Y, N, [D] = N) > Y

Select the solids output print option:
  0 = Return to previous question
  1 = Only after the final answer is reached
  2 = Each time a mineral precipitates or dissolves
      ENTER CHOICE >
```

6.2.9 Edit Level I Option 9: Maximum Number of Iterations

The default number of iterations is 40. Generally this is sufficient for relatively simple problems or those that do not allow solids to precipitate. More iterations may be necessary if the problem is very complex and/or poor activity guesses are provided fo rthe species present. Also, if you suspect that multiple solids will precipitate, then a larger number of iterations will be required.

```
Select maximum number of iterations:
  0 =   40 iterations
  1 =   10 iterations
  2 =  100 iterations
  3 =  200 iterations
       ENTER CHOICE > 0
```

6.2.10 Edit Level I Option 10: Calculation of Activity Coefficients

There are two choices for calculating activity coefficients, the modified Debye-Huckel equation or the Davies equation (consult Appendix A for the details). It should be noted that only a fraction of the species present in the database have the necessary constants for the modified Debye-Huckel equation. When the Debye-Huckel equation is selected, the Davies equation is will be substituted for those species lacking the required constants. By selecting option "1" you will cause all the activity coefficients to be calculated in a consistent manner with Davies equation.

```
Select an activity coefficient algorithm:
  0 = Extended Debye-Huckel
  1 = Davies Equations
      ENTER CHOICE >
```

6.2.11 Edit Level I Option 11: Chemistry Output File Options

You can control the amount of information written to the chemistry output file. Option 1 is the most complete and

Option 3 provides the least information. For transport problems with more than 10 elements, it is recommented that Option 3 be selected. You should experiment with these to determine how much of the information you really need to obtain. In general, Option 2 provides the best combination of brevity and completeness. Care should be used in selecting Option 1 and simultaneously choosing the solids print Option 2 (see EDIT LEVEL I OPTION 8). Very large output files and long run times may result.

```
Select the output option:
  0 =   Return to previous question
  1 =   FULL output file
  2 =   INTERMEDIATE (omit some of the thermodynamic data read from the database
        uncorrected log K values, gfw, etc.)
  3 =   ABBREVIATED (mass distribution at equilibrium only)
        ENTER CHOICE >
```

6.2.12 Edit Level I Option 12: pH

The hydronium ion concentration can be entered as a measured pH, or as total hydrogen. Each of these options also allows you the choice of fixing the pH or letting BLT-EC calculate the equilibrium value.

```
Select pH option:
  1 = Specify EQUILIBRIUM PH
  2 = Allow pH to be computed but specify total hydrogen concentration
  R = Return to previous menu
        ENTER CHOICE > 1
```

Note: The user must specify pH (Option 1) or total hydrogen concentration (Option 2) in the BLT-EC input file (see data sets 9 and 15).

6.2.13 Edit Level I Option 13: Eh

Redox potential is entered as Eh. Note, systems containing redox chemistry can be very sensitive to the initial activity guesses made for the electron or for the components of redox couples.

```
Select redox potential option:
  1 = Specify equilibrium Eh
  R = Return to previous menu
      ENTER CHOICE > 1
```

Note that by selecting 1, the user must specify Eh in the main BLT-EC input file.

6.2.14 Edit Level I Option 99: Choose a Different File to Modify or Return to Output File Name Prompt

This option allows you to abandon any work up to the point it is selected and choose a different existing file to use as a seed file. Once you arrive at the prompt that allows this adjustment, you have the option of returning to the very first prompt of the ECIN session and specifying a different filename for the chemistry input file to be created, or to exit the program.

6.3 Main Menu Option 2: Edit Level II

EDIT LEVEL II is used to specify the chemistry of the system. Total dissolved concentrations or fixed activities of components are specified by selecting the appropriate option from the EDIT LEVEL II menu. Infinite solids, redox couples, and other possible solids may also be specified. Many of the options involving aqueous species and solids provide a facility for searching the database if the user is uncertain whether that species is included. New species may be defined

by following the prompts. EDIT LEVEL II also provides for choosing an adsorption model, specifying its parameters, and defining adsorption reactions. The menu screen for EDIT LEVEL II appears below.

```
_____SELECT OPTION_____

1 =  Specify AQUEOUS COMPONENTS: TOTAL CONCENTRATIONS or FIXED ACTIVITIES
2 =  Specify AQUEOUS SPECIES not in the database, search the database, or alter a database AQUEOUS
     SPECIES equilibrium constant
3 =  Specify and ADSORPTION MODEL and REACTIONS
4 =  Specify GASES at FIXED partial pressure
5 =  Specify REDOX COUPLES with FIXED activity ratios
6 =  Specify INFINITE SOLID phases
7 =  Specify POSSIBLE SOLID phases
8 =  Specify EXCLUDED SPECIES of any type
A =  Specify reactions to be included during calculations
R =  RETURN to MAIN MENU

All choices allow you to browse and return without changing anything;
Most allow you to search or view a directory of the relevant database.
   ENTER CHOICE > 1
```

Each of these selections will prompt you for information in approximately the same way you will find some repetition in the discussion of the different options that follow.

6.3.1 Edit Level II Option 1: Specify an Aqueous Component

This option is used to select the basic components that you will need in the chemistry input file. Components are the building blocks for all other species in the database. A complete list of all components and their ID numbers can be found in Appendix E. When a component is selected, you must specify either its total dissolved concentration or the fixed activity of the free component.

Components are identified to ECIN by specifying the first letter of the component name or the 3-digit component ID number. In the example below, Ca^{+2} is selected from the list of components starting with the letter "C." For Ca^{+2} this ID number would be 150 shown below. To signal that you are finished entering components, enter a zero. You may toggle between the first letter mode of entry and the ID number mode by entering -1 as directed. Note that the names of some components are written as acids. For example, an entry of "S" in the first letter mode will produce a numbered list of components that begin with the letter "S" but the component for silicon will not be among them. That component, H_4Si0_4, is listed under "H". Also, when you enter a total dissolved concentration, an activity guess is made by ECIN unless the entered concentration is zero. In that case you will be asked to supply the activity guess (read the prompt carefully; you may be asked for the "log activity" which should be taken to mean the common logarithm of the free component activity). For components that you specify as having fixed activity, you will likewise be asked to specify the fixed activity. Note that activities, whether fixed or guessed, are always in units of molal (approximately molar) regardless of the concentration units specified in EDIT LEVEL I.

```
_____EDIT LEVEL II_____PROB # 1_____
_____DEFINE COMPONENT SPECIES_____

Specify components for which you know the:
1 = TOTAL DISSOLVED CONCENTRATION
2 = FIXED EQUILIBRIUM ACTIVITY
R = Return to previous options menu (EDIT LEVEL II)
    ENTER CHOICE > 1
- Enter the FIRST LETTER for the COMPONENT:
```

```
    To identify the component you want, enter the first letter in its chemical symbol (inorganic)
  or  name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR press enter to terminate component entry.
    ENTER you choice > c

 1 CO3-2      2 CN-          3 CLIG2          4 Ca+2          5 Cd+2
 6 Cl-1       7 Cr+2         8 Cr(OH)2+       9 Cr04-2  10 Cu+1
11 Cu+2       12 Citrate

Select the number of the appropriate component ( 0 = None) > 3

- Enter the FIRST LETTER for the COMPONENT:
    To identify the component you want, enter the first letter in its chemical symbol (inorganic)
  or  name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR press enter to terminate component entry.
    ENTER you choice > c

 1 CO3-2      2 CN-          3 CLIG2          4 Ca+2          5 Cd+2
 6 Cl-1       7 Cr+2         8 Cr(OH)2+       9 Cr04-2        10 Cu+1
11 Cu+2       12 Citrate

Select the number of the appropriate component ( 0 = None) > 1
```

Note: Concentrations are specified in the main BLT-EC input file (see data set 15)

```
- Enter the FIRST LETTER for the COMPONENT:
      To identify the component you want, enter the first letter in its chemical symbol
      (inorganic) or  name (organic),
      OR enter a minus one (-1) to switch to component entry by ID number,
      OR press enter to terminate component entry.
   ENTER your Choice > OR

Specify components for which you know the :
1 = TOTAL DISSOLVED CONCENTRATION FRACTION
2 = FIXED EQUILIBRIUM ACTIVITY
R = Return to previous options menu (EDIT LEVEL II)
    ENTER CHOICE > R
```

6.3.2 Edit LEVEL II Option 2: Specify an Aqueous Species

There are two reasons for selecting this option. One is to change the equilibrium constant associated with a particular species from the database value to some other value that you have reason to believe is more appropriate. The other reason is to search the database to see whether a particular species is included and, if it is not, to define that species as an added reaction. The series of prompts that assist you in defining the new aqueous species are similar to those encountered in defining a new solid or an adsorption reaction in other EDIT LEVEL II options. You should have the reaction already written out in terms of components so that you can provide the stoichiometry and you should have the log K for the reaction as written as well as the species charge and molar mass. Other entries (enthalpy, Debye-Huckel constants, alkalinity factor) can be entered as zero if you do not have good values.

In identifying the species of interest, the user is asked for both the major cation and anion in a manner that is similar to EDIT LEVEL II OPTION 1 above. The database is searched for complexes that contain both components. If any matches are found, the reactions that contain them and their products are displayed on the screen. You may select any of these reactions. If no match is found or the species you want is not among those found, you are given an opportunity to add a new reaction. Note that you may skip the database search when a new species is to be added, but do this ONLY if you are sure

the species is not in the database already. It is generally best to first search the database by choosing the search option (1) first. An example dialogue for adding a reaction is shown below.

Specify a species that is a product of a:
1 = CONVENTIONAL REACTION
2 = REACTION involving a COMPOSITE LIGAND
R = Return to previous menu

If option 1 or 2 is selected, choose an option:
1 = Search the thermodynamic database for the species you want. If it is in the database, display its log K and enthalpy values for you to change if desired. If not in the database, assist you in defining and adding the species.
2 = Assist you in defining and adding a species that you already know is not in the thermodynamic database.
ENTER CHOICE > 1

The idea of the next series of prompts is to identify the species you want to ECIN. The 7-digit ID number should be used for an existing species (assuming you want to check or change its equilibrium constant).

EDIT LEVEL II PROB # 1
DEFINE AQUEOUS SPECIES

Is the ID # known for AQUEOUS SPECIES? (Y,N) > N

Define MAJOR cation component

- Enter the FIRST LETTER for the COMPONENT:
To identify the component you want, enter the first letter in its chemical symbol (inorganic) or name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR enter a zero (0) to terminate component entry.
ENTER your choice > c

1 CLIG2 2 Ca+2 3 Cd+2 4 Cr+2 5 Cr(OH)2+
6 Cu+1 7 Cu+2

Select the number of the appropriate component (0 = NONE) > 3

Define MAJOR anion component

- Enter the FIRST LETTER for the COMPONENT:
To identify the component you want, enter the first letter in its chemical symbol (inorganic) or name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR enter a zero (0) to terminate component entry.
ENTER your choice > c

1 CO3-2 2 CN- 3 CLIG2 4 Ca+2 5 Cd+2
6 Cl-1 7 Cr+2 8 Cr(OH)2+ 9 Cr04-2 10 Cu+1
11 Cu+2 12 Citrate

Select the number of the appropriate component (0 = NONE) > 3

Once you have completed choosing the major ions, the computer will search the entire database for entries that contain those two major components. In this case, no matches were found. Had one or more species been found that

included both of these components, a numbered menu would appear from which to choose. If none were the species of interest, you would be given opportunity to define a new species just as the case where no matching species was found, as in this example. The dialogue which informs you that no matches were detected and proceeds to prompt you for information for the new species follows.

PATIENCE..Thermodynamic database file 7 is being searched!

No NEAR match found in the database for ID 2101800

Do you want to define a new species comprised at least partly of those constituents you have already specified? (Y, N) > Y

Is ID = 2101801 acceptable for a new AQUEOUS SPECIES? (Y, N, H) > Y
Now Add Reaction Not Yet In Data Base For AQUEOUS SPECIES

Enter Name For AQUEOUS SPECIES >CrCl+

Enter Charge On Species > 1.00

Enter Debye-Huckel A Parameter > 0.00

Enter Debye-Huckel B Parameter > 0.00

Enter Alkalinity Factor > 0.00

Enter Molecular Wt. (GFW) > 87.5

THE REACTION THUS FAR CREATED IS:

0.000 Cl-1 + 0.000Cr+2 <- - - - -> CrCl+

- - - - Specify MASS ACTION and MASS BALANCE stoichiometry- - - -

Reactants (entities ordinarily on the left side) have positive stoichiometry
Products (entities ordinarily on the right side) have negative stoichiometry
Enter the stoichiometry of Cl-1

THE REACTION THUS FAR CREATED IS:

1.000 Cl-1 +0.000Cr+2 <- - - - -> CrCl+

Enter the stoichiometry of Cr+2

THE REACTION THUS FAR CREATED IS:

1.000 Cl-1 +1.000Cr+2 <- - - - -> CrCl+

Are there any other components in this reaction? (Y,N)>N

For The Request That Follows, K Must Be Consistent With Molar Concentrations.

Enter the Log K value for formation of this species > 5.6

Enter the enthalpy for formation of this species > -20.2

ID # 2101800 CrCl+ Chosen. Current LOG10 (KEQ) = 0.56000E+01

EDIT LEVEL TWO PROB # 1
DEFINE AQUEOUS SPECIES

Specify AQUEOUS SPECIES? (Y, N, H) > N

Note that the stoichiometry coefficients requested are for the mass action expression. BLT-EC supports the option of having mass balance stoichiometry that differs from that of the mass actions expression. For added reactions with this characteristic, the mass balance stoichiometry can be specified in EDIT LEVEL III. Also, note that we can tell by examination of the above of the above example that the components Cl^- and Cr^{2+} had not been selected as components for this problem when this reaction was defined.

6.3.3 Edit Level II Option 3: Specify Adsorption Definition

This option is chosen when you want to specify an adsorption model and add adsorption reactions to the problem. Descriptions of input parameters for the available models are provided in Appendix D. In the following example, Ca^{+2} is allowed to adsorb to surface 1 site type 1 by a simple activity Kd sorption algorithm. The adsorption reactions are created and treated similarly to aqueous complexation reactions in the above example.

EDIT LEVEL II PROB # 1
DEFINE Adsorption Problem

Select an adsorption algorithm:
1 = Activity Kd
2 = Activity Langmuir
3 = Activity Freundlich
4 = Ion Exchange Model
5 = Constant Capacitance Model (CCM)
6 = Triple Layer Model (TLM)
7 = Diffuse Layer Model (DLM)
R = Return to edit level 2 menu
ENTER CHOICE > 1

A maximum of five adsorbing surfaces, each with one or two types of binding sites may be defined. Opportunity to define multiple surfaces is presented in a succession of prompts. The identifying surface numbers 1 through 5 serve only to distinguish one surface from another when specifying surface reactions. There is no intrinsic difference between surfaces of different identifying numbers. Similarly, there is no intrinsic difference between sites 1 and 2 on a surface. For both surfaces and sites YOU establish any differences by assigning different characteristics and parameters for different surfaces and different reactions and equilibrium constants for the different sites on a surface.

PRESS ENTER TO CONTINUE

Some of the modifications to be made are material dependent. Please enter the number (1-5) of the material to be modified:
(This can be changed later) > 1

Enter the mass of soil (kg) to which one liter of solution is exposed (Enter zero to return to previous prompt) > 3.177

Once you have selected the adsorption model, a screen displaying the status of currently defined surface and site definitions will appear. This screen will be updated as you set additional parameters. You may define one or more reactions involving each site. The procedure is almost identical to that required to enter a new aqueous species as shown in EDIT

LEVEL II OPTION 2. For the electrostatic models, note that the components that represent electrostatic terms are entered with the proper stoichiometry automatically.

```
_____ADSORPTION STATUS_____

The following binding-site types are defined for 0 surface(s):

----NO SURFACES CURRENTLY DEFINED----

_____ADSORPTION OPTIONS_____
Select an option:
  1 = ADD a NEW SURFACE with a site
  2 = ADD a NEWS SITE on a currently defined surface
  3 = ADD a NEW REACTION for material 1 at a currently defined site
  4 = ATTACH an auxiliary database of adsorption reactions
  5 = DELETE a currently defined site
  6 = Change the material currently being modified
  7 = Characterize OLD SURFACE for CURRENT MATERIAL
  8 = Characterize OLD REACTION for CURRENT MATERIAL
  C = CANCEL adsorption option for material 1 and return
  R = RETURN without changing anything

  Enter Choice > 1

Enter the site type number (1 or 2) > 1

_____ADSORPTION STATUS_____
_____MATERIAL #1_____

The following binding-site types are defined for 1 surface(s):
Surface  Site Type Number      Component Number    Site Conc (moles/l)
   1              1                   811              Infinite Supply

_____ADSORPTION OPTIONS_____
Select an option:
  1 = ADD a NEW SURFACE with a site
  2 = ADD a NEWS SITE on a currently defined surface
  3 = ADD a NEW REACTION for material 1 at a currently defined site
  4 = ATTACH an auxiliary database of adsorption reactions
  5 = DELETE a currently defined site
  6 = Change the material currently being modified
  7 = Characterize OLD SURFACE for CURRENT MATERIAL
  8 = Characterize OLD REACTION for CURRENT MATERIAL
  C = CANCEL adsorption option for material 1 and return
  R = RETURN without changing anything

  Enter Choice:  ([D] = R) > 3

For Material #1:

Enter the ID # (1-5) of the surface to which this operation pertains > 1
Enter the site type number (1 or 2) >1

_____SPECIFICATION OF ADSORPTION REACTIONS ON Site Type 1_____
_____MATERIAL #1_____
_____SURFACE NUMBER ONE_____

>>>>>>Specify tthe Major Aqueous Reactant in ADSORP'N Product>>>>>>>
```

Enter the FIRST LETTER for the COMPONENT:
To identify the component you want, enter the first letter in its chemical symbol (inorganic) or name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR enter a zero (0) to terminate component entry.
ENTER your choice > c

1 C03-2	2 CN-	3 CLIG2	4 Ca+2	5 Cd+2
6 Cl-1	7 Cr+2	8 Cr(OH)2+	9 Cr04-2	10 Cu+1
11 Cu+2	12 Citrate			

Select the number of the appropriate component (0 = None) > 4

Is ID = 8111500 acceptable for a new ADSORBED SPECIES? (Y, N) > Y

Now Add Reaction Not Yet In Data Base For ADSORBED SPECIES

Enter Name For ADSORP'N PRODUCT . > X-Ca

THE REACTION THUS FAR CREATED IS:

0.000ADS1TYP1 + 0.000 Ca+2 <-----> X-Ca

----- Specify MASS ACTION and MASS BALANCE Stoichiometry -----

Reactants (entities ordinarily on the left side) have positive stoichiometry
Products (entities ordinarily on the right side) have negative stoichiometry

Enter the stoichiometric coefficient for ADS1TYP1
ENTER stoichiometry > 1.00

THE REACTION THUS FAR CREATED IS:

1.000 ADS1TYP1 + 0.000 Ca+2 <-----> X-Ca

-----Specify MASS ACTION and MASS BALANCE stoichiometry -----

Reactants (entities ordinarily on the left side) have positive stoichiometry
Products (entities ordinarily on the right side) have negative stoichiometry

Enter the stoichiometric coefficient for Ca+2
ENTER stoichiometry of Ca+2 > 1.00

Are there any other components in this reaction? (Y, N) > N

THE REACTION CORRESPONDING TO MASS ACTION THUS FAR CREATED IS:

1.000 ADS1TYP1 + 1.000 Ca+2 <-----> X-Ca

The distribution coefficient needed for the activity K_d model is expressed in liters/kg. The nulmber of kg of soil with which one liter of solution is in equilibrium has been entered already and will be used to normalize this value to a mg (sorbed) per mg (dissolved) basis for use as an equilibrium constant in the above reaction.

Enter the distribution coefficient, K_d, for this metal for material 1 (l/kg) >1.0

Enter Enthalpy For Reaction To Form X-Ca > 0.00000E+00

ID # 8111500 X-Ca Current LOGK (KEQ) = 0.502

Any MORE ADSORPTION REAC'NS for Site Type 1? (Y, N) > N

ADSORPTION STATUS
MATERIAL #1

The following binding-site types are defined for 1 surface(s):

Surface	Site Type Number	Component Number	Site Conc (moles/1)
1	1	811	Infinite Supply

ADSORPTION OPTIONS

Select an Option:
1 = ADD a NEW SURFACE with a site
2 = ADD a NEWS SITE on a currently defined surface
3 = ADD a NEW REACTION at a currently defined site
4 = ATTACH an auxiliary database of adsorption reactions
5 = DELETE a currently defined site
6 = Change the material currently being modified
7 = Characterize OLD SURFACE for CURRENT MATERIAL
8 = Characterize OLD REACTION for CURRENT MATERIAL
C = CANCEL adsorption option for material 1 and return
R = RETURN without changing anything
Enter Choice: > R

Note that a currently defined site and all added reactions in which it is involved may be deleted by choosing Option 5.

6.3.4 Edit Level II Option 4: Specify a Fixed Gas Species

This option should not be selected for transport calculations. This option is provided only to give the user the option of examining fixed gas species on chemical equilibria in the absence of transport. When this option is chosen, you are prompted with a complete list of the gases present in BLT-EC's database. You then make a selection and enter the fixed equilibrium partial pressure of the gas. You are allowed to change the log K if you desire; otherwise, it is automatically corrected to the partial pressure you have specified (in atm). All gases are automatically defined as EXCLUDED species in BLT-EC unless explicitly entered here.

EDIT LEVEL II PROB # 1
DEFINE GASEOUS SPECIES

Specify FIXED GASES? (Y, N) > Y

1-CH4 (g)	2-CO2 (g)	3-02 (g)	4-Hg (g)
5-Hg2 (g)	6-Hg(CH3)2 (g)	7-HgBr (g)	8-HgCl (g)
9-HgF (g)	10-HgI (g)	11-HGBr2 (g)	12-HgF2 (g)
13-HgI2 (g)			

Enter the number corresponding the gas you want. Enter zero to abort the specification of a gas.
ENTER CHOICE > 2

PATIENCE..thermodynamic database file 9 is being searched!
1 3301403 CO2 (g) <- 1.0 CO3-2 + 2.0 H+1 + -1.0 H2O

Enter the non-zero partial pressure (atm of CO2 (g) > 0.10000E-02

Corrected log K is 21.160

Do you want to Change the Log K value from 21.1600? (Y<N) >N

6.3.5 Edit Level II Option 5: Specify a Redox Couple

When this option is selected, redox couples in the thermodynamic database will be displayed in a numbered menu from which you may choose those you want to include in the BLT-EC problem. It is also a good idea to specify the Eh either as a guess at the equilibrium value (if the true Eh is to be computed) or as a fixed value (if the solution is to be equilibrated to a given Eh).

```
                    EDIT LEVEL II          PROB # 1
                  DEFINE REDOX SPECIES

      ----  CHOOSE FROM THE FOLLOWING REDOX COUPLES:  ----

1 Fe+2/Fe+3        2 NO2/NO3        3 NH4/NO3        4 AsO3/AsO4
5 SbOH3/SbOH6-     6 U+3/UO2+2      7 U+4/UO2+2      8 UO2+/UO2+2
9 Mn+2/Mn+3        10 Cu+1/Cu+2     11 V+2/VO2+1     12 V+3/VO2+1
13 VO+2/VO2+1      14 HS-/SO4-2     15 Tl+/Tl(OH)3   16 HSe-/HSe03-
17 HseO3-/SeO4     18 Hg2/Hg(OH)2   19 Cr+2/Cr(OH)2  20 Cr(OH)2/CrO4

Enter the index corresponding to the couple you want. Enter zero to abort the selection of a redox
couple.
        ENTER CHOICE > 1

PATIENCE..Thermodynamic database file 8 is being searched!
 1 2812810 FE+2/FE+3          <        -1.0 Fe+3          +-1.0 Fe+2  +    1.0 E-1

Do you want To Change Log K value from 13.0320? (Y, N) > N

Do you want To Change the enthalpy value from  -10.00? (Y, N) > N
```

Note that had the electron not already been entered as a component (by specifying the pe or Eh in EDIT LEVEL I OPTION 13 or by simply selecting it as a component in EDIT LEVEL OPTION 1 above), ECIN would have entered it as a component with total dissolved concentration of zero and inquired whether to fix its activity (at the program default value of log activity = -16.0).

6.3.6 Edit Level II Option 6: Specify an Infinite Solid

An infinite solid is one that is not subject to complete dissolution. As such, the solution is required to be at equilibrium with the infinite solid. All precipitated solids, whether infinite or finite, reduce the degrees of freedom by 1 (see Appendix C). As was shown above for EDIT LEVEL II OPTION 2 (Specify Aqueous species), ECIN provides means of searching the database to see whether a particular solid is present, allowing you to specify an equilibrium constant different from the database value if desired, and allowing you to define a new solid species if the one you seek is not found in the database. The method of identifying the solid species you want is the primary difference between the aqueous species procedure and that shown below (which applies to INFINITE and POSSIBLE solids). In general, the major cation and major mineral group as given by a numbered menu are specified. For solids that are known to be included in the database, the 7-digit ID number may be specified instead.

```
                    EDIT LEVEL II          PROB # 1
                  DEFINE MINERAL SPECIES

- - This section allows you to specify minerals that are present in complete dissolution.

Choose an option:
  1 =  Search the thermodynamic database for the species you want.  If it is in the database, display
```

its log K and enthalpy values for you to change if desired. If not in the database, assist you in defining and adding the species.

2 = Assist you in defining and adding a species that you already know is not in the thermodynamic database.

R = Return to the previous question.

ENTER CHOICE > 1

Is the ID # known for the MINERAL? (Y, N) > N

1 Elemental	10 Sulfide	11 Cyanide
12 Selenide	14 Antimonide	20 Oxide or Hydroxide
30 Multiple Oxide	40 Bromide	41 Chloride
42 Fluoride	43 Iodide	50 Carbonate
51 Nitrate	52 Borate	60 Sulfate
61 Selenate or Selenite	70 Phosphate	72 Arsenate
73 Vanadate	80 Orthosilicate	82 Chain Silicate
84 Framework Silicate	86 Sheet Silicate	

Enter the number corresponding to the class to which the mineral belongs.
ENTER CHOICE (0 = none) > 10

>>>>>SPECIFY MAJOR CATION <<<<<

- Enter the FIRST LETTER for the COMPONENT:
To identify the component you want, enter the first letter in its chemical symbol (inorganic) or name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR enter a zero (0) to terminate component entry.
ENTER your choice > f

1 Fe+2 2 Fe+3

Select the number of the appropriate component (0 = NONE) > 1

PATIENCE.. Thermodynamic database file 19 is being searched!

1	1028000 FES PPT	<- -1.0 H+1	+	1.0 Fe+2	+	1.0 HS-1
2	1028001 GREIGITE	<- -4.0 H+1 + 4.0 HS-1	+	2.0 Fe+3	+	1.0 Fe+2
3	1028002 MACKINAWITE	<- -1.0 H+1	+	1.0 Fe+2	+	1.0 HS-1
4	1028003 PYRITE	<- -2.0 H+1 + 2.0 HS-1	+	-2.0 E-1	+	1.0 Fe+2

Enter the number aligned with the species you want. (0 = None of above) > 4

Do you want To Change the Log K value from 18.4790? (Y, N) > N

Do you want to Change the Enthalpy value from -11.3000? (Y, N) > N

Remember that each solid specified, as well as each gas, each redox couple, each finite solid, and each component with fixed activity reduces the number of degrees of freedom for solving this problem by 1. If the degrees of freedom is reduced to zero, phase-rule violation will occur in BLT-EC. ECIN checks the degrees of freedom upon attempting to exit the program and

warns if it is zero at the outset due to the presence of more fixed species than variable components. It may be necessary to remove some constraints such as one or more infinite solids if such a warning occurs.

6.3.7 Edit Level II Option 7: Specify a Possible Solid

POSSIBLE SOLIDS are solids that are permitted to precipitate if equilibrium conditions warrant. All database solids become POSSIBLE SOLIDS when the precipitation flag in EDIT LEVEL I OPTION 8 is so set. In that case there is no need for this option. However, the other setting of the EDIT LEVEL I flag dictates that all solids be EXCLUDED SPECIES except those explicitly designated as POSSIBLE SOLIDS through this option. The manner of identifying POSSIBLE SOLIDS is identical to that for INFINITE SOLIDS above and is not repeated here.

6.3.8 Edit Level II Option 8: Specify an Excluded Species

This option allows you to exclude any type of species from mole balance. In the case of solids, one setting of the precipitation flag in EDIT LEVEL I provides for all database solids to be excluded from precipitating (the equivalent of defining them as EXCLUDED SPECIES). Another provides for all to be permitted to precipitate if equilibrium conditions warrant. This option can be used in conjunction with the latter EDIT LEVEL I option to explicitly exclude certain solids (see EDIT LEVEL II OPTION 8). Any aqueous species may also be excluded including any component as an aqueous species. The user will note that certain species appear in the list of EXCLUDED SPECIES automatically when BLT-EC is executed. These include the electron unless its activity is fixed, all electrostatic components of the adsorption models, all database gases and redox couples not explicitly defined as SPECIES WITH FIXED ACTIVITY. EXCLUDED solids do not appear in the list unless explicitly defined as EXCLUDED SPECIES in BLT-EC.

The procedure for explicitly excluding a species amounts to little more than identifying it to ECIN. The procedures for doing that are basically the same as for identifying species of the various types as shown above. The same questions and rules follow here as well, except a little less information is required. Please refer to the options above for examples of the selection dialogue. An example of excluding a component follows.

EDIT LEVEL II PROB # 1

DEFINE Excluded Species

- - This section allows you to specify component, aqueous, or mineral species that you want to exclude from mass balance calculations. Note that all redox, gas, and adsorbed species are excluded by default except those you enter as TYPE 3 or as ADDED speciles in this input file. Components used for electrostatic potentials are excluded automatically.

Specify the type of species:

1 = COMPONENT species
2 = AQUEOUS species
3 = MINERAL species
4 = ADSORBED species
5 = FIXED RATIO REDOX couple
6 = FIXED GAS species
R = RETURN to EDIT LEVEL II menu
ENTER CHOICE ([D] = R) > 3

Is the ID # known for the EXCLUDED SPECIES? (Y, N) > N

1 Elemental	10 Sulfide	11 Cyanide
12 Selenide	14 Antimonide	20 Oxide or Hydroxide
30 Multiple Oxide	40 Bromide	41 Chloride
42 Fluoride	43 Iodide	50 Carbonate

51 Nitrate	52 Borate	60 Sulfate
61 Selenate or Selenite	70 Phosphate	72 Arsenate
73 Vanadate	80 Orthosilicate	82 Chain Silicate
84 Framework Silicate	86 Sheet Silicate	

Enter the number corresponding to the class to which the mineral belongs.
ENTER CHOICE (0 = none) > 10

>>>>>>>>>SPECIFY MAJOR CATION>>>>>>>>>

- Enter the FIRST LETTER for the COMPONENT:
To identify the component you want, enter the first letter in its chemical symbol (inorganic) or name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR press ENTER to terminate component entry.
ENTER your choice > f

1 Fe+2 2 Fe+3

Select the number of the appropriate component (0 = NONE) > 1

PATIENCE.. Thermodynamic database file 19 is being searched!

1	1028000 FES PPT	<- -1.0 H+1	+	1.0 Fe+2	+	1.0 HS-1
2	1028001 GREIGITE	<- -4.0 H+1 + 4.0 HS-1	+	2.0 Fe+3	+	1.0 Fe+2
3	1028002 MACKINAWITE	<- -1.0 H+1	+	1.0 Fe+2	+	1.0 HS-1
4	1028003 PYRITE	<- -2.0 H+1 + 2.0 HS-1	+	-2.0 E-1	+	1.0 Fe+2

Enter the number aligned with the species you want. (0 = None of above) > 1

6.3.9 Edit Level II Option A: Specify Chemical Reactions

Option A allows the user to specify chemical reactions that are to be included in the BLT-EC calculations. This feature permits the chemistry problem to be limited to choose reactions determined to be important, an important capability in large transport problems.

EDIT LEVEL II PROB # 1
DEFINE REACTIONS

- - This section allows you to specify reactions that will be used for type II, type V, and ligand-bound species during calculations.

Please enter the type of reaction to be added or deleted:
1 = Reaction involving a complex ligand
2 = Type II species (species in solution)
3 = Type V species (possible solid)
R = RETURN to previous options menu (Edit Level II)
ENTER CHOICE ([D] = R) > 2

Please select how you would like to input the reactions:

1 = Input a list of ID numbers
2 = Identify major components and select reaction(s)
3 = Identify only one component and choose from
reactions involving that component
R = RETURN to previous menu
ENTER CHOICE ([D] = R) > 2

>>>>>>>>>SPECIFY MAJOR CATION>>>>>>>>>

- Enter the FIRST LETTER for the COMPONENT:
To identify the component you want, enter the first letter in its chemical symbol (inorganic) or name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR press ENTER to terminate component entry.
ENTER your choice > c

1 CLIG2 2 Ca+2 3 Cd+2 4 Cr+2 5 Cr(OH)2+
6 Cu+1 7 Cu+2

Select the number of the appropriate component (0 = NONE) > 2

>>>>>>>>>SPECIFY OTHER MAJOR ION>>>>>>>>>

Enter the FIRST LETTER for the COMPONENT:
To identify the component you want, enter the first letter in its chemical symbol (inorganic) or name (organic),
OR enter a minus one (-1) to switch to component entry by ID number,
OR press ENTER to terminate component entry.
ENTER your choice > c

1 C03-2 2 CN- 3 CLIG2 4 Ca+2 5 Cd+2
6 Cl-1 7 Cr+2 8 Cr(OH)2+ 9 Cr04-2 10 Cu+1
11 Cu+2 12 Citrate

Select the number of the appropriate component (0 = None) > 1

The following reactions involve those components:
Reaction #1:

501400 CaHCO3 + <- - - - -> 1.00 Ca+2 +1.00 CO3-2 +1.00 H+1
Reaction #2:
501401 CaCO3 AQ <- - - - -> 1.00 Ca+2 +1.00 CO3-2

Enter the number of the reaction you would like to add or <R> to return to the previous menu.

ENTER CHOICE ([D] = R) > 1

The following reactions involve those components:
Reaction #1:

501400 CaHCO3 + <- - - - -> 1.00 Ca+2 +1.00 CO3-2 +1.00 H+1

Enter the number of the reaction you would like to add or <R> to return to the previous menu.

ENTER CHOICE ([D] = R) > R

Are you finished entering reactions?

(Y=yes, N=no, [D]=N) > Y

Select a reaction list option:
1 = See the current list of reactions
2 = Add a reaction to the list of reactions to be used
3 = Delect a reaction from the list
4= Delect the entire list (use whatever reactions are found in thermo.unf)
R = RETURN to previous menu (select different type of species)
ENTER CHOICE ([D] = R) > R

EDIT LEVEL II PROB # 1
DEFINE REACTIONS

- - This section allows you to specify reactions that will be used for type II, type V, and ligand-bound species during calculations.

Please enter the type of reaction to be added or deleted:
1 = Reaction involving a complex ligand
2 = Type II species (species in solution)
3 = Type V species (possible solid)
R = RETURN to previous options menu (Edit Level II)
ENTER CHOICE ([D] = R) > R

6.4 Edit Level III

EDIT LEVEL III functions as a "line editor" in displaying by category or TYPE of data line by line entries of those species that have been explicitly entered through EDIT LEVEL II. The order of data presentation is: 1) COMPONENTS, 2) TYPE II - AQUEOUS SPECIES, 3) TYPE III - SPECIES WITH FIXED ACTIVITY, 4) TYPE V - POSSIBLE SOLIDS, and 5) TYPE VI - EXCLUDED SPECIES. Finally, any new species for which the reaction has been entered in ECIN (referred to as TYPE VII in this listing) is displayed. Note that TYPE I - COMPONENTS AS SPECIES IN SOLUTION are omitted because displaying the components themselves is sufficient here. Also, if no species have been explicitly entered for a particular type, that listing is omitted. For all the data types, the user is given opportunity to change entered values or to delete an entry altogether.

As each screen is displayed, the user is given opportunity to edit specific entries by specifying the number displayed to the left of each entry. Upon selecting an entry for editing, that entry is isolated and a menu of change operations is displayed. The change commands are rather straightforward.

6.5 Main Menu Option X: Exit

Upon selecting the EXIT option, ECIN re-orders the list of TYPE III - SPECIES WITH FIXED ACTIVITY so that fixed components are last in the list. It also checks to be sure that the electron is excluded if it is not a FIXED SPECIES. Finally, as mentioned in the explanation above the EDIT LEVEL II OPTION 4 (infinite solids), ECIN determines the initial degrees of freedom. If found to be zero or less, the user is advised to add more components or remove some of the species from the TYPE III list. Finally, upon exiting ECIN reminds the user of the name of the chemistry input file just created.

7 BLT-EC OUTPUT FILES

BLT-EC 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-EC. At a minimum, two output files will be created, the main BLT-EC output file, and ECHO.DAT, a file which provides an immediate echo print of the BLT-EC input file as it is read. ECHO.DAT is extremely useful in detecting errors in input that cause the program to fail. If chemical reactions are computed a third output file, the chemistry output file is also created by the chemical processes module. At a maximum, BLT-EC can create fifty-three separate output files. For DOS based users, this will cause a problem if the number of files specified in CONFIG.SYS is less than 60. In addition to the three files already discussed, BLT-EC may create a concentration trace file, flux trace file, waste form release rate file, and waste form cumulative mass release file for each contaminant. 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-EC input deck, variables NTRC and NTRF). With the exception of the main output file, the file names are fixed by BLT-EC 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-EC simulations. This section will describe each of the output files, their naming convention, and their structure.

Table 7.1 BLT-EC Output Files

File Name	Contents
ECHO.DAT	List of main BLT-EC input file as it is read.
User Specified	Primary BLT-EC 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 23, variable, KPR.
User Specified	Chemistry output file. This file lists detailed chemistry information at nodes specified by the user in the main BLT-EC input file (see Data Set 23B).
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.

* 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 (ECHO.DAT)

This file contains output written immediately after reading the BLT-EC input file. Therefore, it is quite useful for debugging invalid input decks. In some cases, all of the input is not printed in the ECHO.DAT file. This is done to save space and does not influence the ability to determine the last read statement executed in BLT-EC. The primary output file is not as reliable for locating the source of improper input as ECHO.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-EC. 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 velocity in the z-direction for all 100 nodes in a simulation was equal, one input card could be used to specify the velocity at all points (Data Set 24 in section 6). 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-velocity at each nodal location are explicitly stated. Similar remarks apply to all variables that use formulas 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 23 in section 6). 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, container performance data, the waste-form release rates, cumulative mass released for each release mechanism, and mass flow rate and cumulative mass flow out of the boundary nodes of the system are printed. 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 Darcy 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, velocity, 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 Chemistry Output File

The chemistry output file name is specified by the user when using BLT-EC. This output file is divided into six parts. Some of these parts may appear several times in one file depending on the combination of solid print option and general output file detail. The designations of PARTS 1 through 6 are designed to lend organization rather than sequential ordering although there is logic in the ordering as well.

PART 1 - Reproduction and interpretation of the input file.

PART 2 - Detailed listing of species read from the database files including log K values, enthalpy, molar mass, charge, Bebye-Huckel constants, etc.

PART 3 - Iteration information and detailed information for each species including calculated concentration, activity, adjusted log K values, etc.

PART 4 - Percentage distribution of components among dissolved and adsorbed species.

PART 5 - Provisional or equilibrated mass distribution, provisional or equilibrium ionic strength,

equilibrium pH and pe, electrostatic surface potential and charge for electrostatic adsorption models.

PART 6 - Saturation indices of all database solids with respect to the solution.

The "provisional" designation in PART 5 pertains to the use of solids print option 2 where provisional results are written to the output file each time a solid precipitates. The final results will be designated "equilibrated" in the output file. Only equilibrated results are written when the solids print option is set to 1.

The FULL OUTPUT option in ECIN results in an output file that includes all six parts. The INTERMEDIATE OUTPUT option causes PART 2 to be omitted. The ABBREVIATED OUTPUT option causes PART 2, most of PART 3, and all of PART 6 to be omitted. Appendix B contains an example output file.

7.4 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.

Each LEACHRL file contains a title line which identifies the contaminant and the BLT-EC 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:

Identifier	Definition
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
Difr	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-EC 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	Difr	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-EC is 25. In this case, LEACHR0.DAT would be used to store information pertaining to the tenth contaminant, LEACHR11.DAT for eleventh contaminant and so on.

LEACHRL files can be used in BLTPLOT to display the cumulative mass released from each waste form by release rate mechanism.

7.5 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.

Each LEACHMS file contains a title line which identifies the contaminant and the BLT-EC 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

Identifier	Definition
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-EC is printed. An example of a LEACHMS file is presented in Table 7.2.

When multiple contaminants are simulated, the naming convention is similar to that for the LEACHMS files discussed in section 7.4.

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 spread sheet 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). Version 2.0 is an extension of version 1.0 which works with BLT files. Improvements to version 1 include a new menuing system, ability to plot logarithms of concentrations, and the ability to make paper copies of the plots. 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 velocity
3. Z-direction velocity
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 velocity at each location. The magnitude and direction of the velocity 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.

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, BLTEC.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
leachrl1.dat      : Name of the BLT waste-leaching output file
bltec.out         : Name of the BLT 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 comes 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 deck.

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 is 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-EC computer code has been developed, implemented, and tested. This code is a two-dimensional finite-element computer code capable of simulating the time evolution of chemical concentrations and reactions resulting from the time-dependent release and transport of aqueous phase chemical components in a subsurface soil system. BLT-EC combines portions of three existing computer codes, BLT [Sullivan and Suen, 1989] , HYDROGEOCHEM [Yeh and Tripathi, 1989], and MINTEQA2 [Allison et al., 1991]. Improved container and waste-form performance models (Breach and Leach) from BLT are used in BLT-EC to estimate the time at which release begins and the rate of release of contaminants from waste forms. The transport model in BLT-EC is based on a modified version of the hydrologic tranport module contained in the finite-element code HYDROGEOCHEM. The geochemical model used to solve the chemical equilibrium reaction equations in BLT-EC is a modified version of the geochemical computer code MINTEQA2. In addition, BLT-EC interfaces automatically with MINTEQA2's thermodynamic database. Also provided with BLT-EC is the preprocessor ECIN, an interactive program designed to help the BLT-EC user create BLT-EC's chemistry input file. Water flow is handled through tabular input, or auxiliary files created by hydrological codes.

To permit rapid analysis of the output data created by BLT-EC, 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) velocity 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-EC 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-EC has been verified, this does not mean that the code applies to all situations. Prior to use of BLT-EC, 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-EC 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
LIST OF BLT-EC SUBROUTINES AND ARRAY VARIABLES

This appendix lists major subroutines in BLT-EC and their function. This appendix also provides a listing and definition of array variables and a discussion on the specification of array dimensions.

SUBROUTINE GM2DXZ

The subroutine GM2DXZ controls the entire sequence of operations, a function generally performed by the MAIN program. It is, however, preferable to keep a short MAIN and several subroutines with variable storage allocation. This makes it possible to place most of the FORTRAN deck on a permanent file and to deal with a site-specific problem without making changes in array dimensions throughout all subroutines.

The subroutine GM2DXZ will perform either the steady-state computation alone (KSS = 0 and NTI = 0), a transient state computation using the steady state solution a s the initial conditions (KSS = 0, NTI > 0), or a transient computation using user-supplied initial conditions (KSS = 1, NTI > 0).

GM2DXZ calls to subroutine DATAHT to read and print input data required for hydrologic transport computation and subroutine DATACS to read and print input data required for chemical equilibrium computation; subroutine LNDGEN to generate the relationship between node number and equation number when point wise iteration solution strategies are used; subroutine AFABTA to compute upstream weighting factors; subroutine INTERP to obtain sources/sinks and boundary values; subroutine OCSPIT to obtain total dissolved concentrations, total sorbed concentrations, and total precipitated concentrations of all components at all nodes given the total analytical concentrations; subroutine TACADC to compute the total analytical concentrations of all adsorbent components; subroutine ASEMBL to assemble the element matrices and load vectors over all elements to form a compressed global matrix and global load vectors; subroutine HYRDROT to perform a hydrologic transport computation; subroutine SFLOW to compute net rate of chemicals through open boundaries; subroutine CALKD to compute equivalent K_d; subroutine PRINTT to print out the results; subroutine PRITER to print the intermediate results between hydrologic transport and chemical equilibrium iterations; and subroutine STORE to store the results for plotting.

SUBROUTINE OCSPIT

This subroutine calculates the dissolved concentrations, total sorbed concentrations, and total precipitated concentrations of all components and the values of the negative logarithm of the concentrations of all component species by calling the subroutine EQMOD. The input to this subroutine is the total analytical concentrations of all components and their identification number.

Subroutine DATAHT

Subroutine DATAHT reads Data sets 2 through 22. It also prints all the input information and calls subroutine SURF to identify the boundary segments and boundary nodes and subroutines READR and READN, respectively, to automatically generate real and integer numbers.

Subroutine SURF

Subroutine SURF identifies the boundary sides, sequences the boundary nodes, and computes the directional cosine of the surface sides. The mapping from boundary nodes to global nodes is stored in NPB(I), where NPB(I) is the global node number of I^{th} boundary node. The element number associated with the boundary sides are stored in NBE. The length and directional cosines for each side are stored in NBE. The length and directional cosines for each side are stored in DLB and DCOSXB and DCOSZB, respectively. The local and global nodal number of two nodes of each side are stored in ISB. The information containing in NPB, NBE, ISB, DCOSXB, and DCOSZB, along with the number of boundary nodes and the number of boundary sides, are returned to subroutine DATAHT for use by other subroutines.

Subroutine 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 node-point locations.

Subroutine READN

Reads in a sequence of integers and generates a one-dimensional array based on these numbers.

Subroutine LNDGEN

This subroutine is called by the controlling subroutine GM2DXZ to preprocess the pointer array that is needed to assemble the global matrix in compressed form when pointwise solution methods are used. The pointer array automatically generated in this subroutine is the global node connectivity (stencil) LLNODE (J,N). Here LLNODE(J,N) is the global node number of J^{th} node connected to the global node N. This pointer array is generated based on the element connectivity IE(M,J), which is the global node number of J^{th} node of element M.

Subroutine AFABTA

Subroutine AFABTA is called to compute the optimum weighting factors for all sides of an element. The results are stored in array WETAB (M,J), where M = 1, 2, ..., NEL and J = 1, 2, 3, 4 for quadrilateral elements and J = 1, 2, 3 for triangular elements.

Subroutine INTERP

This subroutine is called by subroutine GM2DXZ to compute the functional values (such as the Dirichlet concentrations, element source/sink, point source/sink, incoming concentrations of fluids through variable boundary segment) at a particular time for all profiles. It uses the linear interpolation of the tabular data.

Subroutine BREACH

This subroutine calculates the fraction of a container that has been breached.

Subroutine LEACH

This subroutine calculates waste-form release rates for each container and each contaminant.

Subroutine SUBELER

This subroutine apportions the rinse source to specific nodes within the element containing a simulated wasteform based on the Darcy flux.

Subroutine LEACHFD

This subroutine is the finite-difference leaching model general manager.

Subroutine FDASSM

This subroutine assembles the matrix equations for the finite-difference leaching model.

Subroutine FDSLV

This subroutine solves the finite-difference leaching equations.

Subroutine PARTCO

This subroutine calculates the time-dependent waste-form partition coefficient.

Subroutine DECAYIN

This subroutine calculates decay and ingrowth of progeny in the waste form.

Subroutine SFLOW

This subroutine is called by subroutine GM2DXZ to compute mass fluxes through all open boundary nodes.

Subroutine CALKD

This subroutine is called by subroutine GM2DXZ to calculate the equivalent K_d for all components.

Subroutine RNODE

This subroutine reads in geometry values to create automatic mesh generation.

Subroutine RELEM

This subroutine generates the finite-element mesh based on input values.

Subroutine SHAP2

This subroutine calculates shape factors for finite-element equations when automatic mesh generation is used.

Subroutine PRINTT

This subroutine is used to line-print the transport variable. These include the total analytical concentrations, total dissolved concentrations, total sorbed concentrations, total precipitated concentrations of all components, and the values of negative logarithm of the concentrations of all component species.

Subroutine PRITER

This subroutine is used to line-print the intermediate total analytical concentrations of all components between hydrologic transport and chemical equilibrium iterations.

Subroutine STORE

This subroutine is used to store the transport variables on Logical Unit 2. It is intended for use for plotting. The information stored includes region geometry and transport variables.

Subroutine LOUT

This subroutine is called by the subroutine EQMOD to line print chemical species distribution at desired nodes at desired time interval. The information printed included concentrations, modified equilibrium constants, and stoichiometric coefficients of all species.

Subroutine TACADC

This subroutine is called by GM2DXZ to compute total concentrations of all adsorbent components.

Subroutine ASEMBL

This subroutine calls Q4 and Q3 to evaluate the element matrices. It then sums over all element matrices to form the compressed global matrices MMTRX, SMTRXD, VMTRX, and DMTRX and the global load vector RLD.

Subroutines Q4 and Q3

These subroutines are called by the subroutine ASEMBL to compute the element matrix. Q4 computes the element integration for quadrilateral elements, whereas Q3 computes those for triangular elements. Subroutines Q4 and Q3 also calculate the element load vector.

Subroutine SHAPE

This subroutine is called by the subroutines Q4 to evaluate the value of the base and weighting functions and the derivatives of the base functions and the derivatives of the base functions at a Gaussian point. The computation is straightforward.

Subroutine HYDROT

This subroutine is called by GM2DXZ to perform hydrologic transport computations. Two additional entries are called by GM2DSXZ: HYTRNI and HTYRNC. When the subroutine HYDROT is called, it simulates the transport of conservative chemical components. At entry point HYTRNI, it makes an initial guess of all nonconservative chemical components by solving the transport equations. At entry point HYTRNC, it simulates the transport of nonconservative chemical components for the new iterates. This subroutine calls to subroutine EQNGEN to obtain the matrix equation out of the compressed matrix and load vector fore each chemical component; subroutine BC to implement the boundary conditions; subroutine SOLVT or subroutine ZITS to solve the resulting matrix equations with direct elimination method or pointwise iteration methods.

Subroutine EQNGEN

This subroutine generates the matrix equation for an aqueous component out of the compressed global matrices and the global load vectors. It utilizes the array of the node connectivity produced in the subroutine LNDGEN to form a banded matrix and load vector for all aqueous components.

Subroutine BC

This subroutine incorporates Dirichlet and variable-boundary conditions. For a Dirichlet boundary condition, an identity algebraic equation is generated for each Dirichlet nodal point. Any other equation having this nodal variable is modified accordingly to simplify the computation. The subroutine BC also implements the variable-boundary conditions. It calls the subroutine Q2VB to compute the contributions of a variable-boundary segment to the global matrix equation.

Subroutine Q2VB

This subroutine is called by the subroutine BC to compute a 2 by 2 matrix BQ and a load vector RQ for each variable boundary segment.

Subroutine SOVLT

This subroutine is called by the subroutine GM2DXZ to solve for the matrix equation of the type

$$[C]\ \{x\} = \{y\},$$

where [C] is the coefficient matrix and {x} and {y} are two vectors. {x} is the unknown to be solved, and {y} is the known

load vector. The computer returns the solution {y} and stores it in {y}. The computation is a standard banded Gaussian direct-elimination procedure.

Subroutine ZITS

This subroutine is called by the subroutine HYDROT to solve the global matrix equation with point iteration solution strategies if desired by setting IPNTS = 1 in Data Set 5.

Subroutine EQMOD

Subroutine EQMOD is called by the subroutine OCSPIT to schedule the chemical equilibrium computation. It initiates the concentrations of all product species, given the guess of component species concentrations from subroutine OCSPIT. It then calls to subroutines PREP2ACT, ADSET, and MAINDB to solve the set of algebraic equations governing mole balance and chemical equilibrium reactions. Finally, total dissolved, total sorbed, and total precipitated concentrations of all components are returned to OCSPIT after concentrations of all species have been found.

Specifications of Array Dimensions

The subscripted variable arrays have to be dimensioned for each site-specific problem in the MAIN program. The listing and definitions of these parameters and their associated subscripts (maximum-control numbers) are given below:

Arrays for Node Coordinates and Element and Node Connectivities

X(MAXNP), Z(MAXNP), IE(MAXEL,5), LRN(JBAND, MAXNP)

MAXEL = maximum number of elements
MAXNP = maximum number of nodes
JBAND = maximum number of non-zero elements in any row of the matrix
X(NP) = x-coordinate of NP^{th} nodal point
Z(NP) = z-coordinate of NP^{th} nodal point
IE(M,I) = global node number for the I^{th} node of the M^{th} element if I is between 1 and 4, integer to indicate the material type of the M^{th} element if I is equal to 5
LRN(I,NP) = global node number of I^{th} node connected to node NP

Arrays for Boundary Surfaces

DLB(MAXBES), DCOSXB(MAXBES), DCOSZB(MAXBES)
MBES(MAXBES), ISB(4, MAAXBES), NPBB(MAXBNP)
MAXBES = maximum number of boundary-element sides
MAXBNP = maximum number of boundary nodal points
DLB(I) = length of the I^{th} boundary element side
DCOSXB(I) = x-directional cosine of I^{th} boundary element side
DCOSZB(I) = z-directional cosine of I^{th} boundary element side
MBES(I) = element number to which the I^{th} boundary element-side belongs
ISB(1,I) = global node number of the first node of I^{th} boundary element surface
ISB(2,I) = global node number of the second node of I^{th} boundary element surface
ISB(3,I) = element NBE(I)'s local node number of the first node of the I^{th} boundary element side
ISB(4,I) = element NBE(I)'s local node number of the second node of the I^{th} boundary element side
NPBB(I) = global node number of I^{th} boundary node

Arrays to Store Compressed Global Matrices and Global Load Vectors

SMTRX(MAXNP, JBAND), BMTRX(MAXNP, JBAND), DMTRX (MAXNP,JBAND), MMTRX (MAXNP, JBAND),

RLD (MAXNP,MXNCC)

SMTRX(N, I) = compressed global matrix from dispersion terms, source terms, and moisture change terms
VMTRX(N,I) = compressed global matrix from the velocity term = sum of QV
DMTRX(N,I) = compressed global matrix from moisture change terms = sum of QC
MMTRX(N,I) = compressed global matrix from moisture terms = sum of QA
RLD(N,K) = compressed global load vector of the N^{th} node for the K^{th} component = sum of QR

Arrays to Store the Global Matrix and Global Load Vector

CMATRX(MAXNP, MAXBHP), RVCTR(MAXNP), RI(MAXNP), RL(MAXNP)
MAXBHP = maximum number of half bandwidth plus 1
CMATRX(NP,I) = an array to store the assembled global matrix
RVCTR(NP) = an array to store the assembled global load vector
RI(NP) = concentration iterate in subroutine ZITS

Arrays to Store Chemical Component Variables

T(MAXNP, MAXN), TP(MAXNP,MAXN), TW(MAXNP, MAXN), C(MAXNP,MAXN), CP(MAXNP, MAXN), S(MAXNP,MAXN), XLOG(MAXNP,MAXN), CNAM(MAXN), INDC(MAXN), IDN(MAXN), TMC(MAXN), DMC(MAXN), SMC(MAXN), PMC(MAXN), XMC(MAXN)

MAXN = Maximum number of chemical components
T(N,K) = total analytical concentration at he N^{th} node for the K^{th} chemical component
TP(N,K) = value of T(N,K) at the previous time step
TW(N,K) = value of T(N,K) for the previous iteration
C(N,K) = total dissolved concentration at the N^{th} node for the K^{th} chemical component,
CP(N,K) = value of C(N,K) at the previous time-step
S(N,K) = total sorbed concentration at the N^{th} node for the K^{th} chemical component
P(N,K,) = total precipitated concentration at the N^{th} node for the K^{th} chemical component
XLOG(N,K) = negative logarithm of free ion concentration at the N^{th} node for the K^{th} chemical component
CNAM(K) = name of the K^{th} chemical component
INDC(K) = index of the type of the K^{th} chemical components
- 0 = mobile conservative chemical (aqueous components)
- 1 = mobile non-conservative chemical (aqueous components)
- 2 = immobile non-conservative chemical (sorbing sites)
- 3 = mobile chemical component with activity specified

IDN(K) = identification number of the K^{th} chemical
TMC(K) = total molar concentration of the K^{th} chemical component at any given node
DMC(K) = total dissolved molar concentration of the K^{th} chemical component at any given node
SMC(K) = total sorbed molar concentration of the K^{th} chemical component at any given node
PMC(K) = total precipitated molar concentration of the K^{th} chemical component at any given node

Arrays for Hydrological Variables and Nonconvergent Nodes

VX(MAXNP), VZ(MAXNP), TH(4,MAXE4L), THP(4,MAXEL), DTH(4,MAXEL), WETAB(4,MAXEL)

VX(NP) = x-component velocity at NP^{th} node,
VZ(NP) = z-component velocity at NP^{th} node,
TH(I,M) = water content of the I^{th} Gaussian point of the M^{th} element,
THP(I,M) = value of TH(I,M) at previous time step,
DTH(I,M) = dTH/dt at the I^{th} Gaussian node of the M^{th} element,
WETAB(I,M) = weighting factor for the I^{th} side of the M^{th} element.

Arrays for Element (Distributed) and Well (Point) Sources/Sinks

SOSF(MXSDP, MXSPR, MAXN1), TSOSF(MXSDP, MXSPR, MAXN1`), SOS(MXSPR, MAXN1), ISTYP(MXSEL, MAXN1), LES(MXSEL), WSSF(MXWDP, MXWPR, MAXN1), TWSSFF (MXWDP, MXWPR, MAXN1), WSS(MXWPR, MAXN1), IWTYP(MXWNP, MAXN1), NPW(MXWNP)

MAXN1 = maximum number of chemical components plus 1
MXSEL = maximum number of source elements
MXSPR = maximum number of source profiles
MXSDP = maximum number of data points on each well-source profile
MXWNP = maximum number of well nodal points
MXWPR = maximum number of well-source profiles
MXWDP = maximum number of data point on each well-source profile
SOSF(I,J,K) = source concentration of I^{th} data point in J^{th} element-source vs time profile for the K^{th} chemical, component; when K = NCC+1, SOSF (I,J,K) is the source flow rate
TSOSF(I,J,K) = time of I^{th} data point in J^{th} element -source vs time profile for the K^{th} chemical component
SOS(I,K) = value of I^{th} element-source profile for the K^{th} chemical component; when K = NCC + 1, SOS(I,K) is the source flow rate
ISTYP(M,K) = source type assigned to M^{th} source-element for the K^{th} chemical component
LES(M) = element number of the M^{th} source-element
WSSF(I,J,K) = source concentration of the I^{th} data point in the J^{th} well-source vs time profile for the K^{th} chemical component; when K = NCC + 1, WSS(I,J,K) is the source flow rate
TWSSF(I,J,K) = time of the I^{th} data point in the J^{th} well-source vs time profile for the K^{th} chemical component
WSS(I,K) = value of I^{th} well-source profile for the K^{th} chemical component; when K = NCC + 1, WSS (I,K) is the source flow rate
IWTYP(N,K)= source type assigned to the N^{th} well source node for the K^{th} chemical component
NPW(N) = global node number of the N^{th} well-source node

Arrays for Dirichlet Boundary Conditions

CDBF(MXDDP, MXDKPR, MAXN) TCDBF (MXDDP, MXDPR, MAXN), CDB (MXDPR, MAXN), IDTYP (MXDNP, MAXN), NPDB(MXDNP)

MXDNP = maximum number of Dirichlet nodal points
MXDPR = maximum number of Dirichlet total head profiles
MXDDP = maximum number of data points on each Dirichlet profile
CDBF(I,J,K) = total concentration of the I^{th} data point in the J^{th} Dirichlet total concentration vs time profile for the K^{th} chemical
TCDBF(I,J,K) = time of the I^{th} data point in the J^{th} Dirichlet total concentration vs time profile for the K^{th} chemical component
CDB(I,K) = value of total concentration at the present time of the I^{th} total concentration vs time profile for K^{th} chemical component
IDTYP(NP,K) = type of Dirichlet total concentration vs time profile assigned to the NP^{th} Dirichlet node for the K^{th} chemical component
NPDB(NP) = global node number of NP^{th} Dirichlet node

Arrays for Variable Boundary Conditions

DLV(XVES), DCOSXV (MXVES), DCOSZV(MXVES), MVES(MXVES, ISV(4, MXVES), IVFTYP(MXVES, MXNCC), NPVB(MXVNP), CVBF(MXVDP, MXVPR, MAXN), TCVBF(MXVDP, MXVPR, MAXN), CVB(MXVPR, MAXN)

MXVES = maximum number of variable boundary element sides

MXVNP = maximum number of variable boundary node points
MXVPR = maximum number of variable boundary profiles
MXVDP = maximum number of data point on each variable profile

DVL(MP) = length of the MP^{th} variable boundary element side
DCOSXV(MP) = x-directional cosine of the MP^{th} variable boundary element side
DCOSZV(MP) = z-directional cosine of the MP^{th} variable boundary element side
MVES(MP) = element number to which the MP^{th} variable boundary element-side belong
IS(1,MP) = Compressed variable boundary node number of the first node of the MP)th variable boundary element side
IS(2,MP) = Compressed variable boundary node number of the second node of the MP^{th} variable boundary element side
IS(3,MP) = Element MVES(MP)'s local node number of the second node of the MP^{th} variable boundary element side
IS(4,MP) = Element MVES(MP)'s local node number of the second node of the MP^{th} variable boundary element side
ISVTYP(MP,K) = type of incoming-fluid-concentration profile assigned to MP^{th} variable boundary side for the K^{th} chemical component
NJPVB(NP) = global node number of the NP^{th} variable boundary node
CVBF(I,J,K) = concentration of incoming fluid of the I^{th} data point in the J^{th} concentration vs time profile for the K^{th} chemical component
TCVBF(I,J,K) = time of the I^{th} data point in the J^{th} incoming concentration vs time profile for the K^{th} chemical component
CVB(I,K) = concentration of the I^{th} profile for the K^{th} chemical component

Arrays for Material Property Array and node indicator

PROP(MXMPPM, MAXMAT), NODEP(MAXNP,2)

MAXMAT = maximum number of material types (medium formations)
MXMPPM = maximum number of material properties per material
PROP(J,I) = J^{th} material property of I^{th} materials
J = 1 = longitudinal dispersivity (L)
J = 2 = lateral dispersivity(L)
J = 3 = effective molecular diffusion coefficient (L**2/T)
J = 4 = bulk density of the medium, (M/L**3)

NODEP(NP,1) = are chemical equilibrium results at the NP^{th} node to be printed? 1 = yes, 0 = no
NODEP(NP,2) = chemical property type assigned to node NP.

Arrays for Output Control and Time Step Size Change

KPR(MAXNTI), KDSK(MAXNTI), TDTCH(MXNDTC)

MAXNTI = maximum number of time steps
MXNDTC = maximum number of DELT changes
KPR(I) = line print for I^{th} time step 1 = yes, 0 = no
KDSK(I) = store results on unit 2 for the I^{th} time step? 1 = yes, 0 = no
TDTCH(I) = time of I^{th} time to reset time step size to original time step size, DELTO

Arrays for Required for Other Computations

RKD(MAXNP,MAXN), IWRK(MAXNP), THN(MAXNP), DTHN(MAXNP), RHOBN(MAXNP), FRATE(MXVNP,MAXN), FLOW(MXVNP, MAXN), TFLOW(MXVNP, MAXN),

RKD(N,K)=computed equivalent Kd at the N^{th} node for the K^{th} chemical component
IWRK(N) = a working array for computing THN(N) and DDTHN(N)
THN(N) = moisture content at the N^{th} node

DTHN(N) = dTH/dt at the N^{th} node
RHOPBN(N) = bulk density at he N^{th} node
FRATE(I,K) = rate of material flux at the I^{th} variable node for the K^{th} chemical component
FLOW(I,K) = FRATE(I,K)*DELT (time step size)
TFLOW(LI,K) = accumulated amount of material per unit area going through the I^{th} variable node for the K^{th} chemical component.

The subscripts (maximum-control numbers) of the above arrays should be specified in the BLOCK DATA in the source program. One should always assign correct numbers to these subscripts so that the program can function properly. If the program fails to function, it is most likely that either the arrays mentioned above are not properly dimensioned or the numbers assigned in the BLOCK DATA to these specification numbers of the arrays are not correct. The following listing represents the BLOCK DATA as it exists in BLT-EC.

```
      BLOCK DATA
    IMPLICIT REAL*8(A-H,O-Z)
     COMMON  /TCONVR/  TIMEYR
COMMON/SGEOM/MAXEL,MAXNP,MAXBES,MAXBNP,MAXBW,JBAND,MAXNTI,
  & MXNDTC
    COMMON /CSEL/ MXSEL,MXSPR,MXSDP,NSEL,NSPR,NSDP
    COMMON /CLEL/ MXLEL,MXLPR,MXLDP,NLEL,NLPR,NLDP
    COMMON /CSNP/ MXWNP,MXWPR,MXWDP,NWNP,NWPR,NWDP
    COMMON /CDBC/ MXDNP,MXDPR,MXDDP,NDNP,NDPR,NDDP
    COMMON /MATL/ MAXMAT,MXMPPM,NMAT,NMPPM
    COMMON/CVBC/MXVES,MXVNP,MXVPR,MXVDP,NVES,NVNP,NVPR,NVDP,
   $ NRSN
    COMMON /DIM/ MAXN,MAXN1,MAXM,MAXMZ,MAXMP,MAXPD,MAXEQ
    DATA MAXEL,MAXNP,MAXBES,MAXBNP,MAXBW,JBAND/550,600,202,203,45,9/
    DATA TIMEYR /3.15576D+07/
    DATA MAXNTI,MXNDTC/1000,20/
    DATA MXSEL,MXSPR,MXSDP/5,2,8/
    DATA MXLEL,MXLPR,MXLDP/50,2,8/
    DATA MXWNP,MXWPR,MXWDP/10,4,8/
    DATA MXDNP,MXDPR,MXDDP/51,2,8/
    DATA MXVES,MXVNP,MXVPR,MXVDP/101,102,2,8/
    DATA MAXMAT,MXMPPM,NMPPM /5,8,4/
    DATA MAXN,MAXN1,MAXM,MAXMZ,MAXMP,MAXPD,MAXEQ/25,26,450,20,
   & 16,78,90/
C
    END
```

In the following, we will demonstrate how to dimension the above arrays in the MAIN and how to specify the maximum-control numbers in the BLOCK DATA with an example.

Let us assume that a region of interest is discretized by 15 by 89 nodes and 14 by 88 elements. In other words, we are discretizing the region with 89 nodes along the longitudinal, or x-direction, and 15 nodes along the vertical, or z-direction. Because we have a total of 15 x 89 = 1,335 nodes, the maximum number of nodes is MAXNP = 1335. The total number of elements is 14 x 88 = 1,232, i.e. MAXEL = 1232. For this simple discretization problem, the maximum connecting number to any of the 1,335 nodes in the region of interest is 9 (i.e., JBAND = 9). There will be 14 element-sides each on the right and left sides and 88 element-sides each on the top and bottom sides of the region. Thus, there will be a total of 204 element-sides (i.e., MAXBES = 204). Similarly, we can compute the boundary nodes to be 220 (i.e., MAXBNP= 220). The bandwidth is equal to twice the minimum number of nodes in the x or z-direction (15 in this example) plus three, therefore, 33 (i.e., MAXBW= 33). We further assume that we are dealing with 12 chemical

components, i.e., (MAXN = 12). Among these 12 components, there will be chemical reactions to result in a maximum of 78 product species, of which a maximum number of 10 species involve ion-exchange and a maximum number 9 of 38 are potentially precipitated species. Thus, we have MAXPD = 78, MAXMZ = 10, MAXMP = 38, and MAXM = 90. Of course, the maximum number of equations will be MAXEQ = MAXN + MAXMZ + MAXMP = 60. With these maximum-control numbers specified, the arrays related to the global region, global boundary, and hydrologic variables can be dimensioned as:

```
DIMENSION  X (1335), Z(1335), IE(1232,5), LRN(9,1335)
DIMENSION  DLB(204), DCOSXB(204)H, DCOSZB(204), MVES(4,204), ISB(4,204)
DIMENSION  NPBB(204)
DIMENSION   SMTRX(1335,9), VMTRX (1335, 9), DMTRX(1335,9), MMTRX(1335, 9)
DIMENSION  RLD(1335, 12)
DIMENSION  CMATRX(335, 33), RVCTR(1335)
DIMENSION  RI(1335), RL(1335)
DIMENSION  T(1335, 12), TP(1335, 12), TW (1335, 12)
DIMENSION  C(1335, 12), CP(1335, 12)
DIMENSION  S(1335, 12), P(1335, 12), XLOG(1335, 12)
DIMENSION  CNAM(12), INDC (12), IDN(12)
DIMENSION  TMC(12), DMC(12), SMC(12), PMC(12)
DIMENSION  SPECN(90)
DIMENSION  VX(1335), VZ(1335), TH(3, 1232), DTH(4, 1232))
DIMENSION  WETAB(4, 1232)
```

We will assume that there will be a maximum of 11 elements that have the distributed sources/sinks (i.e., MXSEL = 11) and a maximum of 10 nodal points that can be considered as well sources/sinks (i.e., MXWSNP = 10). We will also assume that there will be three different distributed source/sink profiles and five distinct point source/sink profiles. Then we will have MXSPR = 3 and MXWPR = 5. Let us further assume four data points are needed to describe the distributed source/sink profiles as function of time and 8 data points are required to described point source/sink profiles, i.e., MXSDP = 4 and MXWSDP = 8. With these assumptions, we can now dimension the arrays related to source/sink conditions.

```
DIMENSION  SOSF(4,3,12), TSOSF(4,3,12), SOS(3,12)
DIMENSION  ISTYP(11,12), LES(11)
DIMENSION  WSSF(8,5,12), TWSSF(8,5,12), WSS(5,12)
DIMENSION  IWTYP(10, 12), NPW(10)
```

To specify arrays for boundary conditions, let us assume that the total analytical concentrations on the left side and the left half of the top side are known. The right half of the top side, bottom side, and right side are specified as variable boundaries.

On the left side there are 15 nodes, and on the left half of the top side there are 44 nodes. Thus, we have a total of 59 Dirichlet nodes. Let us assume that the middle 9 nodes on the left side have a specified total analytical concentration, the bottom 3 nodes on the left side have a different specified concentration, and the other 47 nodes have another specified total analytical concentration. We further assume that both total analytical concentrations can be described by 8 data points as functions of time. We then have MXDNP = 59, MXDPR = 3, and MXDDP = 8; and the Dirichlet boundary condition arrays can be dimensioned as:

```
DIMENSION  CDBF(8,3,11), THDBF(8,3,11), CDB(3,11)
DIMENSION  IDTYP(59,11), NPDB(59)J
```

There are 147 nodes and 146 element-sides on the right half of the top side, bottom side, and right side; thus MXVNP = 147 and MXVES = 146. It is further assumed that there three different incoming fluid concentrations going into the region through the top, bottom, and right sides, respectively, and each of these three concentration is function of time and

can be described by 8 data points. With these descriptions, we have MXVPR = 3 and MXVDP = 8. The variable boundary condition arrays can be specified as:

```
DIMENSION   DLB(146), DCOSXB(146), DCOSZB(11446), MVES(4,146), ISV(4,146)
DIMENSION   IVTYP(146,11), NPVB(147)
DIMENSION   CVBF(8,3,11), TCVBF(8,3,11), CVB(3,11)
```

IN BLT-EC there may be up to 8 material properties per material. We will assume that the whole region of interest is composed of three different kinds of materials. We then have MAXMAT = 3 and MXMPPM = 8. The material property and node-output indicator arrays can be dimensioned as:

```
DIMENSION   PROP (8,3), NODEP(1335,2)
```

If we assume that we will make a 500 time step-simulation and we will re-initiate the change on the time step size for 20 times during our simulation, then we have MAXNTI = 500 and MXNDTC = 20. With this assumption, arrays related to time can be dimensioned as:

```
DIMENSION KPR(500), KDSK(5009), TDTCH(20)
```

Other miscellaneous arrays can be dimensioned as:

```
DIMENSION   RKD(1335,12), IWRK(1335), THN(1335), THN(1335), DTHN(1335), RHOWB(1335)
DIMENSION FRATE(147,12), FLOW(146, 12), TFLOW(147,12)
```

Corresponding to the above dimension specifications, the following data statements must be made in BLOCK DATA to specify the maximum-control integers:

```
DATA MAXEL, MAXNP, MAXBES, MAXBNP, MAXBW, JBAND/1232, 1335, 204, 204,33, 9/
DATA MAXNTI, MXNDTC/500, 20/
DATA MXSEL, MXSPRK, MXSDP/11, 3, 4/
DATA MXWNP, MXWPR, MXWDP/10, 5, 8/
DATA MXDNP, MXDPR, MDDP/59, 3, 4/
DATA MXVES, MXVNP, MXVPR, MXVDP/146, 147, 3, 4/
DATA MAXMAT, MXMPPM/3,8/
DATA MAXN, MAXM, MAXMZ, MAXMP, MAXKPD, PLAXEQ/12,90, 10, 38, 78, 60/
```

If we use the point iteration method to solve the matrix equation in stead of the direct band matrix solver, we should set MAXBW equal to JBAND.

APPENDIX B
EXAMPLE INPUT AND OUTPUT FILES

B.1 BLT-EC Main Input File for the Chain Decay Problem

This appendix presents selected input files and example output files. The first input file provided corresponds to the chain decay problem examined in section 4.1. Note in this problem, use of the geochemistry modules is not required, variable INDC = 0 for all components. Therefore, the input file specifying the geochemical reaction is not required.

```
C ***** DATA SET 1: PROBLEM IDENTIFICATION AND DESCRIPTION -- BLTEC DATA
        3 SPECIES CHAIN DECAY & EMPTY CONTAINERS

C ***** DATA SET 2: INTEGER PARAMETERS FOR INPUT, STORAGE, RESTART AND STEADY
                    STATE CONTROL
         KVI        KSTR       NSTR       KSS
          0         0          0          1

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

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

C ***** DATA SET 5: INTEGER SOLUTION CONTROL PARAMETERS
         NTI        NITER      NDTCHG     NPITER     IPNTS
         273          1          1          1          0

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

C ***** DATA SET 7: INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
         NDNP       NDPR       NDDP
          3         1          4

         NVNP       NVES       NVPR       NVDP
         0          0          0          0

C ***** DATA SET 8: INTEGER PARAMETERS FOR SOURCES
         NSEL       NSPR       NSDP
         0          0          0

         NWNP       NWPR       NWDP
         0          0          0

         NLEL       NLPR       NLDP
         0          0          0
```

```
C ***** DATA SET 9: CHEMICAL COMPONENT INFORMATION
          NON         NONC        LNH       LNE
          3           0           4         10

  CNAM(J)    IND(J)  INDC(J)   CSAT(J)   T(1/2)  JDOTER1 DFRAC1  JDOTER2 DFRAC2
  Am241      1       0         1.0       433.00  2       1.0     0       0.0
  Pu241      2       0         1.0       15.000  3       1.0     0       0.0
  Pu240      3       0         1.0       6540.0  0       0.0     0       0.0

C ***** DATA SET 10: TIME INTEGRATION CONTROL PARAMETERS
          DELT      CHNG    DELMAX     TMAX          W          WV
        1.0         0.0D0   1.0        1e3           1.0D0      1.0D00

          DELTA T CHANGES AT YEAR(SEC):
          1.d38

C ***** DATA SET 11: REAL PARAMETERS FOR NONLINEAR SOLVE
          OME         OMI         TOLA       APHAG
          1.0D0       1.0D00      1.0D-5     1.0D0

C ***** DATA SET 12A: WIDTH OF FACILITY AND NODAL POINT DATA
          WIDFAC
          100.0

          ***KMSH=1, PERFORM AUTOMATIC MESH GENERATION***
          NELX        NELZ        NREG
          70          2           1

          IMIN  JMIN  IMAX  JMAX
            1     1    71     3

       ENTER FOUR COORD. PAIRS STARTING AT LOWER LEFT AND GO CCWSE
      0.0D0  0.0D0  7.0D03  0.0D02  7.0e3  2.0D02  0.0D02  2.0D02

C ***** DATA SET 12B: ELEMENT INCIDENCES
          MI          IE1         IE2         IE3         IE4         IE5
          (DATA SET NOT USED)

C ***** DATA SET 13: POROUS MEDIA PROPERTIES
PR1         PR2         PR3         PR4         PR5         PR6         PR7         PR8
AL          AT          DM          RHOB        CEC         CP1         CP2         SREA
259.0     25.9        0.0D-6        2.34        0.0         0.0         0.0         0.0

C ***** DATA SET 14: MATERIAL TYPE CORRECTION
          MI      NSEQ      MAD      MITYP      MTYPAD
          (DATA SET NOT USED IN THIS SIMULATION)

C ***** DATA SET 15: INITIAL OR PRE-INITIAL CONDITIONS
          NI          NSEQ        NAD         RNI         RAD         RRD
Am241
          1           212         1           0.00D0      0.0D0       0.0D0
          0           0           0           0.0D00      0.0D0       0.0D0
Pu241
```

```
          1          212        1          0.00D-0    0.0D0      0.0D0
          0          0          0          0.0D00     0.0D0      0.0D0
Pu240
          1          212        1          0.0D-0     0.0D0      0.0D0
          0          0          0          0.0D00     0.0D0      0.0D0

a ***** DATA SET 16: VARIABLE BOUNDARY CONDITIONS
            (DATA SET NOT USED IN THIS SIMULATION)

C ***** DATA SET 17: DIRICHLET BOUNDARY CONDITIONS
                    ** B.C. Am241 **
          TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
          0.0D0     1.0D00    91.00  .861   200.0  .725   300.00 0.619

          NI        NSEQ      NAD       NITYP     NTYPAD
          1         2         1         1         0
          0         0         0         0         0

                    ** B.C. Pu241 **
          TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
          0.0D0     0.0D-5    91.0  0.0305  200.0  0.0260 300.0  0.022

          NI        NSEQ      NAD       NITYP     NTYPAD
          1         2         1         1         0
          0         0         0         0         0

                    ** B.C. Pu240 **
          TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
          0.0D0     0.0D-32   91.0  .103  200.0  0.247  300.0 0.353

          NI        NSEQ      NAD       NITYP     NTYPAD
          1         2         1         1         0
          0         0         0         0         0

                    ** GLOBAL DIRICHLET NODES **
          NI        NSEQ      NIAD      NODE      NODEAD
          1          2        1         1         1
          0          0        0         0         0

C ***** DATA SET 18: ELEMENT SOURCE/SINK DATA
           (DATA SET NOT USED)

C ***** DATA SET 19: WELL (POINT) SOURCE/SINK DATA
           (DATA SET NOT USED)

c ***** DATA SET 20: ELEMENT SOURCE/SINK DATA
           (DATA SET NOT USED)

C ***** DATA SET 21: WASTE CONTAINER PARAMETERS
          THICK1    PITN1     PITK1     AREA1     ASCALE1   PITS1
          1.00D0     0.0010   0.007D0   2.1D04    0.2       5.0D03

          GRATE1     CLAY1     SPH1     IAER1
```

```
          0.317D-11  0.15       6.0       2

          THICK1     PITN1      PITK1     AREA1     ASCALE1   PITS1
          1.00D0      0.0010    0.007D0   2.1D04    0.2       5.0D03

          GRATE1     CLAY1      SPH1      IAER1
          0.317D-11  0.15       6.0       2

          NELCON1 NELCON2  X3  X4  X5  X6  X7  X8  X9  X10
          30      40

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

C ***** DATA SET 22A: WASTE FORM LEACHING PARAMETERS
                      WASTE FORM 1
W1-ISO1   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.333     0.333     0.333     1.0D-8    1.0D-03

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO2   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.333     0.333     0.333     1.0D-8    1.0D-03

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO3   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.333     0.333     0.333     1.0D-8    1.0D-03

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

          POREL1    VOLWF1    WWF1
          2.5D1     1.0D6     1.0D0

W2-ISO1   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.333     0.333     0.333     1.0D-8    1.0D-03

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W2-ISO2   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.333     0.333     0.333     1.0D-8    1.0D-03

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W2-ISO3   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.333     0.333     0.333     1.0D-8    1.0D-03
```

```
        PARTK01,1 PARTKI1,1 PARTD1,1
        0.0       0.0       0.0

        POREL1    VOLWF1    WWF1
        2.5D1     1.0D6     1.0D0

C ***** DATA SET 22B: INITIAL MASSES OF EACH WASTE ELEMENT
        WTINIT1,1  X2   X3   X4   X5   X6   X7   X8   X9   X10
             0.0D3   0.0D3

        WTINIT1,2  X2   X3   X4   X5   X6   X7   X8   X9   X10
             0.0   0.0

        WTINIT1,3  X2   X3   X4   X5   X6   X7   X8   X9   X10
             0.0   0.0

C ***** DATA SET 22C: READ WASTE TYPE ASSIGNMENTS
        MI        NSEQ      MAD       MITYP     MTYPAD
        1         1         1         1         1
        0         0         0         0         0

C ***** DATA SET 23A: PRINT AND AUXILIARY STORAGE CONTROL
        INTEGER PRINT PARAMETERS
        IITR      INTER     ICOND     NHGCI
        0         0         0         0

KPR0,KPR(I),I=1,NTI
220002000000000000000000000000000000000000000000000000000000000000000000000000000000000000
000000000000000000002000000000000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000200000200000000000000000000000000000000000000000000000000

KDSK0,KDSK(I),I=1,NTI
110000000000000000000000000001000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000

C ***** DATA SET 23B: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
        NCPRT
        2

        NODEP1,2  NODEP2,2
        1         140

        NI        NSEQ      NAD       NITYP     NTYPAD
        1         212       1         1         0
        0         0         0         0         0

C ***** DATA SET 24: VELOCITY AND MOISTURE CONTENT
        NI        NSEQ      NAD       VXNI      VZNI      VXAD      VZAD
        1         212       1         2.47e-8   -0.000D00 0.0       0.0
        0         0         0         0.0       0.0       0.0       0.0
```

```
NI          NSEQ        NAD         THNI        THNIAD
1           139         1           0.1D0       0.0
0           0           0           0.0         0.0
```

Note that in the above example if ncon in data set 3 was set to 0 then data sets 21, 22A, 22B, and 22C would not have been used. Using empty containers accomplishes the same objective, however, this approach is less computationally efficient. See the next input file for an example with ncon=0.

B.2 BLT-EC Main Input File for One-Dimensional Reactive Transport Problem

The following BLT-EC main input file and chemistry input file correspond to the reactive transport problem given in section 4.7.

Main BLT-EC file:

```
C ***** DATA SET 1: PROBLEM IDENTIFICATION AND DESCRIPTION
 1      1D Reactive transport problem: from Y&T, WRR,vol.27,no.12,1991

C ***** DATA SET 2: INTEGER PARAMETERS FOR INPUT, STORAGE, RESTART AND STEADY
                    STATE CONTROL
          KVI       KSTR        NSTR        KSS
          -1        0           0           1

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

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

C ***** DATA SET 5: INTEGER SOLUTION CONTROL PARAMETERS
          NTI       NITER       NDTCHG      NPITER      IPNTS
          300       2           1           300         0

C ***** DATA SET 6: GRID AND ELEMENT PARAMETERS
          NNP       NEL         NMAT        NCM       KMESH
          202       100         1           0         0

C ***** DATA SET 7: INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
          NDNP      NDPR        NDDP
          0         1           2

          NVNP      NVES        NVPR        NVDP
          4         2           2           6

C ***** DATA SET 8: INTEGER PARAMETERS FOR SOURCES
          NSEL      NSPR        NSDP
          0         0           0
```

```
          NWNP        NWPR        NWDP
          0           0           0

          NLEL        NLPR        NLDP
          0           0           0

C ***** DATA SET 9: CHEMICAL COMPONENT INFORMATION
          NON     NONC      LNH      LNE
          5       5         5        10

  CNAM(J)    IND(J)  INDC(J)   CSAT(J)   DCAY    JDOTER1 DFRAC1   JDOTER2 DFRAC2
  CALCIUM    150     1         0.0       1.d32   0.0     0.0      0.0     0.0
  CARBONATE  140     1         0.0       1.d32   0.0     0.0      0.0     0.0
  MAGNESIUM  460     1         0.0       1.d32   0.0     0.0      0.0     0.0
  SULFATE    732     1         0.0       1.d32   0.0     0.0      0.0     0.0
  HYDROGEN   330     3         0.0       1.d32   0.0     0.0      0.0     0.0

C ***** DATA SET 10: TIME INTEGRATION CONTROL PARAMETERS
          DELT        CHNG       DELMAX     TMAX       W          WV
     0.13689d-2     0.0D0     0.13689d-2    1.0D4      1.0D0      1.0D00

         DELTA T CHANGES AT YEAR(SEC):
         1.d38

C ***** DATA SET 11: REAL PARAMETERS FOR NONLINEAR SOLVE
          OME         OMI         TOLA       APHAG
          1.0D0       1.0D00      1.0D-1     1.0D0

C ***** DATA SET 12A: WIDTH OF FACILITY AND NODE POINT DATA
           WIDFAC
            1.0

                          *** NODE POINT DATA ***
          NI          NSEQ        NAD         XNI         XAD         XRD
          1           100         2           0.0         0.0         0.0
          2           100         2           1.000D0     0.0         0.0
          0           0           0           0.0         0.0         0.0

          NI          NSEQ        NAD         ZNI         ZAD         ZRD
          1           100         2           0.0         1.000D0     0.0
          2           100         2           0.0         1.000D0     0.0
          0           0           0           0.0         0.0         0.0

C ***** DATA SET 12B: ELEMENT INCIDENCES
          MI          IE1         IE2         IE3         IE4         IE5
          1           1           2           4           3           1

          MODL        NLAY
          1           100

C ***** DATA SET 13: POROUS MEDIA PROPERTIES
PR1       PR2         PR3         PR4         PR5         PR6         PR7         PR8
AL        AT          DM          RHOB        CEC         CP1         CP2         SREA
```

```
5.0       0.0D0      0.0D0      1.2        0.0        0.0        0.0        0.0

C ***** DATA SET 14: MATERIAL TYPE CORRECTION
          MI         NSEQ       MAD        MITYP      MTYPAD
          (DATA SET NOT USED)

C ***** DATA SET 15: INITIAL OR PRE-INITIAL CONDITIONS
          NI         NNODE      NAD        RNI        RAD        RRD
CALCIUM
          1          173        1          1.00D-4    0.0D0      0.0D0
          175        7          1          1.00D-4    0.0D0      0.0D0
          183        19         1          1.00D-4    0.0D0      0.0D0
          0          0          0          0.0D00     0.0D0      0.0D0
CARBONATE
          1          84         2          2.00D-4    9.26D-5    0.0D0
          2          84         2          2.00D-4    9.26D-5    0.0D0
          171        15         2          8.00D-3    0.4D-4     0.0D0
          172        15         2          8.00D-3    0.4D-4     0.0D0
          0          0          0          0.0D00     0.0D0      0.0D0
MAGNESIUM
          1          100        2          5.0D-03    -4.0D-5    0.0D0
          2          100        2          5.0D-03    -4.0D-5    0.0D0
          0          0          0          0.0D00     0.0D0      0.0D0
SULFATE
          1          100        2          2.00D-3    -1.9D-5    0.0D0
          2          100        2          2.00D-3    -1.9D-5    0.0D0
          0          0          0          0.0D00     0.0D0      0.0D0
HYDROGEN
          1          100        2          -7.70D00   -0.003D0   0.0D0
          2          100        2          -7.70D0    -0.003D0   0.0D0
          0          0          0          0.0D00     0.0D0      0.0D0

C ***** DATA SET 16: VARIABLE BOUNDARY CONDITIONS
                    ** B.C. CALCIUM **
T1,1 C1,1     T2,1 C2,1     T3,1 C3,1     T4,1 C4,1     T5,1 C5,1     T6,1  C6,1
0.0  1.0D-4  2.7105d-3 1.0D-4  2.7379d-3  9.0D-3  2.5982d-2  9.0D-3  2.6010d-2
1.0D-4  8.21344d-1 1.0D-4
0.0  1.0D-4  2.7105d-3 1.0D-4  2.7379d-3  9.0D-3  2.5982d-2  9.0D-3  2.6010d-2
1.0D-4  8.21344d-1 1.0D-4

          MI         NSEQ       MIAD       MITYP      MTYPAD
          1          0          1          1          0
          2          0          1          2          0
          0          0          0          0          0

                    ** B.C. CARBONATE **
  T1,2 C1,2     T2,2 C2,2     T3,2 C3,2     T4,2 C4,2     T5,2 C5,2     T6,2  C6,2
0.0  2.0D-3  2.7105d-3 2.0D-3  2.7379d-3  2.0D-3  9.5825d-3  2.0D-3  9.6099d-3
2.0D-3  8.21344d-1 2.0D-3
0.0  2.0D-3  2.7105d-3 2.0D-3  2.7379d-3  2.0D-3  9.5825d-3  2.0D-3  9.6099d-3
2.0D-3  8.21344d-1 2.0D-3

          MI         NSEQ       MIAD       MITYP      MTYPAD
```

```
          1          0          1          1          0
          2          0          1          2          0
          0          0          0          0          0

                    ** B.C. MAGNESIUM **
T1,3 C1,3     T2,3 C2,3     T3,3 C3,3     T4,3 C4,3     T5,3 C5,3     T6,3 C6,3
0.0 1.0D-3 2.7105d-3 1.0D-3 2.7379d-3 1.0D-3 9.5825d-3 1.0D-3 9.6099d-3 1.0D-3
8.21344d-1 1.0D-3
0.0   1.0D-3   2.7105d-3 1.0D-3   2.7379d-3 1.0D-3   9.5825d-3 1.0D-3   9.6099d-3
1.0D-3   8.21344d-1 1.0D-3

          MI         NSEQ       MIAD       MITYP      MTYPAD
          1          0          1          1          0
          2          0          1          2          0
          0          0          0          0          0

                    ** B.C. SULFATE **
T1,4 C1,4      T2,4 C2,4      T3,4 C3,4      T4,4 C4,4      T5,4 C5,4      T6,4 C6,4
0.0   2.0D-3   2.7105d-3 2.0D-3   2.7379d-3 2.0D-3   9.5825d-3 2.0D-3    9.6099d-3
2.0D-3   8.21344d-1 2.0D-3
0.0   2.0D-3   2.7105d-3 2.0D-3   2.7379d-3 2.0D-3   9.5825d-3 2.0D-3    9.6099d-3
2.0D-3   8.21344d-1 2.0D-3

          MI         NSEQ       MIAD       MITYP      MTYPAD
          1          0          1          1          0
          2          0          1          2          0
          0          0          0          0          0

                    ** B.C. HYDROGEN **
 T1,5 C1,5     T2,5 C2,5     T3,5 C3,5     T4,5 C4,5     T5,5 C5,5     T6,5 C6,5
0.0   -8.00    2.7105d-3 -8.00    2.7379d-3 -8.00    9.5825d-3 -8.00    9.6099d-3
-8.00   8.21344d-1 -8.00
0.0   -8.00    2.7105d-3 -8.00    2.7379d-3 -8.00    9.5825d-3 -8.00    9.6099d-3
-8.00   8.21344d-1 -8.00

          MI         NSEQ       MIAD       MITYP      MTYPAD
          1          0          1          1          0
          2          0          1          2          0
          0          0          0          0          0

                    ** GLOBAL NODE NUMBER **
          NI         NSEQ       NIAD       NODE       NODEAD
          1          1          1          1          1
          3          1          1          201        1
          0          0          0          0          0

                    ** BOUNDARY ELEMENT SIDES **
    MI      NSEQ    M       IS1     IS2     MIAD    MAD     IS1AD   IA2AD
    1       0       1       1       2       0       0       0       0
    2       0       100     3       4       0       0       0       0
    0       0       0       0       0       0       0       0       0

C ***** DATA SET 17: DIRICHLET BOUNDARY CONDITIONS
```

```
          (DATA SET NOT USED)

C ***** DATA SET 18: ELEMENT SOURCE/SINK DATA
          (DATA SET NOT USED)

C ***** DATA SET 19: WELL (POINT) SOURCE/SINK DATA
          (DATA SET NOT USED)

C ***** DATA SET 20: ELEMENT SOURCE/SINK DATA (LEACHING)
          (DATA SET NOT USED)

C ***** DATA SET 21: WASTE CONTAINER PARAMETERS
          (DATA SET NOT USED)

C ***** DATA SET 22A: WASTE FORM LEACHING PARAMETERS
          (DATA SET NOT USED)

C ***** DATA SET 22B: INITIAL MASSES OF EACH WASTE ELEMENT
          (DATA SET NOT USED)

C ***** DATA SET 22C: READ WASTE TYPE ASSIGNMENTS
          (DATA SET NOT USED)

C ***** DATA SET 23A: PRINT AND AUXILIARY STORAGE CONTROL
          INTEGER PRINT PARAMETERS
          IITR        INTER      ICOND     NHGCI
          0           0          0         0

KPR0,KPR(I),I=1,NTI
2000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000020000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000200000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000200000000000000000

KDSK0,KDSK(I),I=1,NTI
1000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000010000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000010000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000000000000000000000

C ***** DATA SET 23B: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
          NCPRT
          2

          NODEP1,2  NODEP2,2
          1         201

          NI        NSEQ      NAD       NITYP     NTYPAD
          1         201       1         1         0
          0         0         0         0         0

C ***** DATA SET 24: VELOCITY AND MOISTURE CONTENT
          NI        NSEQ      NAD       VXNI      VZNI      VXAD      VZAD
```

```
1          201        1          0.0        -0.5787D-5 0.0        0.0
0          0          0          0.0         0.0        0.0        0.0

NI         NSEQ       NAD        THNI       THNIAD
1          99         1          0.3D0      0.0
0          0          0          0.0        0.0
```

B.2.1 BLT-EC Chemistry Input File for One-Dimensional Reactive Transport Problem

BLT-EC chemistry input file for problem described in section 4.7.

```
Reactive Transport, from Yeh and Tripathi,WRR,vol27,no12,1991
( Mg, Ca, CO3, and SO4)
25.00 MOLAL  0.000  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
0 0 1 2 2 0 0 0 1 2 0 0 0
0   0   0
    330  0.000E+00   -7.76 y                    /H+1
    460  1.111E-04   -3.95 y                    /Mg+2
    732  1.639E-03   -2.78 y                    /SO4-2
    150  1.000E-04   -4.00 y                    /Ca+2
    140  1.959E-03   -2.71 y                    /CO3-2

  20
1503300
1501400
1501401
1507320
4603300
4601400
4601401
4607320
3301400
3301401
3307320
3300020
6015001
5015001
5046000
2046000
5046002
5046001
6046000
2015001
  2   4
1501401     3.2200     4.0300                  /CaCO3 AQ
1501400    11.4300     1.7900                  /CaHCO3 +
1503300   -12.8500    14.5350                  /CaOH +
4603300   -11.4400    15.9350                  /MgOH +
  3   1
    330     7.7000     0.0000                  /H+1
  5   8
5015001     8.4750     2.5850                  /CALCITE
5046002     8.2000     6.1690                  /MAGNESITE
```

```
6015001     4.6200    -0.2610                /GYPSUM
2015001   -21.9000    30.6900                /PORTLANDITE
5046000    -9.6500    28.7420                /ARTINITE
5046001     9.7200    52.2100                /HYDRMAGNESIT
2046000   -16.7920    25.8400                /BRUCITE
6046000     2.1400    -2.8200                /EPSOMITE


 0
```

B.3 BLT-EC Input Files for Two-Dimensional Reactive Transport Problem

The following set of input and output files are for a test problem that was developed to illustrate the complex non-linear behavior that can occur when chemical reactions are modeled. The following files are provided: FEMWATER input file, FEMWATER output file, a REDIMGRD output file, a BLT-EC main input file, a BLT-EC chemistry input file, and BLT-EC main and chemistry output files. The REDIMGRD output file is created by the code REDIMGRD which translates FEMWATER output to a format readable by BLT-EC.

A description of the example problem is as follows. The facility contains 6 waste containers and is surrounded by a concrete vault. The initial pH of the pore water in the region surrounding the facility and the far-field is 7.3. The pH in the facility is initialized at a higher value of 9.5 to reflect cement leaching during the period prior to facility failure. At the time that the facility is assumed to fail, water infiltrates into the facility and transports the higher pH pore water and facility contents downward towards the water table located at 30 meters below the ground surface. Interactions between transport, complexation, precipitation/dissolution, and adsorption of uranium are examined as the elevated pH pore water and released uranium migrate downwards.

The problem domain is taken to be a two-dimensional vertical cross-section perpendicular to the longitudinal axis of a disposal facility. This is the same grid used in MacKinnon et al, [1995]. It is assumed that the length of the facility in the longitudinal direction is much longer than the width of the facility. Therefore, a two-dimensional cross-section provides a reasonable representation for simulating radionuclide migration near the central portion of the facility. Symmetry within the cross section is further assumed, thus requiring only half the problem domain to be modeled. The water table is located approximately 30 meters below the ground surface. The waste containing portion of the facility is taken to be 8 meters deep and 18 meters wide, with the side walls slanting at an angle of approximately 12 degrees from vertical. The facility region is completely enclosed by a concrete vault. The entire disposal facility contains 12 waste containers (6 in the simulated region due to symmetry) that are surrounded by backfill. Above the top portion of the concrete vault is a 1 meter thick clay layer with a low hydraulic conductivity to minimize water intrusion from above. The clay layer is covered by a high conductivity cap layer, which is 2 meters thick and slants off towards the edge of the facility. The soil properties are assumed to be uniform in each facility region and in the underlying unsaturated zone. At the time of infiltration, the clay cover and concrete barrier are assumed to have failed and therefore, there saturated conductivities are set to one order of magnitude less than the value for the undisturbed soil. Values of the hydraulic conductivities (cm/sec) and porosities for the undisturbed soil, backfill, clay layer, and gravel cap, respectively, are: 10^{-4} and 30%, 10^{-3} and 40%, 10^{-5} and 50%, 10^{-5} and 30%.

This problem involves two simulations, a steady-state water-flow simulation and a radionuclide transport simulation. The water-flow problem is simulated over the entire cross section, which is divided into 624 bilinear finite elements and 675 nodes. The steady-state flow problem is solved once for the hydrogeologic data (moisture contents and flow velocities).

The boundary conditions for the flow simulation are as follows. The vertical left and right boundaries are homogeneous Neumann or no-flow boundaries. The bottom horizontal boundary is a Dirichlet boundary with a prescribed 1000 cm hydraulic head. The top boundary (ground surface) is a Neumann boundary with a prescribed rain fall infiltration of 1.25 cm/yr.

The transport problem considers a soil-surface component, SOH, and eight aqueous components including

hydronium, carbonate, calcium, sulfate, phosphate, zinc, magnesium, and uranium in the form of uranium oxide. These components formed 17 chemical species and 1 surface complex. The initial composition of the pore water (in mole/l) was CO_3^{-}=1.0x10^{-4}, SO_4^{-}=3.0x10^{-5}, Ca^{+2}=1.7x10^{-4}, SOH=1.0x10^{-5}, PO_4^{-}=5.0x10^{-7}, Zn=7.6x10^{-7}, Mg=1.2x10^{-4}, and UO_2^{2+}=0.0. The component concentrations in the facility (in mole/l) were similar except for the following, Ca^{+2}=2.5x10^{-4} and H^{+}= 4.0x10^{-5}. These concentrations are specified to represent the impact of cement leaching prior to failure of the facility. At the top infiltration boundary the infiltrating rain water was assumed to have the same composition as the pore water. The vertical and bottom boundaries were no-flow boundaries. The pH of the ground water was initially at 7.3 throughout the problem domain except in the facility where it initially is at 9.5.

The source concentration in each 1.0 m^3 container was 1.0 mole of UO_2. This initial uranium concentration is representative of average uranium concentrations found at Barnwell and Richland LLW disposal facilities. Localized and general corrosion resulted in gradual and complete container breach by 20 years. Release from the waste form occurred by rinse (1% of the inventory) and dissolution release processes. The waste-form degradation rate was set to give a fractional release rate of 0.1% per year for the dissolution mass (99% of the inventory). Note that at this conservative dissolution rate, the waste forms will completely dissolve in 100 years.

B.3.1 FEMWATER Input File

Development of a FEMWATER input file is discussed in detail in the BLT input guide [Sullivan and Suen, 1989]. In this problem, the FEMWATER input file is:

```
    4 2D EXAMPLE FLOW PROBLEM      8/96                                  111
  675  624    4  110    0    0    1    8    5    1    0    1    0   20   25    1
    0    0    0  300    0    1
     300.0        0.5   86400.0     1.0E9        0.0       0.01        0.1        1.0
     980.6      0.013        0.5        1.0        1.0        0.0
55
11
1.0D38
0.         0.         0.3          1.0E-4     1.0E-4
0.         0.         0.4          1.0E-3     1.0E-3
0.         0.         0.5          1.0E-5     1.0E-5
0.         0.         0.3          1.0E-5     1.0E-5
    -800.0     -200.      -100.      -25.      -12.5        0.       100.      2000.
    -800.0     -200.      -100.      -25.      -12.5        0.       100.      2000.
    -800.0     -200.      -100.      -25.      -12.5        0.       100.      2000.
    -800.0     -200.      -100.      -25.      -12.5        0.       100.      2000.
      .100      .1630        .25       .285       .290      .2925      .2995        0.3
      .120      .2000        .30       .380       .387      .3900      .3993        0.4
      .200      .2500        .35       .475       .483      .4875      .4992        0.5
      .100      .1630        .25       .285       .290      .2925      .2995        0.3
 0.0758607 0.1120675 0.2758126 0.9483156 0.9655139 0.9655139 0.9999857 0.9999857
 0.0758607 0.1120675 0.2758126 0.9483156 0.9655139 0.9655139 0.9999857 0.9999857
 0.0758607 0.1120675 0.2758126 0.9483156 0.9655139 0.9655139 0.9999857 0.9999857
 0.0758607 0.1120675 0.2758126 0.9483156 0.9655139 0.9655139 0.9999857 0.9999857
         0.      .10E-3      .32E-2      .40E-3      .20E-3      .10E-3      .26E-6         0.
         0.    1.33E-4    4.27E-3    5.33E-4    2.67E-4    1.33E-4    3.47E-7         0.
         0.    1.33E-4    4.27E-3    5.33E-4    2.67E-4    1.33E-4    3.47E-7         0.
         0.      .10E-3      .32E-2      .40E-3      .20E-3      .10E-3      .26E-6         0.
26 24 15
1    1    6    9
.000D+1 .000D+1 .260D+4 .000d+4 .260d+4 .200d+4 .000d+4 .200d+4
6    1   13    9
.260d+4 .000d+1 .420d+4 .000d+1 .420d+4 .200d+4 .260d+4 .200d+4
```

```
13   1   27    9
.420d+4 .000d+1 .560d+4 .000d+1 .560d+4 .200d+4 .420d+4 .200d+4
1    9    6   15
.000d+1 .200d+4 .260d+4 .200d+4 .260d+4 .260d+4 .000d+4 .260d+4
6    9   10   15
.260d+4 .200d+4 .3514d+4 .200d+4 .3514d+4 .260d+4 .260d+4 .260d+4
10   9    13  15
.3514d+4 .200d+4 .420d+4 .200d+4 .420d+4 .260d+4 .3514d+4 .260d+4
13   9   27   15
.420d+4 .200d+4 .560d+4 .200d+4 .560d+4 .260d+4 .420d+4 .260d+4
1   15    6   23
.000d+1 .260d+4 .260d+4 .260d+4 .260d+4 .335d+4 .000d+4 .335d+4
6   15   10   23
.260d+4 .260d+4 .3514d+4 .260d+4 .340d+4 .335d+4 .260d+4 .335d+4
10   15   13   23
.3514d+4 .260d+4 .420d+4 .260d+4 .400d+4 .340d+4 .340d+4 .335d+4
13  15   27   23
.420d+4 .260d+4 .560d+4 .260d+4 .560d+4 .340d+4 .400d+4 .340d+4
1   23    6   25
.000d+1 .335d+4 .260d+4 .335d+4 .260d+4 .340d+4 .000d+1 .340d+4
6   23   10   25
.260d+4 .335d+4 .340d+4 .335d+4 .340d+4 .340d+4 .260d+4 .340d+4
10   23   13   25
.340d+4 .335d+4 .400d+4 .340d+4 .400d+4 .350d+4 .340d+4 .340d+4
13   23   27   25
.400d+4 .340d+4 .560d+4 .340d+4 .560d+4 .360d+4 .400d+4 .350d+4
  375   10   24    2    0
  376   10   24    2    0
  377   10   24    2    0
  378   10   24    2    0
  379   10   24    2    0
  380   10   24    2    0
  381   10   24    2    0
  382   10   24    3    0
  383   10   24    4    0
  384   10   24    4    0

    1  674    1           0.0       0.0       0.0

    0    0    0    0    0    0    0   27    2    2   27   26    1    2    0    0
    0    0    0    0    0
       0.0    0000.0     1.0E9    0000.0
       0.0    0000.0     1.0E9    0000.0
    1   26   51   76  101  126  151  176  201  226  251  276  301  326  351  376
  401  426  451  476  501  526  551  576  601  626  651
    1   26    1    1    0
                                                              END OF IDTYPE
       0.0 -4.000E-8     1.0E9 -4.000E-8
   25   50   75  100  125  150  175  200  225  250  275  300  325  350  375  400
  425  450  475  500  525  550  575  600  625  650  675
    1   26    1    1    0
                                                              END OF IDTYPE
    1   25    1    2    1    1    1
                                                              END OF SIDES
```

B.3.2 Truncated FEMWATER Output File for Two-Dimensional Reactive Transport Problem

The truncated FEMWATER output file is:

```
1PROBLEM    4..      SPECTRUM 96 FLOW PROBLEM      4/96                    111

0      **** BASIC INTEGER PARAMETERS ****

       NUMBER OF NODAL POINTS. . . . . .  675
       NUMBER OF ELEMENTS. . . . . .  624
       NUMBER OF DIFFERENT MATERIALS . . . . .    4
       NUMBER OF CORRECTION MATERIALS. . . . .  110
       NUMBER OF TIME INCREMENTS . . . . . .    0

       STEADY-STATE I.C. CONTROL . . . . . .    0
       MESH INPUT CONTROL . . . . . .    1
       SOIL-PROPERTY CONTROL . . . . . .    1
       NUMBER OF SOIL PARAMETERS . . . . . .    8
       NUMBER OF MATERIAL PROPERTIES . . . . .    5

       AUXILIARY STORAGE CONTROL . . . . . .    1
       CONDUCTIVITY-PERMEABILITY CONTROL . . .    0
       GRAVITY CONTROL . . . . . .    1
       RESTART PARAMETER . . . . . .    0

       NO. OF ITERATIONS PER CYCLE . . . . . .   20
       NO. OF CYCLES PER TIME STEP . . . . . .   25
       NO. OF TIMES TO RESET TIME STEP SIZE  .    1
       NO. OF POINTWISE ITERATIONS ALLOWED .  300

0      LUMPING INDICATOR, ILUMP. . . . . .    0
       TIME-DIFFERENCE INDICATOR, IMID . . . .    0
       IS POINTWISE ITERATION SOLUTION USED?      0
       IS VELOCITY-SOLVING MATRIX LUMPED? .       0


       TIME INCREMENT. . . . . .  0.300000E+03
       MULTIPLIER FOR INCREASING DELT. . . . .  0.500000E+00
       MAXIMUM VALUE OF DELT . . . . . .  0.864000E+05
       MAXIMUM VALUE OF TIME . . . . . .  0.100000E+10

       DEGREES OF PRIN-AXIS INCLINATION. . . .  0.000000E+00
       STEADY-STATE TOLERANCE. . . . . .  0.100000E-01
       TRANSIENT-STATE TOLERANCE . . . . . .  0.100000E+00

       DENSITY OF WATER. . . . . .  0.100000E+01
       ACCELERATION OF GRAVITY . . . . . .  0.980600E+03
       VISCOSITY OF WATER. . . . . .  0.130000E-01

       TIME-INTEGRATION PARAMETER. . . . . .  0.500000E+00
       ITERATION PARAMETER FOR NONLINEAR EQ.  0.100000E+01
       RELAXATION PARAMETER FOR POINTWISE SOL.  0.100000E+01
```

```
      CYLINDER COORDINATOR PARAMETER . . . .    0.000000E+00



      OUTPUT CONTROL
           5


      DISK OUTPUT CONTROL
           1
0      TIME OF CHANGING DELT
            0.1000E+39
1     **** MATERIAL PROPERTIES ****

 MAT. NO.      ALP         BETAP          POR        KSX/PSX      KSZ/PSZ
        1  0.0000E+00  0.0000E+00  0.3000E+00  0.10 00E-03  0.1000E-03
        2  0.0000E+00  0.0000E+00  0.4000E+00  0.1000E-02   0.1000E-02
        3  0.0000E+00  0.0000E+00  0.5000E+00  0.1000E-04   0.1000E-04
        4  0.0000E+00  0.0000E+00  0.3000E+00  0.1000E-04   0.1000E-04
1     **** SOIL PROPERTY INTERPOLATION VALUES ****

 MAT. NO.       PRESSURE       MOISTURE CONTENT    RELATIVE CONDUCTIVITY      WATER CAPACITY
     1         -0.8000E+03      0.1000E+00              0.7586E-01            0.0000E+00
               -0.2000E+03      0.1630E+00              0.1121E+00            0.1000E-03
               -0.1000E+03      0.2500E+00              0.2758E+00            0.3200E-02
               -0.2500E+02      0.2850E+00              0.9483E+00            0.4000E-03
               -0.1250E+02      0.2900E+00              0.9655E+00            0.2000E-03
                0.0000E+00      0.2925E+00              0.9655E+00            0.1000E-03
                0.1000E+03      0.2995E+00              0.1000E+01            0.2600E-06
                0.2000E+04      0.3000E+00              0.1000E+01            0.0000E+00
1     **** SOIL PROPERTY INTERPOLATION VALUES ****

 MAT. NO.       PRESSURE       MOISTURE CONTENT    RELATIVE CONDUCTIVITY      WATER CAPACITY
     2         -0.8000E+03      0.1200E+00              0.7586E-01            0.0000E+00
               -0.2000E+03      0.2000E+00              0.1121E+00            0.1330E-03
               -0.1000E+03      0.3000E+00              0.2758E+00            0.4270E-02
               -0.2500E+02      0.3800E+00              0.9483E+00            0.5330E-03
               -0.1250E+02      0.3870E+00              0.9655E+00            0.2670E-03
                0.0000E+00      0.3900E+00              0.9655E+00            0.1330E-03
                0.1000E+03      0.3993E+00              0.1000E+01            0.3470E-06
                0.2000E+04      0.4000E+00              0.1000E+01            0.0000E+00
1     **** SOIL PROPERTY INTERPOLATION VALUES ****

 MAT. NO.       PRESSURE       MOISTURE CONTENT    RELATIVE CONDUCTIVITY      WATER CAPACITY
     3         -0.8000E+03      0.2000E+00              0.7586E-01            0.0000E+00
               -0.2000E+03      0.2500E+00              0.1121E+00            0.1330E-03
               -0.1000E+03      0.3500E+00              0.2758E+00            0.4270E-02
               -0.2500E+02      0.4750E+00              0.9483E+00            0.5330E-03
               -0.1250E+02      0.4830E+00              0.9655E+00            0.2670E-03
                0.0000E+00      0.4875E+00              0.9655E+00            0.1330E-03
                0.1000E+03      0.4992E+00              0.1000E+01            0.3470E-06
                0.2000E+04      0.5000E+00              0.1000E+01            0.0000E+00
1     **** SOIL PROPERTY INTERPOLATION VALUES ****
```

MAT. NO.	PRESSURE	MOISTURE CONTENT	RELATIVE CONDUCTIVITY	WATER CAPACITY
4	-0.8000E+03	0.1000E+00	0.7586E-01	0.0000E+00
	-0.2000E+03	0.1630E+00	0.1121E+00	0.1000E-03
	-0.1000E+03	0.2500E+00	0.2758E+00	0.3200E-02
	-0.2500E+02	0.2850E+00	0.9483E+00	0.4000E-03
	-0.1250E+02	0.2900E+00	0.9655E+00	0.2000E-03
	0.0000E+00	0.2925E+00	0.9655E+00	0.1000E-03
	0.1000E+03	0.2995E+00	0.1000E+01	0.2600E-06
	0.2000E+04	0.3000E+00	0.1000E+01	0.0000E+00

B.3.3 Using REDIMGRD to Process the FEMWATER Output File

Often when simulating water flow using FEMWATER, a much larger spatial domain must be simulated than for the transport segment of the simulation. When this occurs, the program REDIMGRD can be used to process the FEMWATER file and reduce the spatial domain.

In this example, the aquifer flow is along the direction of the x-axis. Therefore, symmetry can not be assumed about the center line of the disposal facility during the flow calculation. However, for the wasteform release and contaminant transport segment of the problem, this example focuses on the near field (waste region and vadose zone). In this case, symmetry can be assumed and the resulting simulation domain can be decreased, thereby savings in computational time can be achieved.

When the user runs REDIMGRD to translate FEMWATER output into a format readable by BLT-EC, the user is prompted for spatial coordinates (in cm.) defining the transport region. The following coordinates were input for this example.

Xmin = 3400 Xmax = 5600
Zmin = 0. Zmax = 3600

The resulting REDIMGRD output file contains information on the finite element geometry, flow velocities, and moisture content. The file created by REDIMGRD can be read directly by BLT-EC. In this example, the REDIMGRD output file is:

```
 2D EXAMPLE FLOW PROBLEM      8/96
  4  450  408   82   82    0    0
  1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16
 17   19   20   21   22   23   24   25   26   27   28   29   30   31   32   33
 34   35   37   38   39   40   41   42   43   44   45   46   47   48   49   50
 51   52   53   55   56   57   58   59   60   61   62   63   64   65   66   67
 68   69   70   71   73   74   75   76   77   78   79   80   81   82   83   84
 85   86   87   88   89   91   92   93   94   95   96   97   98   99  100  101
102  103  104  105  106  107  109  110  111  112  113  114  115  116  117  118
119  120  121  122  123  124  125  127  128  129  130  131  132  133  134  135
136  137  138  139  140  141  142  143  145  146  147  148  149  150  151  152
153  154  155  156  157  158  159  160  161  163  164  165  166  167  168  169
170  171  172  173  174  175  176  177  178  179  181  182  183  184  185  186
187  188  189  190  191  192  193  194  195  196  197  199  200  201  202  203
204  205  206  207  208  209  210  211  212  213  214  215  217  218  219  220
221  222  223  224  225  226  227  228  229  230  231  232  233  235  236  237
238  239  240  241  242  243  244  245  246  247  248  249  250  251  253  254
255  256  257  258  259  260  261  262  263  264  265  266  267  268  269  271
272  273  274  275  276  277  278  279  280  281  282  283  284  285  286  287
```

289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304
305	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321
322	323	325	326	327	328	329	330	331	332	333	334	335	336	337	338
339	340	341	343	344	345	346	347	348	349	350	351	352	353	354	355
356	357	358	359	361	362	363	364	365	366	367	368	369	370	371	372
373	374	375	376	377	379	380	381	382	383	384	385	386	387	388	389
390	391	392	393	394	395	397	398	399	400	401	402	403	404	405	406
407	408	409	410	411	412	413	415	416	417	418	419	420	421	422	423
424	425	426	427	428	429	430	431	2	3	4	5	6	7	8	9
10	11	12	13	14	15	16	17	18	20	21	22	23	24	25	26
27	28	29	30	31	32	33	34	35	36	38	39	40	41	42	43
44	45	46	47	48	49	50	51	52	53	54	56	57	58	59	60
61	62	63	64	65	66	67	68	69	70	71	72	74	75	76	77
78	79	80	81	82	83	84	85	86	87	88	89	90	92	93	94
95	96	97	98	99	100	101	102	103	104	105	106	107	108	110	111
112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	128
129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144
146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161
162	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178
179	180	182	183	184	185	186	187	188	189	190	191	192	193	194	195
196	197	198	200	201	202	203	204	205	206	207	208	209	210	211	212
213	214	215	216	218	219	220	221	222	223	224	225	226	227	228	229
230	231	232	233	234	236	237	238	239	240	241	242	243	244	245	246
247	248	249	250	251	252	254	255	256	257	258	259	260	261	262	263
264	265	266	267	268	269	270	272	273	274	275	276	277	278	279	280
281	282	283	284	285	286	287	288	290	291	292	293	294	295	296	297
298	299	300	301	302	303	304	305	306	308	309	310	311	312	313	314
315	316	317	318	319	320	321	322	323	324	326	327	328	329	330	331
332	333	334	335	336	337	338	339	340	341	342	344	345	346	347	348
349	350	351	352	353	354	355	356	357	358	359	360	362	363	364	365
366	367	368	369	370	371	372	373	374	375	376	377	378	380	381	382
383	384	385	386	387	388	389	390	391	392	393	394	395	396	398	399
400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	416
417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432
20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
36	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52
53	54	56	57	58	59	60	61	62	63	64	65	66	67	68	69
70	71	72	74	75	76	77	78	79	80	81	82	83	84	85	86
87	88	89	90	92	93	94	95	96	97	98	99	100	101	102	103
104	105	106	107	108	110	111	112	113	114	115	116	117	118	119	120
121	122	123	124	125	126	128	129	130	131	132	133	134	135	136	137
138	139	140	141	142	143	144	146	147	148	149	150	151	152	153	154
155	156	157	158	159	160	161	162	164	165	166	167	168	169	170	171
172	173	174	175	176	177	178	179	180	182	183	184	185	186	187	188
189	190	191	192	193	194	195	196	197	198	200	201	202	203	204	205
206	207	208	209	210	211	212	213	214	215	216	218	219	220	221	222
223	224	225	226	227	228	229	230	231	232	233	234	236	237	238	239
240	241	242	243	244	245	246	247	248	249	250	251	252	254	255	256
257	258	259	260	261	262	263	264	265	266	267	268	269	270	272	273
274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	290
291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306
308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323
324	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340
341	342	344	345	346	347	348	349	350	351	352	353	354	355	356	357
358	359	360	362	363	364	365	366	367	368	369	370	371	372	373	374

375	376	377	378	380	381	382	383	384	385	386	387	388	389	390	391
392	393	394	395	396	398	399	400	401	402	403	404	405	406	407	408
409	410	411	412	413	414	416	417	418	419	420	421	422	423	424	425
426	427	428	429	430	431	432	434	435	436	437	438	439	440	441	442
443	444	445	446	447	448	449	450	19	20	21	22	23	24	25	26
27	28	29	30	31	32	33	34	35	37	38	39	40	41	42	43
44	45	46	47	48	49	50	51	52	53	55	56	57	58	59	60
61	62	63	64	65	66	67	68	69	70	71	73	74	75	76	77
78	79	80	81	82	83	84	85	86	87	88	89	91	92	93	94
95	96	97	98	99	100	101	102	103	104	105	106	107	109	110	111
112	113	114	115	116	117	118	119	120	121	122	123	124	125	127	128
129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	145
146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161
163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178
179	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195
196	197	199	200	201	202	203	204	205	206	207	208	209	210	211	212
213	214	215	217	218	219	220	221	222	223	224	225	226	227	228	229
230	231	232	233	235	236	237	238	239	240	241	242	243	244	245	246
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-0.4146652E-07-0.3993436E-07-0.3906590E-07-0.3874806E-07-0.3864298E-07
-0.3863963E-07-0.3865947E-07-0.3866942E-07-0.3924829E-07-0.3895157E-07
-0.3944880E-07-0.4106866E-07-0.5014025E-07-0.2083072E-07-0.6497937E-07
-0.7232656E-07-0.3269538E-07-0.3789016E-07-0.3522246E-07-0.3604743E-07
-0.3632551E-07-0.3681720E-07-0.3718719E-07-0.3747153E-07-0.3764078E-07
-0.3769873E-07-0.3958197E-07-0.3944901E-07-0.3991737E-07-0.4367527E-07
-0.5257190E-07-0.6802047E-07-0.8793127E-07-0.1036633E-07-0.2516198E-07
-0.2649366E-07-0.3015385E-07-0.3225740E-07-0.3396676E-07-0.3515067E-07
-0.3598643E-07-0.3652913E-07-0.3683434E-07-0.3692884E-07-0.3978293E-07
-0.3989192E-07-0.3959879E-07-0.4528472E-07-0.4247511E-07-0.1099640E-06
-0.1015743E-06 0.1757076E-07-0.2901118E-07-0.2391173E-07-0.3026362E-07
-0.3208632E-07-0.3406899E-07-0.3527049E-07-0.3613533E-07-0.3667683E-07
-0.3698084E-07-0.3708703E-07-0.3999150E-07-0.4003232E-07-0.3988762E-07
-0.4218283E-07-0.4134845E-07-0.7388612E-07-0.6239805E-07-0.1965578E-07
-0.3565847E-07-0.3384360E-07-0.3609348E-07-0.3680419E-07-0.3754148E-07
-0.3799546E-07-0.3831037E-07-0.3849299E-07-0.3857439E-07-0.3860983E-07
-0.4002343E-07-0.4006166E-07-0.3995731E-07-0.4138960E-07-0.3979177E-07
-0.5935444E-07-0.4972392E-07-0.3439336E-07-0.4240813E-07-0.3960186E-07
-0.4029326E-07-0.3999364E-07-0.3999309E-07-0.3991879E-07-0.3986441E-07
-0.3979824E-07-0.3972276E-07-0.3969809E-07
```

B.3.4 BLT-EC Main Input File for the Two-Dimensional Reactive Transport Problem

The preceeding file is read by BLT-EC during execution, flag KVI=1. The main BLT-EC input file for this two-dimensional example problem is:

```
C ***** DATA SET 1: TWO-DIMENSIONAL EXAMPLE APPLICATION
        USES MESH AND FLOW FROM Prob.5 IN BLT-EC NUREG/CR-6305
```

```
C ***** DATA SET 2: INTEGER PARAMETERS FOR INPUT, STORAGE AND
        RESTART CONTROL
         KVI      KSTR      NSTR      KSS
         1        0         0         1

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

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

C ***** DATA SET 5: INTEGER SOLUTION CONTROL PARAMETERS
         NTI       NITER     NDTCHG    NPITER    IPNTS
         300         1         1         1         0

C ***** DATA SET 6: GRID AND ELEMENT PARAMETERS
         NNP       NEL       NMAT      NCM   KMESH
         450       408         4       140   1

C ***** DATA SET 7: INTEGER PARAMETERS FOR BOUNDARY CONDITIONS
         NDNP      NDPR      NDDP
         18        1         2

         NVNP      NVES      NVPR      NVDP
         18        17        1         2

C ***** DATA SET 8: INTEGER PARAMETERS FOR SOURCES
         NSEL      NSPR      NSDP
         0         0         0

         NWNP      NWPR      NWDP
         0         0         0

         NLEL      NLPR      NLDP
         25        1         2

C ***** DATA SET 9: CHEMICAL COMPONENT INFORMATION
         NON      NONC      LNH      LNE
          9       9          5        11

  CNAM(J)    IND(J)  INDC(J)  CSAT(J)  T(1/2) JDOTER1 DFRAC1 JDOTER2 DFRAC2
  CALCIUM    150     1        1.0d6    1.D32  0       0.0    0       0.0
  CARBONATE  140     1        1.0d6    1.D32  0       0.0    0       0.0
  URANIUM    893     1        1.0d6    1.D32  0       0.0    0       0.0
  SULFATE    732     1        1.0d6    1.D32  0       0.0    0       0.0
  HYDROGEN   330     1        1.0d6    1.D32  0       0.0    0       0.0
  SOH        811     2        1.0d6    1.D32  0       0.0    0       0.0
  MAGNESIUM  460     1        1.0d6    1.D32  0       0.0    0       0.0
  PHOSPHATE  580     1        1.0d6    1.D32  0       0.0    0       0.0
  ZINC       950     1        1.0d6    1.D32  0       0.0    0       0.0
```

```
C ***** DATA SET 10: TIME INTEGRATION CONTROL PARAMETERS
         DELT      CHNG     DELMAX     TMAX       W          WV
         0.50       0.0D0   0.50       102.0    1.0D0      1.0D00

         DELTA T CHANGES AT YEAR (SEC):
         1.0D38

C ***** DATA SET 11: REAL PARAMETERS FOR NONLINEAR SOLVE
         OME        OMI        TOLA       APHAG
         1.0D0      1.0D00     1.0D-9     1.0D0

C ***** DATA SET 12: NODAL POINT COORDINATE
         WIDFAC
         1.0

c ***** DATA SET READ FROM FEMWATER FILE

c ***** DATA SET 12A: AUTOMATIC MESH GENERATION
         (DATA SET NOT USED)

C ***** DATA SET 12B: ELEMENT INCIDENCES
          (DATA SET NOT USED)

C ***** DATA SET 13: POROUS MEDIA PROPERTIES
PR1        PR2        PR3        PR4        PR5        PR6        PR7        PR8
AL         AT         DM         RHOB       CEC        CP1        CP2        SREA
10.       10.       1.0D-5      1.75       0.0        0.0        0.0        0.0
10.       10.       1.0D-5      1.75       0.0        0.0        0.0        0.0
10.       10.       1.0D-5      1.75       0.0        0.0        0.0        0.0
10.       10.       1.0D-5      1.75       0.0        0.0        0.0        0.0

C ***** DATA SET 14: MATERIAL TYPE CORRECTION
          MI         NSEQ       MAD        MITYP      MTYPAD
          242        13         1          2          0
          259        13         1          2          0
          276        13         1          2          0
          293        13         1          2          0
          310        13         1          2          0
          327        13         1          2          0
          344        13         1          2          0
          361        13         1          2          0
          378        13         1          2          0
          395        13         1          2          0
          0          0          0          0          0

C ***** DATA SET 15: INITIAL OR PRE-INITIAL CONDITIONS
          NI         NSEQ       NAD        RNI        RAD        RRD
CALCIUM
          1          269        1          1.7E-04    0.0D0      0.0D0
          271        6          1          1.7E-04    0.0D0      0.0D0
          278        10         1          1.70E-04   0.0D0      0.0D0
          289        6          1          1.7E-04    0.0D0      0.0D0
          296        10         1          2.45E-04   0.0D0      0.0D0
```

307	6	1	1.7E-04	0.0D0	0.0D0
314	10	1	2.45E-04	0.0D0	0.0D0
325	6	1	1.7E-04	0.0D0	0.0D0
332	10	1	2.45E-04	0.0D0	0.0D0
343	6	1	1.7E-04	0.0D0	0.0D0
350	10	1	2.45E-04	0.0D0	0.0D0
361	6	1	1.7E-04	0.0D0	0.0D0
368	10	1	2.45E-04	0.0D0	0.0D0
379	6	1	1.7E-04	0.0D0	0.0D0
386	10	1	2.45E-04	0.0D0	0.0D0
397	6	1	1.7E-04	0.0D0	0.0D0
404	10	1	1.70E-04	0.0D0	0.0D0
415	6	1	1.7E-04	0.0D0	0.0D0
422	10	1	1.70E-04	0.0D0	0.0D0
433	6	1	1.7E-04	0.0D0	0.0D0
440	10	1	1.70E-04	0.0D0	0.0D0
0	0	0	0.0D00	0.0D0	0.0D0
CARBONATE					
1	269	1	1.00D-4	0.0D0	0.0D0
271	3	1	1.00D-4	0.0D0	0.0D0
275	13	1	1.00D-4	0.0D0	0.0D0
289	3	1	1.00D-4	0.0D0	0.0D0
293	13	1	1.00D-4	0.0D0	0.0D0
307	3	1	1.00D-4	0.0D0	0.0D0
311	13	1	1.00D-4	0.0D0	0.0D0
325	3	1	1.00D-4	0.0D0	0.0D0
329	13	1	1.00D-4	0.0D0	0.0D0
343	3	1	1.00D-4	0.0D0	0.0D0
347	13	1	1.00D-4	0.0D0	0.0D0
361	3	1	1.00D-4	0.0D0	0.0D0
365	13	1	1.00D-4	0.0D0	0.0D0
379	3	1	1.00D-4	0.0D0	0.0D0
383	13	1	1.00D-4	0.0D0	0.0D0
397	3	1	1.00D-4	0.0D0	0.0D0
401	13	1	1.00D-4	0.0D0	0.0D0
415	3	1	1.00D-4	0.0D0	0.0D0
419	13	1	1.00D-4	0.0D0	0.0D0
433	3	1	1.00D-4	0.0D0	0.0D0
437	13	1	1.00D-4	0.0D0	0.0D0
0	0	0	0.0D00	0.0D0	0.0D0
URANIUM					
1	269	1	1.0D-20	0.0D0	0.0D0
271	3	1	1.0D-20	0.0D0	0.0D0
275	13	1	1.0d-20	0.0D0	0.0D0
289	3	1	1.0D-20	0.0D0	0.0D0
293	13	1	1.0d-20	0.0D0	0.0D0
307	3	1	1.0D-20	0.0D0	0.0D0
311	13	1	1.0d-20	0.0D0	0.0D0
325	3	1	1.0D-20	0.0D0	0.0D0
329	13	1	1.0d-20	0.0D0	0.0D0
343	3	1	1.0D-20	0.0D0	0.0D0
347	13	1	1.0d-20	0.0D0	0.0D0
361	3	1	1.0D-20	0.0D0	0.0D0

365	13	1	1.0d-20	0.0D0	0.0D0
379	3	1	1.0D-20	0.0D0	0.0D0
383	13	1	1.0d-20	0.0D0	0.0D0
397	3	1	1.0D-20	0.0D0	0.0D0
401	13	1	1.0D-20	0.0D0	0.0D0
415	3	1	1.0D-20	0.0D0	0.0D0
419	13	1	1.0D-20	0.0D0	0.0D0
433	3	1	1.0D-20	0.0D0	0.0D0
437	13	1	1.0D-20	0.0D0	0.0D0
0	0	0	0.0D00	0.0D0	0.0D0
SULFATE					
1	269	1	3.00D-5	0.0D0	0.0D0
271	3	1	3.00D-5	0.0D0	0.0D0
275	13	1	3.00D-5	0.0D0	0.0D0
289	3	1	3.00D-5	0.0D0	0.0D0
293	13	1	3.00D-5	0.0D0	0.0D0
307	3	1	3.00D-5	0.0D0	0.0D0
311	13	1	3.00D-5	0.0D0	0.0D0
325	3	1	3.00D-5	0.0D0	0.0D0
329	13	1	3.00D-5	0.0D0	0.0D0
343	3	1	3.00D-5	0.0D0	0.0D0
347	13	1	3.00D-5	0.0D0	0.0D0
361	3	1	3.00D-5	0.0D0	0.0D0
365	13	1	3.00D-5	0.0D0	0.0D0
379	3	1	3.00D-5	0.0D0	0.0D0
383	13	1	3.00D-5	0.0D0	0.0D0
397	3	1	3.00D-5	0.0D0	0.0D0
401	13	1	3.00D-5	0.0D0	0.0D0
415	3	1	3.00D-5	0.0D0	0.0D0
419	13	1	3.00D-5	0.0D0	0.0D0
433	3	1	3.00D-5	0.0D0	0.0D0
437	13	1	3.00D-5	0.0D0	0.0D0
0	0	0	0.0D00	0.0D0	0.0D0
HYDROGEN					
1	269	1	1.1E-04	0.0D0	0.0D0
271	6	1	1.1E-04	0.0D0	0.0D0
278	10	1	1.1E-04	0.0D0	0.0D0
289	6	1	1.1E-04	0.0D0	0.0D0
296	10	1	4.0E-05	0.0D0	0.0D0
307	6	1	1.1E-04	0.0D0	0.0D0
314	10	1	4.0E-05	0.0D0	0.0D0
325	6	1	1.1E-04	0.0D0	0.0D0
332	10	1	4.0E-05	0.0D0	0.0D0
343	6	1	1.1E-04	0.0D0	0.0D0
350	10	1	4.0E-05	0.0D0	0.0D0
361	6	1	1.1E-04	0.0D0	0.0D0
368	10	1	4.0E-05	0.0D0	0.0D0
379	6	1	1.1E-04	0.0D0	0.0D0
386	10	1	4.0E-05	0.0D0	0.0D0
397	6	1	1.1E-04	0.0D0	0.0D0
404	10	1	1.1E-04	0.0D0	0.0D0
415	6	1	1.1E-04	0.0D0	0.0D0
422	10	1	1.1E-04	0.0D0	0.0D0

```
        433         6           1        1.1E-04     0.0D0       0.0D0
        440         10          1        1.1E-05     0.0D0       0.0D0
        0           0           0         0.0D00     0.0D0       0.0D0
SOH
        1           269         1          1.00d-5    0.0D0       0.0D0
        271         3           1          1.00d-5    0.0D0       0.0D0
        275         13          1          1.00d-5    0.0D0       0.0D0
        289         3           1          1.00d-5    0.0D0       0.0D0
        293         13          1          1.00d-5    0.0D0       0.0D0
        307         3           1          1.00d-5    0.0D0       0.0D0
        311         13          1          1.00d-5    0.0D0       0.0D0
        325         3           1          1.00d-5    0.0D0       0.0D0
        329         13          1          1.00d-5    0.0D0       0.0D0
        343         3           1          1.00d-5    0.0D0       0.0D0
        347         13          1          1.00d-5    0.0D0       0.0D0
        361         3           1          1.00d-5    0.0D0       0.0D0
        365         13          1          1.00d-5    0.0D0       0.0D0
        379         3           1          1.00d-5    0.0D0       0.0D0
        383         13          1          1.00d-5    0.0D0       0.0D0
        397         3           1          1.00d-5    0.0D0       0.0D0
        401         13          1          1.00d-5    0.0D0       0.0D0
        415         3           1          1.00d-5    0.0D0       0.0D0
        419         13          1          1.00d-5    0.0D0       0.0D0
        433         3           1          1.00d-5    0.0D0       0.0D0
        437         13          1          1.00d-5    0.0D0       0.0D0
        0           0           0          0.0D00     0.0D0       0.0D0
MAGNESIUM
        1           269         1          1.20D-4    0.0D0       0.0D0
        271         3           1          1.20D-4    0.0D0       0.0D0
        275         13          1          1.20D-4    0.0D0       0.0D0
        289         3           1          1.20D-4    0.0D0       0.0D0
        293         13          1          1.20D-4    0.0D0       0.0D0
        307         3           1          1.20D-4    0.0D0       0.0D0
        311         13          1          1.20D-4    0.0D0       0.0D0
        325         3           1          1.20D-4    0.0D0       0.0D0
        329         13          1          1.20D-4    0.0D0       0.0D0
        343         3           1          1.20D-4    0.0D0       0.0D0
        347         13          1          1.20D-4    0.0D0       0.0D0
        361         3           1          1.20D-4    0.0D0       0.0D0
        365         13          1          1.20D-4    0.0D0       0.0D0
        379         3           1          1.20D-4    0.0D0       0.0D0
        383         13          1          1.20D-4    0.0D0       0.0D0
        397         3           1          1.20D-4    0.0D0       0.0D0
        401         13          1          1.20D-4    0.0D0       0.0D0
        415         3           1          1.20D-4    0.0D0       0.0D0
        419         13          1          1.20D-4    0.0D0       0.0D0
        433         3           1          1.20D-4    0.0D0       0.0D0
        437         13          1          1.20D-4    0.0D0       0.0D0
        0           0           0          0.0D00     0.0D0       0.0D0
PHOSPHATE
        1           269         1          5.00D-7    0.0D0       0.0D0
        271         3           1          5.00D-7    0.0D0       0.0D0
        275         13          1          5.00D-7    0.0D0       0.0D0
```

```
          289         3           1          5.00D-7    0.0D0      0.0D0
          293         13          1          5.00D-7    0.0D0      0.0D0
          307         3           1          5.00D-7    0.0D0      0.0D0
          311         13          1          5.00D-7    0.0D0      0.0D0
          325         3           1          5.00D-7    0.0D0      0.0D0
          329         13          1          5.00D-7    0.0D0      0.0D0
          343         3           1          5.00D-7    0.0D0      0.0D0
          347         13          1          5.00D-7    0.0D0      0.0D0
          361         3           1          5.00D-7    0.0D0      0.0D0
          365         13          1          5.00D-7    0.0D0      0.0D0
          379         3           1          5.00D-7    0.0D0      0.0D0
          383         13          1          5.00D-7    0.0D0      0.0D0
          397         3           1          5.00D-7    0.0D0      0.0D0
          401         13          1          5.00D-7    0.0D0      0.0D0
          415         3           1          5.00D-7    0.0D0      0.0D0
          419         13          1          5.00D-7    0.0D0      0.0D0
          433         3           1          5.00D-7    0.0D0      0.0D0
          437         13          1          5.00D-7    0.0D0      0.0D0
          0           0           0          0.0D00     0.0D0      0.0D0
ZINC
          1           269         1          7.60D-7    0.0D0      0.0D0
          271         3           1          7.60D-7    0.0D0      0.0D0
          275         13          1          7.60D-7    0.0D0      0.0D0
          289         3           1          7.60D-7    0.0D0      0.0D0
          293         13          1          7.60D-7    0.0D0      0.0D0
          307         3           1          7.60D-7    0.0D0      0.0D0
          311         13          1          7.60D-7    0.0D0      0.0D0
          325         3           1          7.60D-7    0.0D0      0.0D0
          329         13          1          7.60D-7    0.0D0      0.0D0
          343         3           1          7.60D-7    0.0D0      0.0D0
          347         13          1          7.60D-7    0.0D0      0.0D0
          361         3           1          7.60D-7    0.0D0      0.0D0
          365         13          1          7.60D-7    0.0D0      0.0D0
          379         3           1          7.60D-7    0.0D0      0.0D0
          383         13          1          7.60D-7    0.0D0      0.0D0
          397         3           1          7.60D-7    0.0D0      0.0D0
          401         13          1          7.60D-7    0.0D0      0.0D0
          415         3           1          7.60D-7    0.0D0      0.0D0
          419         13          1          7.60D-7    0.0D0      0.0D0
          433         3           1          7.60D-7    0.0D0      0.0D0
          437         13          1          7.60D-7    0.0D0      0.0D0
          0           0           0          0.0D00     0.0D0      0.0D0

C ***** DATA SET 16: VARIABLE BOUNDARY CONDITIONS
                    ** B.C. CALCIUM **
          TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
          0.0D0     1.70D-04   1.0D20    1.70D-04

          MI        NSEQ      MIAD       MITYP      MTYPAD
          1         16        1          1          0
          0         0         0          0          0

                    ** B.C. CARBONATE **
```

```
TCDBF-1,2 CDBF-1,2  TCDBF-2,2 CDBF-2,2
0.0D0     1.0D-04   1.0D20    1.0D-04

MI        NSEQ      MIAD      MITYP     MTYPAD
1         16        1         1         0
0         0         0         0         0

          ** B.C. URANIUM **
TCDBF-1,3 CDBF-1,3  TCDBF-2,3 CDBF-2,3
0.0D0     1.0D-20   1.0D20    1.0D-20

MI        NSEQ      MIAD      MITYP     MTYPAD
1         16        1         1         0
0         0         0         0         0

          ** B.C. SULFATE **
TCDBF-1,3 CDBF-1,3  TCDBF-2,3 CDBF-2,3
0.0D0     3.0D-05   1.0D20    3.0D-05

MI        NSEQ      MIAD      MITYP     MTYPAD
1         16        1         1         0
0         0         0         0         0

          ** B.C. HYDROGEN **
TCDBF-1,5 CDBF-1,5  TCDBF-2,5 CDBF-2,5
0.0D0     1.1D-4    1.0D20   1.1D-4

MI        NSEQ      MIAD      MITYP     MTYPAD
1         16        1         1         0
0         0         0         0         0

          ** B.C. SOH **
TCDBF-1,6 CDBF-1,6  TCDBF-2,6 CDBF-2,6
0.0D0     1.0D-05   1.0D20    1.0D-05

MI        NSEQ      MIAD      MITYP     MTYPAD
1         16        1         1         0
0         0         0         0         0

          ** B.C. MAGNESIUM **
TCDBF-1,5 CDBF-1,5  TCDBF-2,5 CDBF-2,5
0.0D0     1.2D-04   1.0D20   1.2D-04

MI        NSEQ      MIAD      MITYP     MTYPAD
1         16        1         1         0
0         0         0         0         0

          ** B.C. PHOSPHATE **
TCDBF-1,5 CDBF-1,5  TCDBF-2,5 CDBF-2,5
0.0D0     5.0D-07   1.0D20   5.0D-07

MI        NSEQ      MIAD      MITYP     MTYPAD
1         16        1         1         0
```

```
0          0          0          0          0

          ** B.C. ZINC **
TCDBF-1,5 CDBF-1,5  TCDBF-2,5 CDBF-2,5
0.0D0     7.6D-07   1.0D20    7.6D-07

MI        NSEQ      MIAD       MITYP     MTYPAD
1         16        1          1         0
0         0         0          0         0

          ** GLOBAL NODE NUMBER **
NI        NSEQ      NIAD       NODE      NODEAD
1         17        1          433       1
0         0         0          0         0

          ** BOUNDARY ELEMENT SIDES **
 MI   NSEQ   M   IS1   IS2   MIAD   MAD   IS1AD   IA2AD
 1    16     392 1     2     1      1     1       1
 0    0      0   0     0     0      0     0       0

C ***** DATA SET 17: DIRICHLET BOUNDARY CONDITIONS
          ** B.C. CALCIUM **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     1.7D-4    1.0D38    1.7D-4

NI        NSEQ      NAD        NITYP     NTYPAD
1         17        1          1         0
0         0         0          0         0

          ** B.C. CARBONATE **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     1.0D-4    1.0D38    1.0D-4

NI        NSEQ      NAD        NITYP     NTYPAD
1         17        1          1         0
0         0         0          0         0

          ** B.C. URANIUM **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     1.0D-20   1.0D38    1.0D-20

NI        NSEQ      NAD        NITYP     NTYPAD
1         17        1          1         0
0         0         0          0         0

          ** B.C. SULFATE **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     3.0D-5    1.0D38    3.0D-5

NI        NSEQ      NAD        NITYP     NTYPAD
1         17        1          1         0
0         0         0          0         0
```

```
            ** B.C. HYDROGEN **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     1.1D-4     1.0D38    1.1D-4

NI          NSEQ       NAD        NITYP      NTYPAD
1           17         1          1          0
0           0          0          0          0

            ** B.C. SOH**
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     1.0D-5    1.0D38    1.0D-5

NI          NSEQ       NAD        NITYP      NTYPAD
1           17         1          1          0
0           0          0          0          0

            ** B.C. MAGNESIUM **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     1.2D-4     1.0D38    1.2D-4

NI          NSEQ       NAD        NITYP      NTYPAD
1           17         1          1          0
0           0          0          0          0

            ** B.C. PHOSPHATE **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     5.0D-7     1.0D38    5.0d-7

NI          NSEQ       NAD        NITYP      NTYPAD
1           17         1          1          0
0           0          0          0          0

            ** B.C. ZINC **
TCDBF-1,1 CDBF-1,1  TCDBF-2,1 CDBF-2,1
0.0D0     7.6D-7     1.0D38    7.6D-7

NI          NSEQ       NAD        NITYP      NTYPAD
1           17         1          1          0
0           0          0          0          0

            ** GLOBAL DIRICHLET NODES **
NI          NSEQ       NIAD       NODE       NODEAD
1           17         1          433        1
0           0          0          0          0

C ***** DATA SET 18: ELEMENT SOURCE/SINK DATA
          (DATA SET NOT USED)

C ***** DATA SET 19: WELL (POINT) SOURCE/SINK DATA
          (DATA SET NOT USED)

C ***** DATA SET 20: ELEMENT LEACH SOURCE/SINK DATA
          LEACHING ELEMENTS ARE:
```

```
263 264 265 266 267 268 269 270 271 272 280 297 314 331 348
365 366 367 368 369 370 371 372 373 374

            **  CALCIUM **
   TLEA-1,1 QLEA-1,1  TLEA-2,1 QLEA-2,1
   0.0D0     0.65D-14    1.0D38    0.65D-14

   NI        NSEQ      NAD       NITYP     NTYPAD
   1         24        1         1         0
   0         0         0         0         0

            **  CARBONATE **
   TLEA-1,2  QLEA-1,2  TLEA-2,2 QLEA-2,2
   0.0D0     0.0D-14    1.0D38    0.0D-14

   NI        NSEQ      NAD       NITYP     NTYPAD
   1         24        1         1         0
   0         0         0         0         0

            **  URANIUM **
   TLEA-1,3 QLEA-1,3  TLEA-2,3 QLEA-2,3
   0.0D0     0.0D-14    1.0D38    0.0D-14

   NI        NSEQ      NAD       NITYP     NTYPAD
   1         24        1         1         0
   0         0         0         0         0

            **  SULFATE **
   TLEA-1,4 QLEA-1,4  TLEA-2,4 QLEA-2,4
   0.0D0     0.0D-14    1.0D38    0.0D-14

   NI        NSEQ      NAD       NITYP     NTYPAD
   1         24        1         1         0
   0         0         0         0         0

            **  HYDROGEN **
   TLEA-1,5 QLEA-1,5  TLEA-2,5 QLEA-2,5
   0.0D0    -1.3D-14   1.0D38  -1.3D-14

   NI        NSEQ      NAD       NITYP     NTYPAD
   1         24        1         1         0
   0         0         0         0         0

            **  SOH **
   TLEA-1,6 QLEA-1,6  TLEA-2,6 QLEA-2,6
   0.0D0     0.0D-14    1.0D38    0.0D-14

   NI        NSEQ      NAD       NITYP     NTYPAD
   1         24        1         1         0
   0         0         0         0         0

            **  MAGNESIUM **
   TLEA-1,7 QLEA-1,7  TLEA-2,7 QLEA-2,7
```

```
          0.0D0      0.0D-14     1.0D38     0.05D-14

          NI         NSEQ        NAD        NITYP      NTYPAD
          1          24          1          1          0
          0          0           0          0          0

                     **  PHOSPHATE **
          TLEA-1,8 QLEA-1,8   TLEA-2,8 QLEA-2,8
          0.0D0      0.0D-14     1.0D38     0.0D-14

          NI         NSEQ        NAD        NITYP      NTYPAD
          1          24          1          1          0
          0          0           0          0          0

                     **  ZINC **
          TLEA-1,9 QLEA-1,9   TLEA-2,9 QLEA-2,9
          0.0D0      0.0D-14     1.0D38     0.0D-14

          NI         NSEQ        NAD        NITYP      NTYPAD
          1          24          1          1          0
          0          0           0          0          0

C ***** DATA SET 21: WASTE CONTAINER PARAMETERS
          THICK1     PITN1       PITK1      AREA1      ASCALE1    PITS1
          0.127      0.39        0.074      2.1D04     0.2        5.0D03

          GRATE1     CLAY1       SPH1     IAER1
          2.0D-10    0.15        6.0       2

          NELCON1 NELCON2   X3   X4   X5   X6   X7   X8   X9   X10
          299      302       305 333 336 339

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

C ***** DATA SET 22A: WASTE FORM LEACHING PARAMETERS
                           WASTE FORM 1
W1-ISO1   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1    DISOL1,1
          0.000      0.000       0.000      1.0D-8     1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0        0.0         0.0

W1-ISO2   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1    DISOL1,1
          0.000      0.000       0.000      1.0D-8     1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0        0.0         0.0

W1-ISO3   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1    DISOL1,1
          0.00010      0.000     0.99990    1.0D-8     2.0D-7
```

```
          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO4   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.000     0.000     0.000     1.0D-8    1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO5   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.000     0.000     0.000     1.0D-8    1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO6   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.000     0.000     0.000     1.0D-8    1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO7   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.000     0.000     0.000     1.0D-8    1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO8   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.000     0.000     0.000     1.0D-8    1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

W1-ISO9   SFRACT1,1 PFRACT1,1 BFRACT1,1 DEFF1,1   DISOL1,1
          0.000     0.000     0.000     1.0D-8    1.0D-11

          PARTK01,1 PARTKI1,1 PARTD1,1
          0.0       0.0       0.0

          POREL1    VOLWF1    WWF1
          2.5D1     1.0D6     1.0D0

C ***** DATA SET 22B: INITIAL MASSES OF EACH WASTE ELEMENT
          WTINIT1,1  X2   X3   X4   X5   X6   X7   X8   X9   X10
               0.0   0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0

          WTINIT1,2  X2   X3   X4   X5   X6   X7   X8   X9   X10
               0.0   0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0

          WTINIT1,3  X2   X3   X4   X5   X6   X7   X8   X9   X10
               1.0   1.0  1.0  1.0  1.0  1.0 1.0  1.0 1.0  1.0

          WTINIT1,4  X2   X3   X4   X5   X6   X7   X8   X9   X10
```

```
          0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0

        WTINIT1,5  X2    X3    X4    X5    X6    X7    X8    X9    X10
          0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0

        WTINIT1,6  X2    X3    X4    X5    X6    X7    X8    X9    X10
          0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0

        WTINIT1,7  X2    X3    X4    X5    X6    X7    X8    X9    X10
          0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0

        WTINIT1,8  X2    X3    X4    X5    X6    X7    X8    X9    X10
          0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0

        WTINIT1,9  X2    X3    X4    X5    X6    X7    X8    X9    X10
          0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0

C ***** DATA SET 22C: READ WASTE TYPE ASSIGNMENTS
        MI          NSEQ        MAD         MITYP       MTYPAD
        1           2           1           1           0
        4           2           1           1           0
        0           0           0           0           0

C ***** DATA SET 23A: PRINT AND AUXILIARY STORAGE CONTROL
        INTEGER PRINT PARAMETERS
        IITR        INTER       ICOND       NHGCI
        0           0           0           0

KPR0,KPR(I),I=1,NTI
20000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000000000000

KDSK0,KDSK(I),I=1,NTI
00000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000000000000

C ***** DATA SET 22B: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
        NCPRT
        3

        NODEP1,2   NODEP2,2    NODEP3,2
        234        320         321

        NI          NSEQ        NAD         NITYP       NTYPAD
        1           449         1           1           0
        0           0           0           0           0

C ***** DATA SET 23: VELOCITY AND MOISTURE CONTENT
   (DATA SET IS NOT USED)
```

B.3.5 BLT-EC Chemistry Input File for the Two-Dimensional Reactive Transport Problem

The chemistry input file for the two-dimensional example problem is:

```
2D EXAMPLE PROBLEM
SAME MESH AS PROB 5 IN NUREG 6305
25.00  MOLAL    0.000    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
0.00000E+00
0 0 1 1 3 0 1 0 1 2 0 0 0
1   1   2
81
0.000E+00     0.00 0.000 0.000
0.000E+00     0.00 0.000 0.000
0.000E+00     0.00 0.000 0.000
0.000E+00     0.00 0.000 0.000
0.000E+00     0.00 0.000 0.000
    811  0.000E+00     0.00 y                    /ADS1TYP1
    330  1.000E-32   -32.00 y                    /H+1
    150  1.000E-32   -32.00 y                    /Ca+2
    140  1.000E-32   -32.00 y                    /CO3-2
    460  1.000E-32   -32.00 y                    /Mg+2
    580  1.000E-32   -32.00 y                    /PO4-3
    732  1.000E-32   -32.00 y                    /SO4-2
    950  1.000E-32   -32.00 y                    /Zn+2
    893  1.000E-32   -32.00 y                    /UO2+2

   0


   3
8118930 sohm1
   0.000000        3.00000              3    1.00000             811
    1.00000            893   -1.00000            330            0
   0.000000       0.000000                0           0   0.000000
   0.000000              0           0   0.000000       0.000000
          0           0   0.000000       0.000000                0           0
8113300 so
   0.000000       -10.3000             2    1.00000             811
   -1.00000            330           0   0.000000       0.000000
          0           0   0.000000       0.000000                0           0
   0.000000       0.000000                0           0   0.000000
   0.000000              0           0
8113301 sohh
   0.000000        5.40000              2    1.00000             811
    1.00000            330           0   0.000000       0.000000
          0           0   0.000000       0.000000                0           0
   0.000000       0.000000                0           0   0.000000
   0.000000              0           0
```

B.4 BLT-EC Main Output File for the Two-Dimensional Reactive Transport Problem

The partial main output file follows. In this example, the input is read and printed on pages B-51 to B-84. Time-dependent output begins on page B-85 and contains flow rates of each component through the boundaries release rates from the wasteform, and concentration at each nodal point.

```
 PROBLEM. 0..
    USES MESH AND FLOW FROM Prob.5 IN BLT-EC NUREG/CR-6305
      **** INTEGER INPUT, STORAGE, & CONTROL PARAMETERS ****

      STEADY-STATE CONTROL  . . . . . .    1
      VELOCITY INPUT CONTROL  . . . . . .    1


      STORAGE CONTROL . . . . . .    0
      RESTART CONTROL   . . . . . .    0


      **** INTEGER PARAMETERS FOR CONTAINERS AND WASTE ****

      NO. OF WASTE CONTAINING ELEMENTS. . . .    6
      NO. OF CONTAINER TYPES. . . . . .    1
      NO. OF WASTE TYPES. . . . . .    1
      LEACHING SUBROUTINE FLAG. . . . . .    1
      FLAG FOR INVENTORY UNITS. . . . . .    0


      **** INTEGRATION INTEGER PARAMETERS ****

      MASS LUMPING CONTROL  . . . . . .    1
      MID-DIFFERENCE INDICATOR  . . . . . .    0
      UPSTREAM WEIGHTING INDICATOR, IWET. . .    1
      WEIGHTING FACTOR OPTIMIZING INDICATOR .    0


      **** INTEGER SOLUTION CONTROL PARAMETERS ****

      NUMBER OF TIME INCREMENTS . . . . . .  300
      NO. OF ITERATIONS TO SOLVE NONLINEAR EQ    1
      NO. OF TIMES TO RESET TIME STEP SIZE  .    1
      NO. OF POINTWISE ITERATIONS ALLOWED . .    1


      IS POINTWISE ITERATION SOLUTION USED?      0


      **** GRID AND ELEMENT PARAMETERS ****

      OLD(0) OR NEW(1) MESH GENERATOR . . . .    1
      NUMBER OF NODAL POINTS. . . . . .  450
      NUMBER OF ELEMENTS. . . . . .  408
      NUMBER OF DIFFERENT MATERIALS . . . . .    4
      NUMBER OF CORRECTION MATERIALS. . . . .  140
```

**** INTEGER PARAMETERS FOR BOUNDARY CONDITIONS ****

NO. OF DIRICHLET NODAL POINTS	18
NO. OF DIRICHLET BOUNDARY CONDIITION PROFILES .	1
NO. OF DIRICHLET DATA POINTS IN EACH PROFILE . .	2
NO. OF VARIABLE BOUNDARY NODE POINTS	18
NO. OF VARIABLE BOUNDARY ELEMENT-SIDES	17
NO. OF INCOMING CON. PROF. FOR VARIABLE BOUNDARY	1
NO. OF DATA POINTS ON EACH NVPR PROFILES	2

**** INTEGER PARAMETERS FOR SOURCES ****

NO. OF SOURCE ELEMENTS (INJECTION)	0
NO. OF SOURCE PROFILE	0
NO. OF SOURCE DATA POINT IN EACH PROFILE	0
NO. OF SOURCE ELEMENTS (LEACHING).	25
NO. OF SOURCE PROFILE	1
NO. OF SOURCE DATA POINT IN EACH PROFILE	2
NO. OF WELL (POINT) SOURCE/SINK NODE POINTS. . .	0
NO. OF WELL (POINT) SOURCE/SINK PROFILE	0
NO. OF DATA POINTS IN WELL SOURCE/SINK PROFILE .	0

**** COMPONENT INFORMATION ****

NO. OF COMPONENTS, NON 9

NO. OF NON CONSERVATIVE COMP.S, NONC . . 9

HYDROGEN COMPONENT NO., LNH 5

ELECTRON COMPONENT NO., LNE 11

K	COMPONENT	IDEN	INDC	CSAT	DCAY	JDOTER1	DFRAC1	JDOTER2	DFRAC2
1	CALCIUM	150	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
2	CARBONATE	140	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
3	URANIUM	893	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
4	SULFATE	732	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
5	HYDROGEN	330	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
6	SOH	811	2	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
7	MAGNESIUM	460	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
8	PHOSPHATE	580	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00
9	ZINC	950	1	1.00E+06	2.20E-40	0	0.00E+00	0	0.00E+00

**** TIME INTEGRATION CONTROL PARAMETERS ****

TIME INCREMENT. 5.000000E-01

```
 MULTIPLIER FOR INCREASING DELT. . . . .   0.000000E+00
 MAXIMUM VALUE OF DELT . . . . . .         5.000000E-01
 MAXIMUM VALUE OF TIME . . . . . .         1.020000E+02
 TIME-INTEGRATION PARAMETER. . . . . .     1.000000E+00
 TIME-INTEGRATION PARAMETER FOR V  . . .   1.000000E+00


 TIME OF CHANGING DELT
       1.0000E+38


 **** REAL PARAMETERS FOR NONLINEAR SOLVE ****

 ITERATION  PARAMETER FOR NONLINEAR EQ..   1.000000E+00
 RELAXATION PARAMETER FOR POINTWISE SOL.   1.000000E+00
 ERROR ALLOWANCE FOR NONLINEAR SOL . . .   1.000000E-09
 GIVEN UPSTREAM WEIGHTING FACTOR . . . .   1.000000E+00


2D EXAMPLE FLOW PROBLEM      8/96


 FACILITY WIDTH (cm) -   1.00E+00


            **** NODAL COORDINATES ****

NODE          X           Z    NODE          X           Z
----          -           -    ----          -           -
   1  3.514E+03  0.000E+00       2  3.743E+03  0.000E+00
   3  3.971E+03  0.000E+00       4  4.200E+03  0.000E+00
   5  4.300E+03  0.000E+00       6  4.400E+03  0.000E+00
   7  4.500E+03  0.000E+00       8  4.600E+03  0.000E+00
   9  4.700E+03  0.000E+00      10  4.800E+03  0.000E+00
  11  4.900E+03  0.000E+00      12  5.000E+03  0.000E+00
  13  5.100E+03  0.000E+00      14  5.200E+03  0.000E+00
  15  5.300E+03  0.000E+00      16  5.400E+03  0.000E+00
  17  5.500E+03  0.000E+00      18  5.600E+03  0.000E+00
  19  3.514E+03  2.500E+02      20  3.743E+03  2.500E+02
  21  3.971E+03  2.500E+02      22  4.200E+03  2.500E+02
  23  4.300E+03  2.500E+02      24  4.400E+03  2.500E+02
  25  4.500E+03  2.500E+02      26  4.600E+03  2.500E+02
  27  4.700E+03  2.500E+02      28  4.800E+03  2.500E+02
  29  4.900E+03  2.500E+02      30  5.000E+03  2.500E+02
  31  5.100E+03  2.500E+02      32  5.200E+03  2.500E+02
  33  5.300E+03  2.500E+02      34  5.400E+03  2.500E+02
  35  5.500E+03  2.500E+02      36  5.600E+03  2.500E+02
  37  3.514E+03  5.000E+02      38  3.743E+03  5.000E+02
  39  3.971E+03  5.000E+02      40  4.200E+03  5.000E+02
  41  4.300E+03  5.000E+02      42  4.400E+03  5.000E+02
  43  4.500E+03  5.000E+02      44  4.600E+03  5.000E+02
  45  4.700E+03  5.000E+02      46  4.800E+03  5.000E+02
  47  4.900E+03  5.000E+02      48  5.000E+03  5.000E+02
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49	5.100E+03	5.000E+02	50	5.200E+03	5.000E+02
51	5.300E+03	5.000E+02	52	5.400E+03	5.000E+02
53	5.500E+03	5.000E+02	54	5.600E+03	5.000E+02
55	3.514E+03	7.500E+02	56	3.743E+03	7.500E+02
57	3.971E+03	7.500E+02	58	4.200E+03	7.500E+02
59	4.300E+03	7.500E+02	60	4.400E+03	7.500E+02
61	4.500E+03	7.500E+02	62	4.600E+03	7.500E+02
63	4.700E+03	7.500E+02	64	4.800E+03	7.500E+02
65	4.900E+03	7.500E+02	66	5.000E+03	7.500E+02
67	5.100E+03	7.500E+02	68	5.200E+03	7.500E+02
69	5.300E+03	7.500E+02	70	5.400E+03	7.500E+02
71	5.500E+03	7.500E+02	72	5.600E+03	7.500E+02
73	3.514E+03	1.000E+03	74	3.743E+03	1.000E+03
75	3.971E+03	1.000E+03	76	4.200E+03	1.000E+03
77	4.300E+03	1.000E+03	78	4.400E+03	1.000E+03
79	4.500E+03	1.000E+03	80	4.600E+03	1.000E+03
81	4.700E+03	1.000E+03	82	4.800E+03	1.000E+03
83	4.900E+03	1.000E+03	84	5.000E+03	1.000E+03
85	5.100E+03	1.000E+03	86	5.200E+03	1.000E+03
87	5.300E+03	1.000E+03	88	5.400E+03	1.000E+03
89	5.500E+03	1.000E+03	90	5.600E+03	1.000E+03
91	3.514E+03	1.250E+03	92	3.743E+03	1.250E+03
93	3.971E+03	1.250E+03	94	4.200E+03	1.250E+03
95	4.300E+03	1.250E+03	96	4.400E+03	1.250E+03
97	4.500E+03	1.250E+03	98	4.600E+03	1.250E+03
99	4.700E+03	1.250E+03	100	4.800E+03	1.250E+03

**** NODAL COORDINATES ****

NODE	X	Z	NODE	X	Z
101	4.900E+03	1.250E+03	102	5.000E+03	1.250E+03
103	5.100E+03	1.250E+03	104	5.200E+03	1.250E+03
105	5.300E+03	1.250E+03	106	5.400E+03	1.250E+03
107	5.500E+03	1.250E+03	108	5.600E+03	1.250E+03
109	3.514E+03	1.500E+03	110	3.743E+03	1.500E+03
111	3.971E+03	1.500E+03	112	4.200E+03	1.500E+03
113	4.300E+03	1.500E+03	114	4.400E+03	1.500E+03
115	4.500E+03	1.500E+03	116	4.600E+03	1.500E+03
117	4.700E+03	1.500E+03	118	4.800E+03	1.500E+03
119	4.900E+03	1.500E+03	120	5.000E+03	1.500E+03
121	5.100E+03	1.500E+03	122	5.200E+03	1.500E+03
123	5.300E+03	1.500E+03	124	5.400E+03	1.500E+03
125	5.500E+03	1.500E+03	126	5.600E+03	1.500E+03
127	3.514E+03	1.750E+03	128	3.743E+03	1.750E+03
129	3.971E+03	1.750E+03	130	4.200E+03	1.750E+03
131	4.300E+03	1.750E+03	132	4.400E+03	1.750E+03
133	4.500E+03	1.750E+03	134	4.600E+03	1.750E+03
135	4.700E+03	1.750E+03	136	4.800E+03	1.750E+03
137	4.900E+03	1.750E+03	138	5.000E+03	1.750E+03
139	5.100E+03	1.750E+03	140	5.200E+03	1.750E+03
141	5.300E+03	1.750E+03	142	5.400E+03	1.750E+03
143	5.500E+03	1.750E+03	144	5.600E+03	1.750E+03
145	3.514E+03	2.000E+03	146	3.743E+03	2.000E+03

147	3.971E+03	2.000E+03	148	4.200E+03	2.000E+03
149	4.300E+03	2.000E+03	150	4.400E+03	2.000E+03
151	4.500E+03	2.000E+03	152	4.600E+03	2.000E+03
153	4.700E+03	2.000E+03	154	4.800E+03	2.000E+03
155	4.900E+03	2.000E+03	156	5.000E+03	2.000E+03
157	5.100E+03	2.000E+03	158	5.200E+03	2.000E+03
159	5.300E+03	2.000E+03	160	5.400E+03	2.000E+03
161	5.500E+03	2.000E+03	162	5.600E+03	2.000E+03
163	3.514E+03	2.100E+03	164	3.743E+03	2.100E+03
165	3.971E+03	2.100E+03	166	4.200E+03	2.100E+03
167	4.300E+03	2.100E+03	168	4.400E+03	2.100E+03
169	4.500E+03	2.100E+03	170	4.600E+03	2.100E+03
171	4.700E+03	2.100E+03	172	4.800E+03	2.100E+03
173	4.900E+03	2.100E+03	174	5.000E+03	2.100E+03
175	5.100E+03	2.100E+03	176	5.200E+03	2.100E+03
177	5.300E+03	2.100E+03	178	5.400E+03	2.100E+03
179	5.500E+03	2.100E+03	180	5.600E+03	2.100E+03
181	3.514E+03	2.200E+03	182	3.743E+03	2.200E+03
183	3.971E+03	2.200E+03	184	4.200E+03	2.200E+03
185	4.300E+03	2.200E+03	186	4.400E+03	2.200E+03
187	4.500E+03	2.200E+03	188	4.600E+03	2.200E+03
189	4.700E+03	2.200E+03	190	4.800E+03	2.200E+03
191	4.900E+03	2.200E+03	192	5.000E+03	2.200E+03
193	5.100E+03	2.200E+03	194	5.200E+03	2.200E+03
195	5.300E+03	2.200E+03	196	5.400E+03	2.200E+03
197	5.500E+03	2.200E+03	198	5.600E+03	2.200E+03
199	3.514E+03	2.300E+03	200	3.743E+03	2.300E+03

**** NODAL COORDINATES ****

NODE	X	Z	NODE	X	Z
201	3.971E+03	2.300E+03	202	4.200E+03	2.300E+03
203	4.300E+03	2.300E+03	204	4.400E+03	2.300E+03
205	4.500E+03	2.300E+03	206	4.600E+03	2.300E+03
207	4.700E+03	2.300E+03	208	4.800E+03	2.300E+03
209	4.900E+03	2.300E+03	210	5.000E+03	2.300E+03
211	5.100E+03	2.300E+03	212	5.200E+03	2.300E+03
213	5.300E+03	2.300E+03	214	5.400E+03	2.300E+03
215	5.500E+03	2.300E+03	216	5.600E+03	2.300E+03
217	3.514E+03	2.400E+03	218	3.743E+03	2.400E+03
219	3.971E+03	2.400E+03	220	4.200E+03	2.400E+03
221	4.300E+03	2.400E+03	222	4.400E+03	2.400E+03
223	4.500E+03	2.400E+03	224	4.600E+03	2.400E+03
225	4.700E+03	2.400E+03	226	4.800E+03	2.400E+03
227	4.900E+03	2.400E+03	228	5.000E+03	2.400E+03
229	5.100E+03	2.400E+03	230	5.200E+03	2.400E+03
231	5.300E+03	2.400E+03	232	5.400E+03	2.400E+03
233	5.500E+03	2.400E+03	234	5.600E+03	2.400E+03
235	3.514E+03	2.500E+03	236	3.743E+03	2.500E+03
237	3.971E+03	2.500E+03	238	4.200E+03	2.500E+03
239	4.300E+03	2.500E+03	240	4.400E+03	2.500E+03
241	4.500E+03	2.500E+03	242	4.600E+03	2.500E+03
243	4.700E+03	2.500E+03	244	4.800E+03	2.500E+03

245	4.900E+03	2.500E+03	246	5.000E+03	2.500E+03
247	5.100E+03	2.500E+03	248	5.200E+03	2.500E+03
249	5.300E+03	2.500E+03	250	5.400E+03	2.500E+03
251	5.500E+03	2.500E+03	252	5.600E+03	2.500E+03
253	3.514E+03	2.600E+03	254	3.743E+03	2.600E+03
255	3.971E+03	2.600E+03	256	4.200E+03	2.600E+03
257	4.300E+03	2.600E+03	258	4.400E+03	2.600E+03
259	4.500E+03	2.600E+03	260	4.600E+03	2.600E+03
261	4.700E+03	2.600E+03	262	4.800E+03	2.600E+03
263	4.900E+03	2.600E+03	264	5.000E+03	2.600E+03
265	5.100E+03	2.600E+03	266	5.200E+03	2.600E+03
267	5.300E+03	2.600E+03	268	5.400E+03	2.600E+03
269	5.500E+03	2.600E+03	270	5.600E+03	2.600E+03
271	3.500E+03	2.694E+03	272	3.725E+03	2.696E+03
273	3.950E+03	2.698E+03	274	4.175E+03	2.700E+03
275	4.277E+03	2.700E+03	276	4.379E+03	2.700E+03
277	4.480E+03	2.700E+03	278	4.582E+03	2.700E+03
279	4.684E+03	2.700E+03	280	4.786E+03	2.700E+03
281	4.888E+03	2.700E+03	282	4.989E+03	2.700E+03
283	5.091E+03	2.700E+03	284	5.193E+03	2.700E+03
285	5.295E+03	2.700E+03	286	5.396E+03	2.700E+03
287	5.498E+03	2.700E+03	288	5.600E+03	2.700E+03
289	3.486E+03	2.788E+03	290	3.707E+03	2.792E+03
291	3.929E+03	2.796E+03	292	4.150E+03	2.800E+03
293	4.254E+03	2.800E+03	294	4.357E+03	2.800E+03
295	4.461E+03	2.800E+03	296	4.564E+03	2.800E+03
297	4.668E+03	2.800E+03	298	4.771E+03	2.800E+03
299	4.875E+03	2.800E+03	300	4.979E+03	2.800E+03

**** NODAL COORDINATES ****

NODE	X	Z	NODE	X	Z
301	5.082E+03	2.800E+03	302	5.186E+03	2.800E+03
303	5.289E+03	2.800E+03	304	5.393E+03	2.800E+03
305	5.496E+03	2.800E+03	306	5.600E+03	2.800E+03
307	3.471E+03	2.881E+03	308	3.689E+03	2.888E+03
309	3.907E+03	2.894E+03	310	4.125E+03	2.900E+03
311	4.230E+03	2.900E+03	312	4.336E+03	2.900E+03
313	4.441E+03	2.900E+03	314	4.546E+03	2.900E+03
315	4.652E+03	2.900E+03	316	4.757E+03	2.900E+03
317	4.863E+03	2.900E+03	318	4.968E+03	2.900E+03
319	5.073E+03	2.900E+03	320	5.179E+03	2.900E+03
321	5.284E+03	2.900E+03	322	5.389E+03	2.900E+03
323	5.495E+03	2.900E+03	324	5.600E+03	2.900E+03
325	3.457E+03	2.975E+03	326	3.671E+03	2.983E+03
327	3.886E+03	2.992E+03	328	4.100E+03	3.000E+03
329	4.207E+03	3.000E+03	330	4.314E+03	3.000E+03
331	4.421E+03	3.000E+03	332	4.529E+03	3.000E+03
333	4.636E+03	3.000E+03	334	4.743E+03	3.000E+03
335	4.850E+03	3.000E+03	336	4.957E+03	3.000E+03
337	5.064E+03	3.000E+03	338	5.171E+03	3.000E+03
339	5.279E+03	3.000E+03	340	5.386E+03	3.000E+03
341	5.493E+03	3.000E+03	342	5.600E+03	3.000E+03

343	3.443E+03	3.069E+03	344	3.654E+03	3.079E+03
345	3.864E+03	3.090E+03	346	4.075E+03	3.100E+03
347	4.184E+03	3.100E+03	348	4.293E+03	3.100E+03
349	4.402E+03	3.100E+03	350	4.511E+03	3.100E+03
351	4.620E+03	3.100E+03	352	4.729E+03	3.100E+03
353	4.838E+03	3.100E+03	354	4.946E+03	3.100E+03
355	5.055E+03	3.100E+03	356	5.164E+03	3.100E+03
357	5.273E+03	3.100E+03	358	5.382E+03	3.100E+03
359	5.491E+03	3.100E+03	360	5.600E+03	3.100E+03
361	3.429E+03	3.163E+03	362	3.636E+03	3.175E+03
363	3.843E+03	3.188E+03	364	4.050E+03	3.200E+03
365	4.161E+03	3.200E+03	366	4.271E+03	3.200E+03
367	4.382E+03	3.200E+03	368	4.493E+03	3.200E+03
369	4.604E+03	3.200E+03	370	4.714E+03	3.200E+03
371	4.825E+03	3.200E+03	372	4.936E+03	3.200E+03
373	5.046E+03	3.200E+03	374	5.157E+03	3.200E+03
375	5.268E+03	3.200E+03	376	5.379E+03	3.200E+03
377	5.489E+03	3.200E+03	378	5.600E+03	3.200E+03
379	3.414E+03	3.256E+03	380	3.618E+03	3.271E+03
381	3.821E+03	3.285E+03	382	4.025E+03	3.300E+03
383	4.138E+03	3.300E+03	384	4.250E+03	3.300E+03
385	4.363E+03	3.300E+03	386	4.475E+03	3.300E+03
387	4.588E+03	3.300E+03	388	4.700E+03	3.300E+03
389	4.813E+03	3.300E+03	390	4.925E+03	3.300E+03
391	5.038E+03	3.300E+03	392	5.150E+03	3.300E+03
393	5.263E+03	3.300E+03	394	5.375E+03	3.300E+03
395	5.488E+03	3.300E+03	396	5.600E+03	3.300E+03
397	3.400E+03	3.350E+03	398	3.600E+03	3.367E+03
399	3.800E+03	3.383E+03	400	4.000E+03	3.400E+03

**** NODAL COORDINATES ****

NODE	X	Z	NODE	X	Z
401	4.114E+03	3.400E+03	402	4.229E+03	3.400E+03
403	4.343E+03	3.400E+03	404	4.457E+03	3.400E+03
405	4.571E+03	3.400E+03	406	4.686E+03	3.400E+03
407	4.800E+03	3.400E+03	408	4.914E+03	3.400E+03
409	5.029E+03	3.400E+03	410	5.143E+03	3.400E+03
411	5.257E+03	3.400E+03	412	5.371E+03	3.400E+03
413	5.486E+03	3.400E+03	414	5.600E+03	3.400E+03
415	3.400E+03	3.375E+03	416	3.600E+03	3.400E+03
417	3.800E+03	3.425E+03	418	4.000E+03	3.450E+03
419	4.114E+03	3.454E+03	420	4.229E+03	3.457E+03
421	4.343E+03	3.461E+03	422	4.457E+03	3.464E+03
423	4.571E+03	3.468E+03	424	4.686E+03	3.471E+03
425	4.800E+03	3.475E+03	426	4.914E+03	3.479E+03
427	5.029E+03	3.482E+03	428	5.143E+03	3.486E+03
429	5.257E+03	3.489E+03	430	5.371E+03	3.493E+03
431	5.486E+03	3.496E+03	432	5.600E+03	3.500E+03
433	3.400E+03	3.400E+03	434	3.600E+03	3.433E+03
435	3.800E+03	3.467E+03	436	4.000E+03	3.500E+03
437	4.114E+03	3.507E+03	438	4.229E+03	3.514E+03
439	4.343E+03	3.521E+03	440	4.457E+03	3.529E+03

441	4.571E+03	3.536E+03	442	4.686E+03	3.543E+03
443	4.800E+03	3.550E+03	444	4.914E+03	3.557E+03
445	5.029E+03	3.564E+03	446	5.143E+03	3.571E+03
447	5.257E+03	3.579E+03	448	5.371E+03	3.586E+03
449	5.486E+03	3.593E+03	450	5.600E+03	3.600E+03

**** MATERIAL PROPERTIES ****

M	AL	AT	DM	RHOB
1	1.000E+01	1.000E+01	1.000E-05	1.750E+00
2	1.000E+01	1.000E+01	1.000E-05	1.750E+00
3	1.000E+01	1.000E+01	1.000E-05	1.750E+00
4	1.000E+01	1.000E+01	1.000E-05	1.750E+00

**** VARIABLE BOUNDARY CONDITIONS ****

$$$ FOR CHEMICAL NO. 1(CALCIUM) $$$

--- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

TIME	CIN	TIME	CIN	TIME	CIN
0.000E+00	1.700E-04	1.000E+20	1.700E-04		

--- TYPE OF FLOW-IN CONCENTRATION ---

MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1						

$$$ FOR CHEMICAL NO. 2(CARBONATE) $$$

--- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

TIME	CIN	TIME	CIN	TIME	CIN

```
  0.000E+00  1.000E-04  1.000E+20  1.000E-04


--- TYPE OF FLOW-IN CONCENTRATION ---

  MP CTYP     MP CTYP     MP CTYP     MP CTYP     MP CTYP
  -- ----     -- ----     -- ----     -- ----     -- ----
   1    1      2    1      3    1      4    1      5    1
   6    1      7    1      8    1      9    1     10    1
  11    1     12    1     13    1     14    1     15    1
  16    1     17    1


 $$$ FOR CHEMICAL NO. 3(URANIUM     ) $$$


     --- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

    TIME        CIN       TIME        CIN       TIME        CIN
    ----        ---       ----        ---       ----        ---
  0.000E+00  1.000E-20  1.000E+20  1.000E-20


--- TYPE OF FLOW-IN CONCENTRATION ---

  MP CTYP     MP CTYP     MP CTYP     MP CTYP     MP CTYP
  -- ----     -- ----     -- ----     -- ----     -- ----
   1    1      2    1      3    1      4    1      5    1
   6    1      7    1      8    1      9    1     10    1
  11    1     12    1     13    1     14    1     15    1
  16    1     17    1


 $$$ FOR CHEMICAL NO. 4(SULFATE     ) $$$


     --- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

    TIME        CIN       TIME        CIN       TIME        CIN
    ----        ---       ----        ---       ----        ---
  0.000E+00  3.000E-05  1.000E+20  3.000E-05


--- TYPE OF FLOW-IN CONCENTRATION ---

  MP CTYP     MP CTYP     MP CTYP     MP CTYP     MP CTYP
  -- ----     -- ----     -- ----     -- ----     -- ----
   1    1      2    1      3    1      4    1      5    1
   6    1      7    1      8    1      9    1     10    1
  11    1     12    1     13    1     14    1     15    1
  16    1     17    1
```

$$$ FOR CHEMICAL NO. 5(HYDROGEN) $$$

--- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

TIME	CIN	TIME	CIN	TIME	CIN
0.000E+00	1.100E-04	1.000E+20	1.100E-04		

--- TYPE OF FLOW-IN CONCENTRATION ---

MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1						

$$$ FOR CHEMICAL NO. 6(SOH) $$$

--- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

TIME	CIN	TIME	CIN	TIME	CIN
0.000E+00	1.000E-05	1.000E+20	1.000E-05		

--- TYPE OF FLOW-IN CONCENTRATION ---

MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1						

$$$ FOR CHEMICAL NO. 7(MAGNESIUM) $$$

--- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

TIME	CIN	TIME	CIN	TIME	CIN
0.000E+00	1.200E-04	1.000E+20	1.200E-04		

--- TYPE OF FLOW-IN CONCENTRATION ---

MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1						

$$$ FOR CHEMICAL NO. 8(PHOSPHATE) $$$

--- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

TIME	CIN	TIME	CIN	TIME	CIN
0.000E+00	5.000E-07	1.000E+20	5.000E-07		

--- TYPE OF FLOW-IN CONCENTRATION ---

MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1						

$$$ FOR CHEMICAL NO. 9(ZINC) $$$

--- INCOMING FLUID CONCENTRATION PROFILE ---

PROFILE NO. 1

TIME	CIN	TIME	CIN	TIME	CIN
0.000E+00	7.600E-07	1.000E+20	7.600E-07		

--- TYPE OF FLOW-IN CONCENTRATION ---

MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP	MP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1						

--- LIST OF VB-NODAL POINTS ---

NP	NPVB	NP	NPVB	NP	NPVB	NP	NPVB	NP	NPVB
1	433	2	434	3	435	4	436	5	437
6	438	7	439	8	440	9	441	10	442
11	443	12	444	13	445	14	446	15	447
16	448	17	449	18	450				

--- RS ELEMENT-SIDES INFORMATION ---

SIDE	ELEMENT	NODE1	NODE2	SIDE	ELEMENT	NODE1	NODE2
1	392	1	2	2	393	2	3
3	394	3	4	4	395	4	5
5	396	5	6	6	397	6	7
7	398	7	8	8	399	8	9
9	400	9	10	10	401	10	11
11	402	11	12	12	403	12	13
13	404	13	14	14	405	14	15
15	406	15	16	16	407	16	17
17	408	17	18				

*** COMPUTED RAINFALL SEEPAGE ELEMENT SIDE INFORMATION ***

MP	M	NP1	NP2	L1	L2	DL(MP)	DCOSX(MP)	DCOSZ(MP)
1	392	2	1	3	4	2.028E+02	-1.644E-01	9.864E-01
2	393	3	2	3	4	2.028E+02	-1.644E-01	9.864E-01
3	394	4	3	3	4	2.028E+02	-1.644E-01	9.864E-01
4	395	5	4	3	4	1.145E+02	-6.238E-02	9.981E-01
5	396	6	5	3	4	1.145E+02	-6.238E-02	9.981E-01
6	397	7	6	3	4	1.145E+02	-6.238E-02	9.981E-01
7	398	8	7	3	4	1.145E+02	-6.237E-02	9.981E-01
8	399	9	8	3	4	1.145E+02	-6.238E-02	9.981E-01
9	400	10	9	3	4	1.145E+02	-6.238E-02	9.981E-01
10	401	11	10	3	4	1.145E+02	-6.238E-02	9.981E-01
11	402	12	11	3	4	1.145E+02	-6.238E-02	9.981E-01
12	403	13	12	3	4	1.145E+02	-6.238E-02	9.981E-01
13	404	14	13	3	4	1.145E+02	-6.238E-02	9.981E-01
14	405	15	14	3	4	1.145E+02	-6.237E-02	9.981E-01
15	406	16	15	3	4	1.145E+02	-6.238E-02	9.981E-01
16	407	17	16	3	4	1.145E+02	-6.238E-02	9.981E-01
17	408	18	17	3	4	1.145E+02	-6.238E-02	9.981E-01

**** DIRICHLET BOUNDARY CONDITIONS ****

$$$ FOR CHEMICAL NO. 1(CALCIUM) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	1.700E-04	1.000E+38	1.700E-04		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 2(CARBONATE) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	1.000E-04	1.000E+38	1.000E-04		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 3(URANIUM) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	1.000E-20	1.000E+38	1.000E-20		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 4(SULFATE) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	3.000E-05	1.000E+38	3.000E-05		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 5(HYDROGEN) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	1.100E-04	1.000E+38	1.100E-04		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 6(SOH) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	1.000E-05	1.000E+38	1.000E-05		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 7(MAGNESIUM) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	1.200E-04	1.000E+38	1.200E-04		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 8(PHOSPHATE) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	5.000E-07	1.000E+38	5.000E-07		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

$$$ FOR CHEMICAL NO. 9(ZINC) $$$

--- DIRICHLET CONCENTRATION PROFILES ---

PROFILE NO. 1

TIME	DCON	TIME	DCON	TIME	DCON
0.000E+00	7.600E-07	1.000E+38	7.600E-07		

--- CONCENTRATION TYPE OF DIRICHLET NODES

NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP	NP	CTYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1				

--- NODE NUMBER OF DIRICHLET NODES

NP	NPDB	NP	NPDB	NP	NPDB	NP	NPDB	NP	NPDB
1	433	2	434	3	435	4	436	5	437
6	438	7	439	8	440	9	441	10	442
11	443	12	444	13	445	14	446	15	447
16	448	17	449	18	450				

*** ELEMENT SOURCE INFORMATION ***

- ELEMENT NUMBER OF SOURCE/SINK ELEMENT (L)

MP	MLEA	MP	MLEA	MP	MLEA	MP	MLEA	MP	MLEA
1	263	2	264	3	265	4	266	5	267
6	268	7	269	8	270	9	271	10	272
11	280	12	297	13	314	14	331	15	348
16	365	17	366	18	367	19	368	20	369
21	370	22	371	23	372	24	373	25	374

$$$ FOR CHEMICAL NO. 1(CALCIUM) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	6.500E-15	1.000E+38	6.500E-15		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 2(CARBONATE) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	0.000E+00	1.000E+38	0.000E+00		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 3(URANIUM) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	0.000E+00	1.000E+38	0.000E+00		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1

11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 4(SULFATE) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	0.000E+00	1.000E+38	0.000E+00		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 5(HYDROGEN) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	-1.300E-14	1.000E+38	-1.300E-14		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 6(SOH) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	0.000E+00	1.000E+38	0.000E+00		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 7(MAGNESIUM) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	0.000E+00	1.000E+38	5.000E-16		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 8(PHOSPHATE) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE
0.000E+00	0.000E+00	1.000E+38	0.000E+00		

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

$$$ FOR CHEMICAL NO. 9(ZINC) $$$

--- ELEMENT SOURCE/SINK PROFILES ---
PROFILE NO. 1

TIME	SOURCE	TIME	SOURCE	TIME	SOURCE

```
  ----      ------      ----      ------      ----      ------
0.000E+00  0.000E+00  1.000E+38  0.000E+00
```

--- SOURCE TYPE ASSIGNED TO ELEMENT ---

MP	STYP	MP	STYP	MP	STYP	MP	STYP	MP	STYP
1	1	2	1	3	1	4	1	5	1
6	1	7	1	8	1	9	1	10	1
11	1	12	1	13	1	14	1	15	1
16	1	17	1	18	1	19	1	20	1
21	1	22	1	23	1	24	1	25	1

*** CONTAINER/PACKAGE AND WASTE TYPE INFORMATION ***

TYPE	THICKNESS	PARAM_N	PARAM_K	AREA	ASCALE	PITS	GRATE	CLAY
SPH	AERA_IND							
1	1.270E-01	3.900E-01	7.400E-02	2.100E+04	2.000E-01	5.000E+03	2.000E-10	
1.500E-01	6.000E+00	2						

GLOBAL ELEMENT NUMBER AND CONTAINER/PACKAGE TYPE SOURCE

I	ELEMENT NO.	TYPE
1	299	1
2	302	1
3	305	1
4	333	1
5	336	1
6	339	1

TYPE	COMP	SURF_FRACT	PORE_FRACT	BULK FRACT	EFFECT_D	DISOL_FRACT_REL_RATE
1	1	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11
1	2	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11
1	3	1.000E-04	0.000E+00	9.999E-01	1.000E-08	2.000E-07
1	4	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11
1	5	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11
1	6	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11
1	7	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11
1	8	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11
1	9	0.000E+00	0.000E+00	0.000E+00	1.000E-08	1.000E-11

TYPE	COMP	VOL_WF	VOL_RATIO	KD(0)	KD(INF)	KD-DECAY	PORE_LEN
1	1	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	2	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	3	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	4	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	5	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	6	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	7	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	8	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01
1	9	1.000E+06	1.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E+01

GLOBAL ELEM. NO. AND WASTE SOURCE(URANIUM)

I	ELEMENT_NO.	WF_TYPE	SURF_MASS	PORE_MASS	BULK_MASS	TOTAL_MASS
1	299	1	1.000E-04	0.000E+00	9.999E-01	1.000E+00
2	302	1	1.000E-04	0.000E+00	9.999E-01	1.000E+00
3	305	1	1.000E-04	0.000E+00	9.999E-01	1.000E+00
4	333	1	1.000E-04	0.000E+00	9.999E-01	1.000E+00
5	336	1	1.000E-04	0.000E+00	9.999E-01	1.000E+00
6	339	1	1.000E-04	0.000E+00	9.999E-01	1.000E+00

INITIAL DARCY VELOCITY (L/T)

NODE	VX	VZ	NODE	VX	VZ
1	-4.491E-11	-7.581E-08	2	-5.324E-11	-7.603E-08
3	-5.967E-11	-7.629E-08	4	-6.261E-11	-7.657E-08
5	-6.311E-11	-7.669E-08	6	-6.243E-11	-7.682E-08
7	-6.099E-11	-7.694E-08	8	-5.867E-11	-7.706E-08
9	-5.552E-11	-7.717E-08	10	-5.157E-11	-7.727E-08
11	-4.687E-11	-7.737E-08	12	-4.149E-11	-7.746E-08
13	-3.551E-11	-7.754E-08	14	-2.904E-11	-7.760E-08
15	-2.209E-11	-7.765E-08	16	-1.509E-11	-7.769E-08
17	-6.934E-12	-7.771E-08	18	-2.178E-12	-7.772E-08
19	-2.738E-11	-1.787E-08	20	-3.244E-11	-1.792E-08
21	-3.633E-11	-1.798E-08	22	-3.811E-11	-1.805E-08
23	-3.841E-11	-1.808E-08	24	-3.799E-11	-1.811E-08
25	-3.711E-11	-1.814E-08	26	-3.570E-11	-1.817E-08
27	-3.378E-11	-1.819E-08	28	-3.138E-11	-1.822E-08
29	-2.852E-11	-1.824E-08	30	-2.525E-11	-1.826E-08
31	-2.161E-11	-1.828E-08	32	-1.768E-11	-1.830E-08
33	-1.345E-11	-1.831E-08	34	-9.183E-12	-1.832E-08
35	-4.221E-12	-1.832E-08	36	-1.326E-12	-1.833E-08
37	-1.430E-10	-4.631E-08	38	-1.711E-10	-4.645E-08
39	-1.931E-10	-4.662E-08	40	-2.035E-10	-4.680E-08
41	-2.057E-10	-4.688E-08	42	-2.036E-10	-4.696E-08
43	-1.991E-10	-4.704E-08	44	-1.917E-10	-4.712E-08
45	-1.814E-10	-4.719E-08	46	-1.685E-10	-4.726E-08
47	-1.531E-10	-4.732E-08	48	-1.355E-10	-4.738E-08
49	-1.159E-10	-4.743E-08	50	-9.478E-11	-4.747E-08
51	-7.208E-11	-4.751E-08	52	-4.921E-11	-4.753E-08
53	-2.261E-11	-4.755E-08	54	-7.100E-12	-4.755E-08
55	-2.215E-10	-3.733E-08	56	-2.691E-10	-3.745E-08
57	-3.077E-10	-3.759E-08	58	-3.266E-10	-3.775E-08
59	-3.314E-10	-3.783E-08	60	-3.287E-10	-3.790E-08
61	-3.219E-10	-3.798E-08	62	-3.100E-10	-3.805E-08
63	-2.935E-10	-3.812E-08	64	-2.726E-10	-3.819E-08
65	-2.475E-10	-3.825E-08	66	-2.189E-10	-3.830E-08
67	-1.871E-10	-3.835E-08	68	-1.528E-10	-3.839E-08
69	-1.161E-10	-3.842E-08	70	-7.920E-11	-3.844E-08
71	-3.638E-11	-3.845E-08	72	-1.142E-11	-3.846E-08
73	-3.369E-10	-4.058E-08	74	-4.204E-10	-4.071E-08
75	-4.913E-10	-4.089E-08	76	-5.278E-10	-4.110E-08
77	-5.392E-10	-4.119E-08	78	-5.361E-10	-4.129E-08
79	-5.260E-10	-4.139E-08	80	-5.070E-10	-4.148E-08

81	-4.798E-10	-4.157E-08	82	-4.450E-10	-4.166E-08
83	-4.033E-10	-4.173E-08	84	-3.558E-10	-4.180E-08
85	-3.034E-10	-4.186E-08	86	-2.472E-10	-4.191E-08
87	-1.874E-10	-4.195E-08	88	-1.276E-10	-4.198E-08
89	-5.857E-11	-4.199E-08	90	-1.838E-11	-4.200E-08
91	-4.611E-10	-3.956E-08	92	-5.992E-10	-3.970E-08
93	-7.239E-10	-3.990E-08	94	-7.918E-10	-4.015E-08
95	-8.166E-10	-4.028E-08	96	-8.142E-10	-4.040E-08
97	-8.004E-10	-4.053E-08	98	-7.710E-10	-4.065E-08
99	-7.282E-10	-4.077E-08	100	-6.730E-10	-4.087E-08

INITIAL DARCY VELOCITY (L/T)

NODE	VX	VZ	NODE	VX	VZ
101	-6.072E-10	-4.097E-08	102	-5.329E-10	-4.105E-08
103	-4.518E-10	-4.112E-08	104	-3.662E-10	-4.118E-08
105	-2.764E-10	-4.123E-08	106	-1.875E-10	-4.126E-08
107	-8.587E-11	-4.128E-08	108	-2.691E-11	-4.128E-08
109	-5.707E-10	-3.961E-08	110	-7.915E-10	-3.975E-08
111	-1.008E-09	-3.999E-08	112	-1.135E-09	-4.032E-08
113	-1.187E-09	-4.049E-08	114	-1.187E-09	-4.066E-08
115	-1.169E-09	-4.084E-08	116	-1.123E-09	-4.100E-08
117	-1.053E-09	-4.116E-08	118	-9.649E-10	-4.130E-08
119	-8.611E-10	-4.143E-08	120	-7.466E-10	-4.153E-08
121	-6.255E-10	-4.162E-08	122	-5.012E-10	-4.168E-08
123	-3.746E-10	-4.173E-08	124	-2.522E-10	-4.177E-08
125	-1.150E-10	-4.179E-08	126	-3.594E-11	-4.179E-08
127	-6.379E-10	-3.923E-08	128	-9.856E-10	-3.931E-08
129	-1.374E-09	-3.957E-08	130	-1.621E-09	-4.005E-08
131	-1.735E-09	-4.032E-08	132	-1.743E-09	-4.061E-08
133	-1.713E-09	-4.091E-08	134	-1.630E-09	-4.118E-08
135	-1.507E-09	-4.142E-08	136	-1.352E-09	-4.162E-08
137	-1.177E-09	-4.177E-08	138	-9.942E-10	-4.189E-08
139	-8.118E-10	-4.197E-08	140	-6.355E-10	-4.202E-08
141	-4.660E-10	-4.206E-08	142	-3.092E-10	-4.208E-08
143	-1.398E-10	-4.209E-08	144	-4.348E-11	-4.209E-08
145	-5.904E-10	-3.895E-08	146	-1.107E-09	-3.892E-08
147	-1.829E-09	-3.915E-08	148	-2.365E-09	-3.979E-08
149	-2.658E-09	-4.019E-08	150	-2.690E-09	-4.064E-08
151	-2.630E-09	-4.109E-08	152	-2.436E-09	-4.150E-08
153	-2.156E-09	-4.183E-08	154	-1.835E-09	-4.208E-08
155	-1.510E-09	-4.224E-08	156	-1.207E-09	-4.234E-08
157	-9.371E-10	-4.239E-08	158	-7.027E-10	-4.241E-08
159	-4.980E-10	-4.242E-08	160	-3.223E-10	-4.241E-08
161	-1.436E-10	-4.241E-08	162	-4.431E-11	-4.241E-08
163	-5.135E-10	-3.865E-08	164	-1.094E-09	-3.847E-08
165	-2.021E-09	-3.858E-08	166	-2.775E-09	-3.935E-08
167	-3.231E-09	-3.995E-08	168	-3.292E-09	-4.064E-08
169	-3.177E-09	-4.136E-08	170	-2.873E-09	-4.193E-08
171	-2.480E-09	-4.238E-08	172	-2.031E-09	-4.264E-08
173	-1.610E-09	-4.277E-08	174	-1.241E-09	-4.280E-08
175	-9.349E-10	-4.279E-08	176	-6.839E-10	-4.275E-08
177	-4.754E-10	-4.270E-08	178	-3.034E-10	-4.267E-08
179	-1.342E-10	-4.264E-08	180	-4.120E-11	-4.263E-08

181	-3.900E-10	-3.848E-08	182	-1.014E-09	-3.816E-08
183	-2.191E-09	-3.810E-08	184	-3.267E-09	-3.892E-08
185	-4.016E-09	-3.968E-08	186	-4.103E-09	-4.067E-08
187	-4.016E-09	-4.154E-08	188	-3.552E-09	-4.245E-08
189	-2.846E-09	-4.289E-08	190	-2.202E-09	-4.313E-08
191	-1.641E-09	-4.317E-08	192	-1.203E-09	-4.312E-08
193	-8.681E-10	-4.303E-08	194	-6.133E-10	-4.294E-08
195	-4.148E-10	-4.286E-08	196	-2.594E-10	-4.280E-08
197	-1.134E-10	-4.276E-08	198	-3.460E-11	-4.274E-08
199	-2.121E-10	-3.829E-08	200	-8.326E-10	-3.777E-08

INITIAL DARCY VELOCITY (L/T)

NODE	VX	VZ	NODE	VX	VZ
201	-2.284E-09	-3.741E-08	202	-3.836E-09	-3.811E-08
203	-5.118E-09	-3.919E-08	204	-5.408E-09	-4.055E-08
205	-4.859E-09	-4.237E-08	206	-3.919E-09	-4.302E-08
207	-3.134E-09	-4.379E-08	208	-2.211E-09	-4.383E-08
209	-1.558E-09	-4.371E-08	210	-1.088E-09	-4.352E-08
211	-7.562E-10	-4.333E-08	212	-5.177E-10	-4.316E-08
213	-3.416E-10	-4.303E-08	214	-2.097E-10	-4.293E-08
215	-9.067E-11	-4.288E-08	216	-2.749E-11	-4.286E-08
217	2.591E-11	-3.813E-08	218	-5.216E-10	-3.739E-08
219	-2.194E-09	-3.659E-08	220	-4.390E-09	-3.675E-08
221	-6.848E-09	-3.811E-08	222	-7.178E-09	-4.076E-08
223	-7.628E-09	-4.227E-08	224	-6.184E-09	-4.552E-08
225	-3.405E-09	-4.505E-08	226	-2.086E-09	-4.478E-08
227	-1.232E-09	-4.428E-08	228	-7.388E-10	-4.390E-08
229	-4.314E-10	-4.358E-08	230	-2.460E-10	-4.333E-08
231	-1.342E-10	-4.314E-08	232	-6.880E-11	-4.302E-08
233	-2.624E-11	-4.294E-08	234	-7.328E-12	-4.292E-08
235	3.219E-10	-3.800E-08	236	-5.340E-11	-3.704E-08
237	-1.819E-09	-3.562E-08	238	-4.473E-09	-3.469E-08
239	-9.163E-09	-3.490E-08	240	-1.216E-08	-3.977E-08
241	-7.084E-09	-4.833E-08	242	-1.871E-09	-4.590E-08
243	-1.813E-09	-4.678E-08	244	-9.899E-10	-4.528E-08
245	-8.107E-10	-4.473E-08	246	-5.949E-10	-4.415E-08
247	-4.567E-10	-4.376E-08	248	-3.373E-10	-4.345E-08
249	-2.384E-10	-4.323E-08	250	-1.539E-10	-4.308E-08
251	-6.862E-11	-4.299E-08	252	-2.116E-11	-4.297E-08
253	6.805E-10	-3.797E-08	254	5.201E-10	-3.681E-08
255	-8.709E-10	-3.496E-08	256	-4.144E-09	-3.180E-08
257	-7.721E-09	-3.251E-08	258	-2.197E-08	-2.551E-08
259	-3.077E-08	-5.791E-08	260	-1.393E-08	-5.898E-08
261	-3.265E-09	-4.717E-08	262	-1.469E-09	-4.717E-08
263	4.211E-10	-4.524E-08	264	1.020E-09	-4.451E-08
265	1.265E-09	-4.385E-08	266	1.203E-09	-4.344E-08
267	9.912E-10	-4.315E-08	268	7.043E-10	-4.296E-08
269	3.296E-10	-4.286E-08	270	1.044E-10	-4.282E-08
271	1.025E-09	-3.803E-08	272	1.214E-09	-3.678E-08
273	5.146E-10	-3.465E-08	274	-1.493E-09	-2.921E-08
275	-5.648E-09	-2.981E-08	276	-1.292E-08	-1.132E-08
277	-1.383E-08	-4.950E-08	278	-1.044E-08	-7.620E-08
279	-6.386E-09	-5.178E-08	280	2.588E-11	-5.049E-08

281	1.990E-09	-4.659E-08	282	3.108E-09	-4.505E-08
283	3.227E-09	-4.384E-08	284	2.915E-09	-4.314E-08
285	2.322E-09	-4.269E-08	286	1.622E-09	-4.242E-08
287	7.522E-10	-4.228E-08	288	2.372E-10	-4.223E-08
289	1.364E-09	-3.818E-08	290	1.827E-09	-3.705E-08
291	2.242E-09	-3.483E-08	292	1.675E-09	-2.849E-08
293	1.624E-10	-2.667E-08	294	-5.663E-09	-8.689E-09
295	4.910E-10	-4.410E-08	296	7.210E-09	-7.993E-08
297	3.199E-09	-5.706E-08	298	4.439E-09	-5.295E-08
299	4.724E-09	-4.772E-08	300	4.543E-09	-4.524E-08

INITIAL DARCY VELOCITY (L/T)

NODE	VX	VZ	NODE	VX	VZ
301	3.998E-09	-4.354E-08	302	3.283E-09	-4.257E-08
303	2.480E-09	-4.198E-08	304	1.677E-09	-4.165E-08
305	7.655E-10	-4.148E-08	306	2.393E-10	-4.143E-08
307	1.663E-09	-3.838E-08	308	2.314E-09	-3.746E-08
309	3.867E-09	-3.563E-08	310	5.267E-09	-2.930E-08
311	6.430E-09	-2.658E-08	312	2.522E-09	-6.935E-09
313	8.584E-09	-4.385E-08	314	1.543E-08	-7.940E-08
315	1.161E-08	-5.765E-08	316	1.016E-08	-5.328E-08
317	8.329E-09	-4.737E-08	318	6.842E-09	-4.455E-08
319	5.430E-09	-4.269E-08	320	4.171E-09	-4.167E-08
321	3.016E-09	-4.108E-08	322	1.984E-09	-4.077E-08
323	8.926E-10	-4.062E-08	324	2.769E-10	-4.057E-08
325	1.913E-09	-3.864E-08	326	2.621E-09	-3.796E-08
327	5.004E-09	-3.688E-08	328	8.463E-09	-3.228E-08
329	1.339E-08	-2.891E-08	330	1.077E-08	-7.120E-09
331	2.036E-08	-4.512E-08	332	2.830E-08	-7.923E-08
333	2.094E-08	-5.549E-08	334	1.686E-08	-5.107E-08
335	1.239E-08	-4.529E-08	336	9.223E-09	-4.279E-08
337	6.792E-09	-4.118E-08	338	4.932E-09	-4.038E-08
339	3.427E-09	-3.995E-08	340	2.194E-09	-3.975E-08
341	9.733E-10	-3.966E-08	342	2.996E-10	-3.963E-08
343	2.085E-09	-3.893E-08	344	2.816E-09	-3.850E-08
345	5.233E-09	-3.820E-08	346	1.013E-08	-3.705E-08
347	1.978E-08	-3.584E-08	348	2.287E-08	-1.008E-08
349	2.962E-08	-4.302E-08	350	3.662E-08	-8.102E-08
351	3.091E-08	-5.008E-08	352	2.194E-08	-4.584E-08
353	1.529E-08	-4.147E-08	354	1.076E-08	-3.993E-08
355	7.575E-09	-3.907E-08	356	5.300E-09	-3.875E-08
357	3.582E-09	-3.864E-08	358	2.249E-09	-3.864E-08
359	9.871E-10	-3.866E-08	360	3.021E-10	-3.867E-08
361	2.207E-09	-3.925E-08	362	2.837E-09	-3.895E-08
363	5.015E-09	-3.945E-08	364	7.807E-09	-4.107E-08
365	2.311E-08	-5.014E-08	366	3.383E-08	-2.083E-08
367	7.149E-08	-6.498E-08	368	8.499E-08	-7.233E-08
369	4.666E-08	-3.270E-08	370	2.956E-08	-3.789E-08
371	1.926E-08	-3.522E-08	372	1.278E-08	-3.605E-08
373	8.617E-09	-3.633E-08	374	5.814E-09	-3.682E-08
375	3.827E-09	-3.719E-08	376	2.360E-09	-3.747E-08
377	1.026E-09	-3.764E-08	378	3.119E-10	-3.770E-08
379	2.196E-09	-3.958E-08	380	3.070E-09	-3.945E-08

381	3.516E-09	-3.992E-08	382	6.593E-09	-4.368E-08
383	2.308E-09	-5.257E-08	384	4.913E-08	-6.802E-08
385	1.162E-07	-8.793E-08	386	7.161E-08	-1.037E-08
387	2.174E-08	-2.516E-08	388	1.964E-08	-2.649E-08
389	1.100E-08	-3.015E-08	390	7.852E-09	-3.226E-08
391	5.183E-09	-3.397E-08	392	3.549E-09	-3.515E-08
393	2.331E-09	-3.599E-08	394	1.441E-09	-3.653E-08
395	6.261E-10	-3.683E-08	396	1.919E-10	-3.693E-08
397	2.210E-09	-3.978E-08	398	2.992E-09	-3.989E-08
399	3.207E-09	-3.960E-08	400	1.894E-09	-4.528E-08

INITIAL DARCY VELOCITY (L/T)

NODE	VX	VZ	NODE	VX	VZ
401	-2.431E-09	-4.248E-08	402	-8.024E-09	-1.100E-07
403	-5.461E-08	-1.016E-07	404	-6.203E-08	1.757E-08
405	-2.852E-08	-2.901E-08	406	-2.366E-08	-2.391E-08
407	-1.561E-08	-3.026E-08	408	-1.142E-08	-3.209E-08
409	-8.034E-09	-3.407E-08	410	-5.655E-09	-3.527E-08
411	-3.803E-09	-3.614E-08	412	-2.375E-09	-3.668E-08
413	-1.036E-09	-3.698E-08	414	-3.190E-10	-3.709E-08
415	2.210E-09	-3.999E-08	416	3.053E-09	-4.003E-08
417	3.035E-09	-3.989E-08	418	6.432E-10	-4.218E-08
419	-5.517E-09	-4.135E-08	420	-3.699E-08	-7.389E-08
421	-8.856E-08	-6.240E-08	422	-9.243E-08	-1.966E-08
423	-6.271E-08	-3.566E-08	424	-4.473E-08	-3.384E-08
425	-3.200E-08	-3.609E-08	426	-2.278E-08	-3.680E-08
427	-1.615E-08	-3.754E-08	428	-1.123E-08	-3.800E-08
429	-7.478E-09	-3.831E-08	430	-4.592E-09	-3.849E-08
431	-1.961E-09	-3.857E-08	432	-5.857E-10	-3.861E-08
433	2.231E-09	-4.002E-08	434	3.000E-09	-4.006E-08
435	3.171E-09	-3.996E-08	436	-4.846E-10	-4.139E-08
437	-4.990E-09	-3.979E-08	438	-5.373E-08	-5.935E-08
439	-1.113E-07	-4.972E-08	440	-8.607E-08	-3.439E-08
441	-5.008E-08	-4.241E-08	442	-3.909E-08	-3.960E-08
443	-2.679E-08	-4.029E-08	444	-1.942E-08	-3.999E-08
445	-1.368E-08	-3.999E-08	446	-9.543E-09	-3.992E-08
447	-6.342E-09	-3.986E-08	448	-3.865E-09	-3.980E-08
449	-1.621E-09	-3.972E-08	450	-4.648E-10	-3.970E-08

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
1	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
2	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
3	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
4	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
5	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
6	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
7	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
8	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
9	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01
10	2.7204E-01	2.7204E-01	1.6563E-01	1.6563E-01

11	2.7204E-01	2.7204E-01	1.6564E-01	1.6563E-01
12	2.7204E-01	2.7204E-01	1.6564E-01	1.6564E-01
13	2.7204E-01	2.7204E-01	1.6564E-01	1.6564E-01
14	2.7204E-01	2.7204E-01	1.6564E-01	1.6564E-01
15	2.7204E-01	2.7204E-01	1.6564E-01	1.6564E-01
16	2.7204E-01	2.7204E-01	1.6564E-01	1.6564E-01
17	2.7204E-01	2.7204E-01	1.6564E-01	1.6564E-01
18	1.5225E-01	1.5225E-01	1.3715E-01	1.3715E-01
19	1.5225E-01	1.5225E-01	1.3716E-01	1.3715E-01
20	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
21	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
22	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
23	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
24	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
25	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
26	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
27	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
28	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
29	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
30	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
31	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
32	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
33	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
34	1.5225E-01	1.5225E-01	1.3716E-01	1.3716E-01
35	1.2611E-01	1.2611E-01	1.1102E-01	1.1102E-01
36	1.2611E-01	1.2611E-01	1.1102E-01	1.1102E-01
37	1.2611E-01	1.2611E-01	1.1102E-01	1.1102E-01
38	1.2611E-01	1.2611E-01	1.1102E-01	1.1102E-01
39	1.2611E-01	1.2611E-01	1.1103E-01	1.1102E-01
40	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
41	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
42	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
43	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
44	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
45	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
46	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
47	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
48	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
49	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
50	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
51	1.2611E-01	1.2611E-01	1.1103E-01	1.1103E-01
52	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
53	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
54	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
55	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
56	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
57	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
58	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
59	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
60	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

61	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
62	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
63	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
64	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
65	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
66	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
67	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
68	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
69	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
70	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
71	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
72	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
73	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
74	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
75	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
76	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
77	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
78	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
79	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
80	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
81	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
82	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
83	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
84	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
85	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
86	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
87	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
88	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
89	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
90	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
91	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
92	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
93	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
94	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
95	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
96	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
97	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
98	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
99	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
100	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
101	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
102	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
103	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
104	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
105	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
106	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
107	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
108	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
109	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
110	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

111	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
112	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
113	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
114	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
115	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
116	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
117	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
118	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
119	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
120	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
121	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
122	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
123	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
124	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
125	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
126	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
127	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
128	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
129	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
130	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
131	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
132	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
133	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
134	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
135	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
136	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
137	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
138	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
139	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
140	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
141	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
142	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
143	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
144	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
145	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
146	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
147	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
148	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
149	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
150	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
151	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
152	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
153	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
154	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
155	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
156	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
157	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
158	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
159	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
160	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

161	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
162	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
163	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
164	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
165	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
166	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
167	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
168	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
169	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
170	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
171	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
172	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
173	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
174	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
175	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
176	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
177	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
178	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
179	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
180	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
181	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
182	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
183	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
184	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
185	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
186	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
187	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
188	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
189	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
190	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
191	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
192	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
193	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
194	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
195	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
196	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
197	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
198	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
199	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
200	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
201	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
202	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
203	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
204	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
205	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
206	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
207	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
208	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
209	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
210	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

211	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
212	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
213	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
214	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
215	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
216	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
217	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
218	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
219	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
220	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
221	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
222	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
223	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
224	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
225	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
226	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
227	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
228	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
229	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
230	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
231	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
232	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
233	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
234	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
235	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
236	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
237	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
238	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
239	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
240	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
241	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
242	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
243	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
244	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
245	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
246	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
247	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
248	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
249	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
250	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
251	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
252	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
253	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
254	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
255	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
256	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
257	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
258	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
259	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
260	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

261	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
262	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
263	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
264	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
265	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
266	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
267	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
268	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
269	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
270	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
271	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
272	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
273	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
274	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
275	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
276	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
277	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
278	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
279	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
280	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
281	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
282	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
283	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
284	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
285	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
286	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
287	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
288	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
289	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
290	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
291	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
292	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
293	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
294	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
295	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
296	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
297	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
298	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
299	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
300	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
301	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
302	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
303	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
304	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
305	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
306	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
307	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
308	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
309	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
310	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

311	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
312	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
313	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
314	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
315	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
316	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
317	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
318	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
319	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
320	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
321	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
322	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
323	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
324	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
325	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
326	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
327	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
328	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
329	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
330	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
331	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
332	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
333	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
334	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
335	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
336	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
337	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
338	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
339	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
340	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
341	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
342	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
343	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
344	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
345	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
346	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
347	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
348	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
349	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
350	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
351	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
352	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
353	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
354	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
355	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
356	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
357	1.2000E-01	1.2000E-01	1.2000E-01	1.2000E-01
358	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
359	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
360	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

361	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
362	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
363	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
364	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
365	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
366	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
367	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
368	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
369	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
370	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
371	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
372	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
373	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
374	2.0000E-01	2.0000E-01	2.0000E-01	2.0000E-01
375	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
376	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
377	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
378	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
379	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
380	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
381	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
382	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
383	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
384	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
385	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
386	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
387	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
388	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
389	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
390	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
391	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
392	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
393	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
394	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
395	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
396	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
397	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
398	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
399	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
400	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

INITIAL MOISTURE CONTENT (L**3/L**3)

ELEMENT	MC PT. 1	MC PT. 2	MC PT. 3	MC PT. 4
401	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
402	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
403	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
404	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
405	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
406	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
407	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
408	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01

OUTPUT TABLE 11.. MASS FLOW AT TIME = 6.0000E+01
(DELT = 5.0000E-01), ITIM = 120, ITER = 1

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 1

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-6.88E-10	-4.05E-10	-1.56E-26	-1.21E-10	-4.45E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-4.85E-10	-2.02E-12	-3.07E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 1

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.09E-02	-6.38E-03	-2.46E-19	-1.91E-03	-7.01E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-7.66E-03	-3.19E-05	-4.85E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 1

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.30E+00	-7.66E-01	-2.95E-17	-2.30E-01	-8.42E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-9.19E-01	-3.83E-03	-5.82E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 2

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.38E-09	-8.10E-10	-3.12E-26	-2.43E-10	-8.91E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-9.73E-10	-4.05E-12	-6.16E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 2

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-2.17E-02	-1.28E-02	-4.93E-19	-3.84E-03	-1.41E-02	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.53E-02	-6.39E-05	-9.72E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 2

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-2.61E+00	-1.53E+00	-5.91E-17	-4.60E-01	-1.69E+00	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.84E+00	-7.67E-03	-1.17E-02			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 3

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.38E-09	-8.13E-10	-3.13E-26	-2.44E-10	-8.93E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-9.75E-10	-4.06E-12	-6.18E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 3

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-2.18E-02	-1.28E-02	-4.94E-19	-3.85E-03	-1.41E-02	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.54E-02	-6.41E-05	-9.75E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 3

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-2.62E+00	-1.54E+00	-5.93E-17	-4.62E-01	-1.69E+00	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.85E+00	-7.69E-03	-1.17E-02			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 4

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.09E-09	-6.43E-10	-2.48E-26	-1.93E-10	-7.07E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-7.72E-10	-3.22E-12	-4.89E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 4

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.73E-02	-1.01E-02	-3.91E-19	-3.04E-03	-1.12E-02	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.22E-02	-5.07E-05	-7.71E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 4

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-2.07E+00	-1.22E+00	-4.69E-17	-3.65E-01	-1.34E+00	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.46E+00	-6.09E-03	-9.25E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 5

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-8.27E-10	-4.86E-10	-1.87E-26	-1.46E-10	-5.34E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.83E-10	-2.43E-12	-3.70E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 5

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.30E-02	-7.67E-03	-2.96E-19	-2.30E-03	-8.43E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-9.21E-03	-3.84E-05	-5.83E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 5

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.57E+00	-9.21E-01	-3.55E-17	-2.76E-01	-1.01E+00	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-1.10E+00	-4.60E-03	-7.00E-03

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 6

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-9.92E-10	-5.83E-10	-2.25E-26	-1.75E-10	-6.41E-10	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-7.00E-10	-2.92E-12	-4.43E-12

FLOW (M/L) AT LOCAL BOUNDARY NODE 6

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.56E-02	-9.20E-03	-3.55E-19	-2.76E-03	-1.01E-02	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-1.10E-02	-4.60E-05	-6.99E-05

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 6

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.88E+00	-1.10E+00	-4.26E-17	-3.31E-01	-1.21E+00	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-1.33E+00	-5.52E-03	-8.39E-03

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 7

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-8.29E-10	-4.88E-10	-1.88E-26	-1.46E-10	-5.36E-10	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-5.85E-10	-2.44E-12	-3.71E-12

FLOW (M/L) AT LOCAL BOUNDARY NODE 7

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.31E-02	-7.70E-03	-2.97E-19	-2.31E-03	-8.46E-03	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-9.24E-03	-3.85E-05	-5.85E-05

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 7

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.57E+00	-9.24E-01	-3.56E-17	-2.77E-01	-1.01E+00	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-1.11E+00	-4.62E-03	-7.02E-03

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 8

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-6.41E-10	-3.77E-10	-1.45E-26	-1.13E-10	-4.15E-10	0.00E+00

MAGNESIUM	PHOSPHATE	ZINC
-4.53E-10	-1.89E-12	-2.87E-12

FLOW (M/L) AT LOCAL BOUNDARY NODE 8

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.01E-02	-5.95E-03	-2.29E-19	-1.79E-03	-6.54E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-7.14E-03	-2.98E-05	-4.52E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 8

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.21E+00	-7.14E-01	-2.75E-17	-2.14E-01	-7.85E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.57E-01	-3.57E-03	-5.43E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 9

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.23E-10	-4.25E-10	-1.64E-26	-1.28E-10	-4.67E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.10E-10	-2.13E-12	-3.23E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 9

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.14E-02	-6.71E-03	-2.59E-19	-2.01E-03	-7.37E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.05E-03	-3.36E-05	-5.10E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 9

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.37E+00	-8.05E-01	-3.10E-17	-2.42E-01	-8.85E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-9.66E-01	-4.03E-03	-6.12E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 10

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.34E-10	-4.31E-10	-1.66E-26	-1.29E-10	-4.74E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.18E-10	-2.16E-12	-3.28E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 10

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.16E-02	-6.81E-03	-2.62E-19	-2.04E-03	-7.48E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.17E-03	-3.40E-05	-5.17E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 10

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.39E+00	-8.17E-01	-3.15E-17	-2.45E-01	-8.98E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			

-9.80E-01 -4.09E-03 -6.21E-03

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 11

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.46E-10	-4.39E-10	-1.69E-26	-1.32E-10	-4.82E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.27E-10	-2.19E-12	-3.34E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 11

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.18E-02	-6.93E-03	-2.67E-19	-2.08E-03	-7.61E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.31E-03	-3.46E-05	-5.26E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 11

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.41E+00	-8.31E-01	-3.20E-17	-2.49E-01	-9.13E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-9.97E-01	-4.16E-03	-6.32E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 12

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.54E-10	-4.44E-10	-1.71E-26	-1.33E-10	-4.87E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.32E-10	-2.22E-12	-3.37E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 12

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.19E-02	-7.00E-03	-2.70E-19	-2.10E-03	-7.69E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.40E-03	-3.50E-05	-5.32E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 12

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.43E+00	-8.40E-01	-3.24E-17	-2.52E-01	-9.23E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.01E+00	-4.20E-03	-6.38E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 13

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.60E-10	-4.47E-10	-1.72E-26	-1.34E-10	-4.91E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.36E-10	-2.23E-12	-3.40E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 13

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.20E-02	-7.05E-03	-2.72E-19	-2.12E-03	-7.75E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.46E-03	-3.53E-05	-5.36E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 13

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.44E+00	-8.46E-01	-3.26E-17	-2.54E-01	-9.30E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.02E+00	-4.23E-03	-6.43E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 14

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.64E-10	-4.49E-10	-1.73E-26	-1.35E-10	-4.94E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.39E-10	-2.25E-12	-3.41E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 14

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.21E-02	-7.09E-03	-2.73E-19	-2.13E-03	-7.79E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.51E-03	-3.54E-05	-5.39E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 14

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.45E+00	-8.51E-01	-3.28E-17	-2.55E-01	-9.35E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.02E+00	-4.25E-03	-6.47E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 15

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.67E-10	-4.51E-10	-1.74E-26	-1.35E-10	-4.96E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.41E-10	-2.25E-12	-3.43E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 15

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.21E-02	-7.12E-03	-2.74E-19	-2.13E-03	-7.82E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.54E-03	-3.56E-05	-5.41E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 15

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.45E+00	-8.54E-01	-3.29E-17	-2.56E-01	-9.38E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			

-1.02E+00 -4.27E-03 -6.49E-03

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 16

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.68E-10	-4.52E-10	-1.74E-26	-1.36E-10	-4.97E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.42E-10	-2.26E-12	-3.44E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 16

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.21E-02	-7.13E-03	-2.75E-19	-2.14E-03	-7.84E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.56E-03	-3.57E-05	-5.42E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 16

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.46E+00	-8.56E-01	-3.30E-17	-2.57E-01	-9.41E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.03E+00	-4.28E-03	-6.50E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 17

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.70E-10	-4.53E-10	-1.74E-26	-1.36E-10	-4.98E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.43E-10	-2.26E-12	-3.44E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 17

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.21E-02	-7.14E-03	-2.75E-19	-2.14E-03	-7.85E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-8.57E-03	-3.57E-05	-5.43E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 17

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-1.46E+00	-8.57E-01	-3.30E-17	-2.57E-01	-9.42E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-1.03E+00	-4.29E-03	-6.52E-03			

FLOW RATE (M/T/L) AT LOCAL BOUNDARY NODE 18

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-3.85E-10	-2.27E-10	-8.73E-27	-6.80E-11	-2.49E-10	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-2.72E-10	-1.13E-12	-1.72E-12			

FLOW (M/L) AT LOCAL BOUNDARY NODE 18

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-6.08E-03	-3.58E-03	-1.38E-19	-1.07E-03	-3.93E-03	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-4.29E-03	-1.79E-05	-2.72E-05			

TOTAL FLOW (M/L) AT LOCAL BOUNDARY NODE 18

CALCIUM	CARBONATE	URANIUM	SULFATE	HYDROGEN	SOH
-7.29E-01	-4.29E-01	-1.65E-17	-1.29E-01	-4.71E-01	0.00E+00
MAGNESIUM	PHOSPHATE	ZINC			
-5.15E-01	-2.15E-03	-3.26E-03			

URANIUM CHEMICAL = 3

CONTAINER BREACH

ELEMENT	CONTAINER TYPE	TIME BREACH	BREACHED AREA	CONTAINER AREA	RATIO
299	1	5.00E-01	2.10E+04	2.10E+04	1.00E+00
302	1	5.00E-01	2.10E+04	2.10E+04	1.00E+00
305	1	5.00E-01	2.10E+04	2.10E+04	1.00E+00
333	1	5.00E-01	2.10E+04	2.10E+04	1.00E+00
336	1	5.00E-01	2.10E+04	2.10E+04	1.00E+00
339	1	5.00E-01	2.10E+04	2.10E+04	1.00E+00

SOURCE TERM TO THE TRANSPORT CALCULATION --- IN MOLE/LITER-S

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL REL RATE	RINSE REL RATE	DIFFUSION REL RATE	DISSOLUTION REL RATE
299	1	1	5.96E-16	0.00E+00	0.00E+00	5.96E-16
302	1	1	5.96E-16	0.00E+00	0.00E+00	5.96E-16
305	1	1	5.96E-16	0.00E+00	0.00E+00	5.96E-16
333	1	1	5.77E-16	0.00E+00	0.00E+00	5.77E-16
336	1	1	5.77E-16	0.00E+00	0.00E+00	5.77E-16
339	1	1	5.77E-16	0.00E+00	0.00E+00	5.77E-16

CUMULATIVE RELEASE FROM THE MIXING BATH AVAILABLE FOR TRANSPORT ---- IN MOLES

ELEMENT	CUM. REL
299	1.11E-04
302	1.11E-04

305	1.11E-04
333	1.11E-04
336	1.11E-04
339	1.11E-04

CUMULATIVE MASS RELEASED FROM THE WASTE FORM ---- IN MOLES

ELEMENT	CONTAINER TYPE	WASTE TYPE	TOTAL RELEASED	RINSE RELEASE	DIFFUSION RELEASE	DISSOLUTION RELEASE
299	1	1	1.11E-04	9.89E-05	0.00E+00	1.19E-05
302	1	1	1.11E-04	9.91E-05	0.00E+00	1.19E-05
305	1	1	1.11E-04	9.91E-05	0.00E+00	1.19E-05
333	1	1	1.11E-04	9.90E-05	0.00E+00	1.19E-05
336	1	1	1.11E-04	9.91E-05	0.00E+00	1.19E-05
339	1	1	1.11E-04	9.91E-05	0.00E+00	1.19E-05

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
1	7.3364E-19	2.8271E-19	-18.13	4.5093E-19	0.0000E+00	2.4795E-01
2	1.3230E-18	5.0980E-19	-17.88	8.1317E-19	0.0000E+00	2.4795E-01
3	3.5215E-18	1.3570E-18	-17.45	2.1646E-18	0.0000E+00	2.4796E-01
4	8.5067E-18	3.2777E-18	-17.07	5.2289E-18	0.0000E+00	2.4799E-01
5	1.7497E-17	6.7413E-18	-16.76	1.0756E-17	0.0000E+00	2.4802E-01
6	2.8778E-17	1.1087E-17	-16.54	1.7691E-17	0.0000E+00	2.4805E-01
7	4.2017E-17	1.6186E-17	-16.38	2.5832E-17	0.0000E+00	2.4809E-01
8	5.6166E-17	2.1634E-17	-16.25	3.4532E-17	0.0000E+00	2.4812E-01
9	6.9666E-17	2.6833E-17	-16.16	4.2833E-17	0.0000E+00	2.4814E-01
10	8.0880E-17	3.1150E-17	-16.09	4.9729E-17	0.0000E+00	2.4816E-01
11	8.8631E-17	3.4135E-17	-16.05	5.4496E-17	0.0000E+00	2.4817E-01
12	9.2587E-17	3.5658E-17	-16.03	5.6929E-17	0.0000E+00	2.4818E-01
13	9.3280E-17	3.5925E-17	-16.03	5.7355E-17	0.0000E+00	2.4818E-01
14	9.1811E-17	3.5359E-17	-16.04	5.6452E-17	0.0000E+00	2.4818E-01
15	8.9413E-17	3.4436E-17	-16.05	5.4977E-17	0.0000E+00	2.4818E-01
16	8.7093E-17	3.3542E-17	-16.06	5.3551E-17	0.0000E+00	2.4818E-01
17	8.5494E-17	3.2927E-17	-16.07	5.2568E-17	0.0000E+00	2.4818E-01
18	8.4932E-17	3.2710E-17	-16.07	5.2222E-17	0.0000E+00	2.4818E-01
19	3.9064E-18	1.5053E-18	-17.41	2.4011E-18	0.0000E+00	1.4487E-01
20	7.5875E-18	2.9237E-18	-17.12	4.6638E-18	0.0000E+00	1.4488E-01
21	2.1652E-17	8.3422E-18	-16.66	1.3310E-17	0.0000E+00	1.4491E-01
22	5.5378E-17	2.1332E-17	-16.26	3.4046E-17	0.0000E+00	1.4495E-01
23	1.1841E-16	4.5602E-17	-15.93	7.2813E-17	0.0000E+00	1.4502E-01
24	1.9967E-16	7.6873E-17	-15.70	1.2280E-16	0.0000E+00	1.4509E-01
25	2.9683E-16	1.1424E-16	-15.53	1.8259E-16	0.0000E+00	1.4516E-01
26	4.0215E-16	1.5473E-16	-15.40	2.4742E-16	0.0000E+00	1.4522E-01
27	5.0319E-16	1.9357E-16	-15.30	3.0962E-16	0.0000E+00	1.4528E-01
28	5.8656E-16	2.2560E-16	-15.23	3.6095E-16	0.0000E+00	1.4531E-01
29	6.4270E-16	2.4718E-16	-15.19	3.9553E-16	0.0000E+00	1.4534E-01

30	6.6917E-16	2.5734E-16	-15.17	4.1183E-16	0.0000E+00	1.4535E-01
31	6.7074E-16	2.5794E-16	-15.17	4.1279E-16	0.0000E+00	1.4535E-01
32	6.5664E-16	2.5253E-16	-15.18	4.0412E-16	0.0000E+00	1.4535E-01
33	6.3672E-16	2.4487E-16	-15.20	3.9185E-16	0.0000E+00	1.4534E-01
34	6.1849E-16	2.3786E-16	-15.21	3.8063E-16	0.0000E+00	1.4534E-01
35	6.0634E-16	2.3319E-16	-15.22	3.7315E-16	0.0000E+00	1.4534E-01
36	6.0213E-16	2.3157E-16	-15.22	3.7056E-16	0.0000E+00	1.4533E-01
37	4.0182E-17	1.5481E-17	-16.40	2.4701E-17	0.0000E+00	1.2001E-01
38	8.5219E-17	3.2827E-17	-16.07	5.2392E-17	0.0000E+00	1.2005E-01
39	2.6684E-16	1.0272E-16	-15.57	1.6412E-16	0.0000E+00	1.2018E-01
40	7.1516E-16	2.7494E-16	-15.15	4.4022E-16	0.0000E+00	1.2044E-01
41	1.6244E-15	6.2339E-16	-14.79	1.0011E-15	0.0000E+00	1.2079E-01
42	2.8226E-15	1.0810E-15	-14.55	1.7416E-15	0.0000E+00	1.2118E-01
43	4.2973E-15	1.6426E-15	-14.37	2.6547E-15	0.0000E+00	1.2157E-01
44	5.9291E-15	2.2623E-15	-14.23	3.6669E-15	0.0000E+00	1.2192E-01
45	7.5091E-15	2.8611E-15	-14.12	4.6481E-15	0.0000E+00	1.2220E-01
46	8.8058E-15	3.3518E-15	-14.06	5.4540E-15	0.0000E+00	1.2239E-01
47	9.6532E-15	3.6723E-15	-14.02	5.9809E-15	0.0000E+00	1.2250E-01
48	1.0013E-14	3.8084E-15	-14.00	6.2047E-15	0.0000E+00	1.2255E-01
49	9.9761E-15	3.7943E-15	-14.00	6.1818E-15	0.0000E+00	1.2255E-01
50	9.7064E-15	3.6921E-15	-14.01	6.0143E-15	0.0000E+00	1.2253E-01

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
51	9.3681E-15	3.5638E-15	-14.03	5.8043E-15	0.0000E+00	1.2251E-01
52	9.0763E-15	3.4532E-15	-14.04	5.6231E-15	0.0000E+00	1.2249E-01
53	8.8889E-15	3.3821E-15	-14.05	5.5068E-15	0.0000E+00	1.2247E-01
54	8.8253E-15	3.3580E-15	-14.05	5.4674E-15	0.0000E+00	1.2247E-01
55	2.3133E-16	8.9093E-17	-15.64	1.4224E-16	0.0000E+00	9.6256E-02
56	5.3830E-16	2.0718E-16	-15.27	3.3111E-16	0.0000E+00	9.6357E-02
57	1.8548E-15	7.1219E-16	-14.73	1.1426E-15	0.0000E+00	9.6732E-02
58	5.3695E-15	2.0513E-15	-14.27	3.3182E-15	0.0000E+00	9.7533E-02
59	1.2822E-14	4.8651E-15	-13.89	7.9572E-15	0.0000E+00	9.8614E-02
60	2.3026E-14	8.6703E-15	-13.64	1.4356E-14	0.0000E+00	9.9829E-02
61	3.6030E-14	1.3463E-14	-13.44	2.2567E-14	0.0000E+00	1.0107E-01
62	5.0796E-14	1.8849E-14	-13.29	3.1947E-14	0.0000E+00	1.0219E-01
63	6.5301E-14	2.4099E-14	-13.19	4.1202E-14	0.0000E+00	1.0308E-01
64	7.7209E-14	2.8390E-14	-13.11	4.8819E-14	0.0000E+00	1.0368E-01
65	8.4812E-14	3.1124E-14	-13.07	5.3688E-14	0.0000E+00	1.0400E-01
66	8.7732E-14	3.2174E-14	-13.06	5.5559E-14	0.0000E+00	1.0412E-01
67	8.6942E-14	3.1887E-14	-13.06	5.5056E-14	0.0000E+00	1.0410E-01
68	8.4129E-14	3.0868E-14	-13.08	5.3261E-14	0.0000E+00	1.0403E-01
69	8.0883E-14	2.9691E-14	-13.09	5.1192E-14	0.0000E+00	1.0396E-01
70	7.8219E-14	2.8724E-14	-13.11	4.9495E-14	0.0000E+00	1.0389E-01
71	7.6564E-14	2.8123E-14	-13.12	4.8441E-14	0.0000E+00	1.0385E-01
72	7.6012E-14	2.7923E-14	-13.12	4.8089E-14	0.0000E+00	1.0384E-01
73	1.0992E-15	4.2299E-16	-14.96	6.7617E-16	0.0000E+00	9.1345E-02
74	2.8349E-15	1.0889E-15	-14.55	1.7460E-15	0.0000E+00	9.1623E-02
75	1.0840E-14	4.1332E-15	-13.96	6.7071E-15	0.0000E+00	9.2728E-02
76	3.4524E-14	1.2943E-14	-13.46	2.1582E-14	0.0000E+00	9.5283E-02
77	8.8487E-14	3.2425E-14	-13.05	5.6063E-14	0.0000E+00	9.8800E-02

78	1.6734E-13	5.9726E-14	-12.78	1.0761E-13	0.0000E+00	1.0296E-01
79	2.7430E-13	9.5267E-14	-12.56	1.7903E-13	0.0000E+00	1.0739E-01
80	4.0195E-13	1.3617E-13	-12.40	2.6579E-13	0.0000E+00	1.1154E-01
81	5.3156E-13	1.7658E-13	-12.27	3.5498E-13	0.0000E+00	1.1487E-01
82	6.3918E-13	2.0962E-13	-12.19	4.2956E-13	0.0000E+00	1.1710E-01
83	7.0651E-13	2.3020E-13	-12.15	4.7632E-13	0.0000E+00	1.1824E-01
84	7.2949E-13	2.3723E-13	-12.14	4.9227E-13	0.0000E+00	1.1858E-01
85	7.1857E-13	2.3384E-13	-12.14	4.8473E-13	0.0000E+00	1.1845E-01
86	6.9093E-13	2.2524E-13	-12.16	4.6570E-13	0.0000E+00	1.1815E-01
87	6.6151E-13	2.1603E-13	-12.18	4.4548E-13	0.0000E+00	1.1783E-01
88	6.3859E-13	2.0884E-13	-12.19	4.2975E-13	0.0000E+00	1.1759E-01
89	6.2484E-13	2.0452E-13	-12.20	4.2032E-13	0.0000E+00	1.1744E-01
90	6.2033E-13	2.0310E-13	-12.21	4.1723E-13	0.0000E+00	1.1739E-01
91	4.2198E-15	1.6220E-15	-14.37	2.5978E-15	0.0000E+00	9.1520E-02
92	1.2266E-14	4.6939E-15	-13.91	7.5724E-15	0.0000E+00	9.2185E-02
93	5.2295E-14	1.9632E-14	-13.28	3.2663E-14	0.0000E+00	9.5074E-02
94	1.8904E-13	6.7614E-14	-12.72	1.2143E-13	0.0000E+00	1.0262E-01
95	5.4627E-13	1.8254E-13	-12.26	3.6373E-13	0.0000E+00	1.1386E-01
96	1.1473E-12	3.5235E-13	-11.94	7.9495E-13	0.0000E+00	1.2892E-01
97	2.0893E-12	5.8438E-13	-11.68	1.5050E-12	0.0000E+00	1.4716E-01
98	3.3652E-12	8.6126E-13	-11.47	2.5039E-12	0.0000E+00	1.6613E-01
99	4.7738E-12	1.1376E-12	-11.32	3.6362E-12	0.0000E+00	1.8265E-01
100	5.9852E-12	1.3603E-12	-11.22	4.6249E-12	0.0000E+00	1.9428E-01

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
101	6.7234E-12	1.4917E-12	-11.17	5.2318E-12	0.0000E+00	2.0042E-01
102	6.9352E-12	1.5297E-12	-11.16	5.4055E-12	0.0000E+00	2.0192E-01
103	6.7693E-12	1.4998E-12	-11.17	5.2695E-12	0.0000E+00	2.0077E-01
104	6.4460E-12	1.4396E-12	-11.19	5.0064E-12	0.0000E+00	1.9872E-01
105	6.1319E-12	1.3800E-12	-11.21	4.7520E-12	0.0000E+00	1.9678E-01
106	5.9015E-12	1.3357E-12	-11.23	4.5658E-12	0.0000E+00	1.9532E-01
107	5.7678E-12	1.3099E-12	-11.24	4.4579E-12	0.0000E+00	1.9447E-01
108	5.7244E-12	1.3015E-12	-11.24	4.4229E-12	0.0000E+00	1.9419E-01
109	1.3910E-14	5.3395E-15	-13.86	8.5702E-15	0.0000E+00	9.1716E-02
110	4.8437E-14	1.8421E-14	-13.31	3.0015E-14	0.0000E+00	9.3107E-02
111	2.2985E-13	8.3576E-14	-12.64	1.4627E-13	0.0000E+00	1.0001E-01
112	9.9453E-13	3.1648E-13	-12.00	6.7805E-13	0.0000E+00	1.2243E-01
113	3.6757E-12	9.4851E-13	-11.43	2.7272E-12	0.0000E+00	1.6430E-01
114	1.0032E-11	1.8980E-12	-11.00	8.1342E-12	0.0000E+00	2.4489E-01
115	2.4505E-11	3.1671E-12	-10.61	2.1338E-11	0.0000E+00	3.8500E-01
116	5.0177E-11	4.6046E-12	-10.30	4.5572E-11	0.0000E+00	5.6554E-01
117	8.3355E-11	5.8500E-12	-10.08	7.7505E-11	0.0000E+00	7.5707E-01
118	1.1359E-10	6.3475E-12	-9.94	1.0724E-10	0.0000E+00	9.6547E-01
119	1.3130E-10	6.8421E-12	-9.88	1.2446E-10	0.0000E+00	1.0394E+00
120	1.3477E-10	6.9548E-12	-9.87	1.2782E-10	0.0000E+00	1.0502E+00
121	1.2915E-10	6.7636E-12	-9.89	1.2239E-10	0.0000E+00	1.0340E+00
122	1.2080E-10	6.4802E-12	-9.92	1.1432E-10	0.0000E+00	1.0080E+00
123	1.1350E-10	6.2391E-12	-9.94	1.0726E-10	0.0000E+00	9.8240E-01
124	1.0847E-10	6.0793E-12	-9.96	1.0239E-10	0.0000E+00	9.6241E-01
125	1.0564E-10	5.9935E-12	-9.98	9.9651E-11	0.0000E+00	9.5009E-01

126	1.0474E-10	5.9667E-12	-9.98	9.8775E-11	0.0000E+00	9.4596E-01
127	3.4077E-14	1.3075E-14	-13.47	2.1003E-14	0.0000E+00	9.1794E-02
128	1.7014E-13	6.4234E-14	-12.77	1.0590E-13	0.0000E+00	9.4209E-02
129	9.5350E-13	3.2833E-13	-12.02	6.2517E-13	0.0000E+00	1.0880E-01
130	5.1317E-12	1.2290E-12	-11.29	3.9027E-12	0.0000E+00	1.8146E-01
131	3.3846E-11	4.1224E-12	-10.47	2.9724E-11	0.0000E+00	4.1202E-01
132	1.4700E-10	7.0595E-12	-9.83	1.3994E-10	0.0000E+00	1.1327E+00
133	4.4775E-10	2.8941E-11	-9.35	4.1880E-10	0.0000E+00	8.2692E-01
134	9.7835E-10	9.0803E-11	-9.01	8.8755E-10	0.0000E+00	5.5854E-01
135	1.6301E-09	1.8611E-10	-8.79	1.4440E-09	0.0000E+00	4.4336E-01
136	2.1825E-09	2.7602E-10	-8.66	1.9065E-09	0.0000E+00	3.9468E-01
137	2.4699E-09	3.2452E-10	-8.61	2.1454E-09	0.0000E+00	3.7777E-01
138	2.4938E-09	3.2865E-10	-8.60	2.1652E-09	0.0000E+00	3.7647E-01
139	2.3725E-09	3.0882E-10	-8.62	2.0636E-09	0.0000E+00	3.8185E-01
140	2.2222E-09	2.8471E-10	-8.65	1.9375E-09	0.0000E+00	3.8887E-01
141	2.1010E-09	2.6547E-10	-8.68	1.8356E-09	0.0000E+00	3.9511E-01
142	2.0209E-09	2.5278E-10	-8.69	1.7682E-09	0.0000E+00	3.9971E-01
143	1.9767E-09	2.4577E-10	-8.70	1.7309E-09	0.0000E+00	4.0246E-01
144	1.9626E-09	2.4353E-10	-8.71	1.7191E-09	0.0000E+00	4.0337E-01
145	4.8727E-14	1.8719E-14	-13.31	3.0008E-14	0.0000E+00	9.1605E-02
146	4.5740E-13	1.7194E-13	-12.34	2.8546E-13	0.0000E+00	9.4870E-02
147	3.8064E-12	1.2174E-12	-11.42	2.5890E-12	0.0000E+00	1.2152E-01
148	3.1382E-11	4.0455E-12	-10.50	2.7337E-11	0.0000E+00	3.8614E-01
149	3.2093E-10	1.7515E-11	-9.49	3.0342E-10	0.0000E+00	9.8990E-01
150	1.4849E-09	1.7344E-10	-8.83	1.3114E-09	0.0000E+00	4.3207E-01

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
151	4.4688E-09	8.0366E-10	-8.35	3.6651E-09	0.0000E+00	2.6060E-01
152	9.5673E-09	2.1817E-09	-8.02	7.3856E-09	0.0000E+00	1.9344E-01
153	1.5583E-08	4.0360E-09	-7.81	1.1547E-08	0.0000E+00	1.6348E-01
154	2.0380E-08	5.6063E-09	-7.69	1.4773E-08	0.0000E+00	1.5058E-01
155	2.2584E-08	6.3409E-09	-7.65	1.6243E-08	0.0000E+00	1.4638E-01
156	2.2506E-08	6.3179E-09	-7.65	1.6188E-08	0.0000E+00	1.4642E-01
157	2.1370E-08	5.9512E-09	-7.67	1.5419E-08	0.0000E+00	1.4805E-01
158	2.0149E-08	5.5611E-09	-7.70	1.4588E-08	0.0000E+00	1.4990E-01
159	1.9232E-08	5.2691E-09	-7.72	1.3963E-08	0.0000E+00	1.5142E-01
160	1.8651E-08	5.0838E-09	-7.73	1.3567E-08	0.0000E+00	1.5250E-01
161	1.8332E-08	4.9820E-09	-7.74	1.3350E-08	0.0000E+00	1.5312E-01
162	1.8228E-08	4.9488E-09	-7.74	1.3279E-08	0.0000E+00	1.5333E-01
163	2.1266E-14	8.1843E-15	-13.67	1.3082E-14	0.0000E+00	9.1340E-02
164	6.9787E-13	2.6308E-13	-12.16	4.3479E-13	0.0000E+00	9.4441E-02
165	8.9125E-12	2.7109E-12	-11.05	6.2017E-12	0.0000E+00	1.3073E-01
166	1.3874E-10	9.5037E-12	-9.86	1.2924E-10	0.0000E+00	7.7707E-01
167	1.6177E-09	1.5391E-10	-8.79	1.4638E-09	0.0000E+00	5.4346E-01
168	6.9061E-09	1.2608E-09	-8.16	5.6453E-09	0.0000E+00	2.5586E-01
169	1.9206E-08	4.9176E-09	-7.72	1.4289E-08	0.0000E+00	1.6604E-01
170	3.8837E-08	1.1987E-08	-7.41	2.6850E-08	0.0000E+00	1.2800E-01
171	6.1005E-08	2.0827E-08	-7.21	4.0178E-08	0.0000E+00	1.1023E-01
172	7.8033E-08	2.7936E-08	-7.11	5.0097E-08	0.0000E+00	1.0247E-01
173	8.5322E-08	3.1018E-08	-7.07	5.4305E-08	0.0000E+00	1.0004E-01

174	8.4600E-08	3.0733E-08	-7.07	5.3867E-08	0.0000E+00	1.0016E-01
175	8.0612E-08	2.9106E-08	-7.09	5.1506E-08	0.0000E+00	1.0112E-01
176	7.6648E-08	2.7503E-08	-7.12	4.9145E-08	0.0000E+00	1.0211E-01
177	7.3803E-08	2.6356E-08	-7.13	4.7447E-08	0.0000E+00	1.0287E-01
178	7.2076E-08	2.5657E-08	-7.14	4.6418E-08	0.0000E+00	1.0338E-01
179	7.1120E-08	2.5272E-08	-7.15	4.5848E-08	0.0000E+00	1.0367E-01
180	7.0790E-08	2.5140E-08	-7.15	4.5650E-08	0.0000E+00	1.0376E-01
181	-4.3203E-15	3.8513E-33	-32.00	6.1487E-33	0.0000E+00	9.1143E-02
182	6.8949E-13	2.6135E-13	-12.16	4.2814E-13	0.0000E+00	9.3612E-02
183	1.4398E-11	4.3638E-12	-10.84	1.0034E-11	0.0000E+00	1.3140E-01
184	3.5566E-10	1.6982E-11	-9.45	3.3868E-10	0.0000E+00	1.1396E+00
185	4.1558E-09	5.2179E-10	-8.38	3.6340E-09	0.0000E+00	3.9797E-01
186	1.6595E-08	3.7018E-09	-7.78	1.2893E-08	0.0000E+00	1.9902E-01
187	4.3720E-08	1.3099E-08	-7.36	3.0621E-08	0.0000E+00	1.3358E-01
188	8.5511E-08	3.0203E-08	-7.07	5.5308E-08	0.0000E+00	1.0464E-01
189	1.3213E-07	5.1097E-08	-6.88	8.1029E-08	0.0000E+00	9.0618E-02
190	1.6737E-07	6.7559E-08	-6.78	9.9811E-08	0.0000E+00	8.4422E-02
191	1.8162E-07	7.4288E-08	-6.74	1.0733E-07	0.0000E+00	8.2560E-02
192	1.7950E-07	7.3334E-08	-6.75	1.0617E-07	0.0000E+00	8.2728E-02
193	1.7165E-07	6.9748E-08	-6.77	1.0190E-07	0.0000E+00	8.3489E-02
194	1.6432E-07	6.6432E-08	-6.78	9.7888E-08	0.0000E+00	8.4201E-02
195	1.5924E-07	6.4148E-08	-6.80	9.5090E-08	0.0000E+00	8.4705E-02
196	1.5633E-07	6.2840E-08	-6.81	9.3494E-08	0.0000E+00	8.5019E-02
197	1.5468E-07	6.2101E-08	-6.81	9.2579E-08	0.0000E+00	8.5188E-02
198	1.5403E-07	6.1817E-08	-6.81	9.2214E-08	0.0000E+00	8.5242E-02
199	-1.1300E-14	3.8517E-33	-32.00	6.1483E-33	0.0000E+00	9.1143E-02
200	4.6524E-13	1.7741E-13	-12.33	2.8782E-13	0.0000E+00	9.2705E-02

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
201	1.8032E-11	5.6110E-12	-10.74	1.2421E-11	0.0000E+00	1.2650E-01
202	7.2787E-10	3.4961E-11	-9.14	6.9291E-10	0.0000E+00	1.1325E+00
203	8.5815E-09	1.2554E-09	-8.07	7.3261E-09	0.0000E+00	3.3347E-01
204	3.2486E-08	8.0879E-09	-7.49	2.4398E-08	0.0000E+00	1.7238E-01
205	8.1765E-08	2.6639E-08	-7.09	5.5126E-08	0.0000E+00	1.1825E-01
206	1.5636E-07	5.9423E-08	-6.81	9.6941E-08	0.0000E+00	9.3222E-02
207	2.3976E-07	9.9549E-08	-6.62	1.4022E-07	0.0000E+00	8.0486E-02
208	3.0276E-07	1.3119E-07	-6.52	1.7157E-07	0.0000E+00	7.4731E-02
209	3.2675E-07	1.4342E-07	-6.49	1.8333E-07	0.0000E+00	7.3045E-02
210	3.2210E-07	1.4117E-07	-6.49	1.8092E-07	0.0000E+00	7.3233E-02
211	3.0945E-07	1.3493E-07	-6.51	1.7452E-07	0.0000E+00	7.3912E-02
212	2.9829E-07	1.2948E-07	-6.53	1.6881E-07	0.0000E+00	7.4496E-02
213	2.9072E-07	1.2584E-07	-6.54	1.6488E-07	0.0000E+00	7.4871E-02
214	2.8689E-07	1.2399E-07	-6.54	1.6290E-07	0.0000E+00	7.5078E-02
215	2.8453E-07	1.2287E-07	-6.55	1.6166E-07	0.0000E+00	7.5182E-02
216	2.8333E-07	1.2232E-07	-6.55	1.6101E-07	0.0000E+00	7.5216E-02
217	-2.6783E-14	3.8511E-33	-32.00	6.1489E-33	0.0000E+00	9.1143E-02
218	2.5685E-13	9.8398E-14	-12.59	1.5846E-13	0.0000E+00	9.2020E-02
219	1.7119E-11	5.6042E-12	-10.77	1.1515E-11	0.0000E+00	1.1741E-01
220	1.1563E-09	5.5861E-11	-8.94	1.1005E-09	0.0000E+00	1.1257E+00
221	1.4596E-08	2.2867E-09	-7.84	1.2309E-08	0.0000E+00	3.0759E-01

222	5.3832E-08	1.4125E-08	-7.27	3.9707E-08	0.0000E+00	1.6063E-01
223	1.3088E-07	4.4252E-08	-6.88	8.6630E-08	0.0000E+00	1.1187E-01
224	2.4535E-07	9.6551E-08	-6.61	1.4880E-07	0.0000E+00	8.8066E-02
225	3.7734E-07	1.6312E-07	-6.42	2.1423E-07	0.0000E+00	7.5047E-02
226	4.7768E-07	2.1629E-07	-6.32	2.6139E-07	0.0000E+00	6.9059E-02
227	5.1308E-07	2.3568E-07	-6.29	2.7740E-07	0.0000E+00	6.7257E-02
228	5.0452E-07	2.3149E-07	-6.30	2.7303E-07	0.0000E+00	6.7395E-02
229	4.8775E-07	2.2264E-07	-6.31	2.6511E-07	0.0000E+00	6.8046E-02
230	4.7359E-07	2.1526E-07	-6.32	2.5834E-07	0.0000E+00	6.8579E-02
231	4.6389E-07	2.1033E-07	-6.33	2.5356E-07	0.0000E+00	6.8887E-02
232	4.6023E-07	2.0843E-07	-6.34	2.5179E-07	0.0000E+00	6.9029E-02
233	4.5744E-07	2.0707E-07	-6.34	2.5037E-07	0.0000E+00	6.9094E-02
234	4.5527E-07	2.0605E-07	-6.34	2.4923E-07	0.0000E+00	6.9118E-02
235	-8.7482E-15	3.8518E-33	-32.00	6.1482E-33	0.0000E+00	9.1182E-02
236	-7.5573E-14	3.8367E-33	-32.00	6.1633E-33	0.0000E+00	9.1143E-02
237	1.5175E-11	5.2795E-12	-10.82	9.8959E-12	0.0000E+00	1.0711E-01
238	1.3282E-09	6.3515E-11	-8.88	1.2647E-09	0.0000E+00	1.1378E+00
239	2.0064E-08	3.0861E-09	-7.70	1.6977E-08	0.0000E+00	3.1436E-01
240	7.6658E-08	2.0258E-08	-7.12	5.6400E-08	0.0000E+00	1.5909E-01
241	1.8327E-07	6.1879E-08	-6.74	1.2139E-07	0.0000E+00	1.1210E-01
242	3.3919E-07	1.3447E-07	-6.47	2.0472E-07	0.0000E+00	8.6997E-02
243	5.2837E-07	2.3312E-07	-6.28	2.9525E-07	0.0000E+00	7.2373E-02
244	6.7269E-07	3.1250E-07	-6.17	3.6019E-07	0.0000E+00	6.5864E-02
245	7.1558E-07	3.3868E-07	-6.15	3.7690E-07	0.0000E+00	6.3590E-02
246	7.0096E-07	3.3194E-07	-6.15	3.6902E-07	0.0000E+00	6.3526E-02
247	6.8275E-07	3.2161E-07	-6.17	3.6114E-07	0.0000E+00	6.4166E-02
248	6.6790E-07	3.1327E-07	-6.18	3.5463E-07	0.0000E+00	6.4687E-02
249	6.5716E-07	3.0753E-07	-6.18	3.4963E-07	0.0000E+00	6.4966E-02
250	6.5539E-07	3.0646E-07	-6.18	3.4893E-07	0.0000E+00	6.5060E-02

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
251	6.5282E-07	3.0516E-07	-6.19	3.4766E-07	0.0000E+00	6.5100E-02
252	6.4922E-07	3.0342E-07	-6.19	3.4580E-07	0.0000E+00	6.5125E-02
253	6.9980E-14	2.6955E-14	-13.16	4.3026E-14	0.0000E+00	9.1213E-02
254	-1.5783E-13	3.8451E-33	-32.00	6.1549E-33	0.0000E+00	9.1191E-02
255	8.5770E-12	3.0762E-12	-11.07	5.5008E-12	0.0000E+00	1.0218E-01
256	1.0296E-09	8.4840E-11	-8.99	9.4481E-10	0.0000E+00	6.3636E-01
257	2.0619E-08	2.6857E-09	-7.69	1.7933E-08	0.0000E+00	3.8156E-01
258	8.9333E-08	2.2354E-08	-7.05	6.6979E-08	0.0000E+00	1.7122E-01
259	2.2038E-07	7.1802E-08	-6.66	1.4857E-07	0.0000E+00	1.2415E-01
260	4.1945E-07	1.6521E-07	-6.38	2.5424E-07	0.0000E+00	9.6729E-02
261	6.7766E-07	3.0187E-07	-6.17	3.7578E-07	0.0000E+00	7.8247E-02
262	8.6478E-07	4.0536E-07	-6.06	4.5942E-07	0.0000E+00	7.1241E-02
263	8.9489E-07	4.3136E-07	-6.05	4.6353E-07	0.0000E+00	6.7544E-02
264	8.7254E-07	4.2281E-07	-6.06	4.4973E-07	0.0000E+00	6.6859E-02
265	8.5618E-07	4.1282E-07	-6.07	4.4336E-07	0.0000E+00	6.7507E-02
266	8.4326E-07	4.0480E-07	-6.07	4.3847E-07	0.0000E+00	6.8086E-02
267	8.3351E-07	3.9919E-07	-6.08	4.3432E-07	0.0000E+00	6.8388E-02
268	8.3439E-07	3.9947E-07	-6.08	4.3492E-07	0.0000E+00	6.8436E-02
269	8.3288E-07	3.9868E-07	-6.08	4.3420E-07	0.0000E+00	6.8458E-02

270	8.2836E-07	3.9637E-07	-6.08	4.3199E-07	0.0000E+00	6.8506E-02
271	-4.8213E-14	3.8537E-33	-32.00	6.1463E-33	0.0000E+00	9.1143E-02
272	3.4289E-13	1.3183E-13	-12.46	2.1107E-13	0.0000E+00	9.1493E-02
273	-4.5069E-13	3.7413E-33	-32.00	6.2587E-33	0.0000E+00	9.2744E-02
274	3.7327E-10	7.6616E-11	-9.43	2.9666E-10	0.0000E+00	2.2126E-01
275	9.8703E-09	5.8573E-10	-8.01	9.2845E-09	0.0000E+00	9.0578E-01
276	5.4570E-08	9.4988E-09	-7.26	4.5071E-08	0.0000E+00	2.7114E-01
277	1.5927E-07	4.2413E-08	-6.80	1.1685E-07	0.0000E+00	1.7318E-01
278	3.9068E-07	1.4616E-07	-6.41	2.4452E-07	0.0000E+00	1.1472E-01
279	7.7480E-07	3.4577E-07	-6.11	4.2903E-07	0.0000E+00	8.5083E-02
280	1.0641E-06	4.7881E-07	-5.97	5.6043E-07	2.4905E-08	8.0260E-02
281	1.1601E-06	4.8469E-07	-5.94	5.2791E-07	1.4747E-07	7.4685E-02
282	1.0764E-06	4.9060E-07	-5.97	4.9541E-07	9.0411E-08	6.9244E-02
283	1.1182E-06	4.7661E-07	-5.95	4.9118E-07	1.5037E-07	7.0667E-02
284	1.1233E-06	4.6914E-07	-5.95	4.8857E-07	1.6554E-07	7.1412E-02
285	1.0538E-06	4.6527E-07	-5.98	4.8671E-07	1.0181E-07	7.1732E-02
286	1.1028E-06	4.6546E-07	-5.96	4.8715E-07	1.5021E-07	7.1767E-02
287	1.1037E-06	4.6549E-07	-5.96	4.8714E-07	1.5108E-07	7.1762E-02
288	1.0420E-06	4.6454E-07	-5.98	4.8634E-07	9.1112E-08	7.1789E-02
289	2.6921E-14	1.0374E-14	-13.57	1.6547E-14	0.0000E+00	9.1147E-02
290	-5.9769E-14	3.8492E-33	-32.00	6.1508E-33	0.0000E+00	9.1143E-02
291	2.1020E-12	7.9684E-13	-11.68	1.3051E-12	0.0000E+00	9.3594E-02
292	8.4735E-11	2.5620E-11	-10.07	5.9115E-11	0.0000E+00	1.3185E-01
293	1.9776E-09	2.6812E-10	-8.70	1.7095E-09	0.0000E+00	3.6434E-01
294	1.7875E-08	1.3879E-09	-7.75	1.6487E-08	0.0000E+00	6.7881E-01
295	9.4318E-08	1.6633E-08	-7.03	7.7684E-08	0.0000E+00	2.9357E-01
296	2.5653E-07	8.4468E-08	-6.59	1.7207E-07	0.0000E+00	1.3968E-01
297	9.3655E-07	3.8421E-07	-6.03	5.5233E-07	0.0000E+00	9.8576E-02
298	6.7389E-06	5.1873E-07	-5.17	9.8238E-07	5.2378E-06	1.2986E-01
299	8.7638E-06	5.2255E-07	-5.06	1.0460E-06	7.1952E-06	1.3727E-01
300	4.1252E-06	5.0231E-07	-5.38	7.6699E-07	2.8559E-06	1.0470E-01

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
301	6.3822E-06	5.0533E-07	-5.20	8.3456E-07	5.0423E-06	1.1325E-01
302	7.3946E-06	5.0576E-07	-5.13	8.6808E-07	6.0207E-06	1.1769E-01
303	3.7580E-06	4.9211E-07	-5.43	7.2047E-07	2.5455E-06	1.0039E-01
304	6.6571E-06	5.0193E-07	-5.18	8.3465E-07	5.3205E-06	1.1403E-01
305	7.0121E-06	5.0319E-07	-5.15	8.5156E-07	5.6573E-06	1.1604E-01
306	3.6080E-06	4.9148E-07	-5.44	7.1771E-07	2.3989E-06	1.0013E-01
307	-7.6876E-15	3.8535E-33	-32.00	6.1465E-33	0.0000E+00	9.1143E-02
308	3.4368E-14	1.3238E-14	-13.46	2.1130E-14	0.0000E+00	9.1209E-02
309	5.0421E-13	1.9242E-13	-12.30	3.1179E-13	0.0000E+00	9.2595E-02
310	2.9174E-11	1.0123E-11	-10.54	1.9051E-11	0.0000E+00	1.0754E-01
311	2.7097E-10	7.2838E-11	-9.57	1.9813E-10	0.0000E+00	1.5544E-01
312	4.8365E-09	4.0738E-10	-8.32	4.4291E-09	0.0000E+00	6.2126E-01
313	3.5187E-08	3.4058E-09	-7.45	3.1781E-08	0.0000E+00	5.8655E-01
314	2.1003E-07	5.4701E-08	-6.68	1.5533E-07	0.0000E+00	1.9472E-01
315	6.4235E-07	2.1849E-07	-6.19	4.2386E-07	0.0000E+00	1.3302E-01
316	2.7988E-05	1.2627E-06	-4.55	8.7380E-06	1.7987E-05	4.7453E-01
317	3.2505E-05	2.0531E-06	-4.49	9.3672E-06	2.1085E-05	3.1286E-01

318	1.5426E-06	5.1899E-07	-5.81	1.0077E-06	1.5884E-08	1.3314E-01
319	3.1249E-05	1.5317E-06	-4.51	9.0560E-06	2.0661E-05	4.0542E-01
320	3.3548E-05	1.9815E-06	-4.47	9.3381E-06	2.2228E-05	3.2316E-01
321	1.3745E-06	4.7320E-07	-5.86	9.0130E-07	0.0000E+00	1.3061E-01
322	3.2213E-05	1.7342E-06	-4.49	9.2078E-06	2.1270E-05	3.6409E-01
323	3.2885E-05	1.8919E-06	-4.48	9.2962E-06	2.1697E-05	3.3693E-01
324	1.2907E-06	4.3980E-07	-5.89	8.5085E-07	0.0000E+00	1.3266E-01
325	4.3165E-15	1.6633E-15	-14.36	2.6532E-15	0.0000E+00	9.1147E-02
326	-8.2443E-15	3.8530E-33	-32.00	6.1470E-33	0.0000E+00	9.1143E-02
327	4.2267E-13	1.6204E-13	-12.37	2.6063E-13	0.0000E+00	9.1911E-02
328	8.6474E-12	3.1603E-12	-11.06	5.4871E-12	0.0000E+00	9.9216E-02
329	9.2582E-11	3.0147E-11	-10.03	6.2434E-11	0.0000E+00	1.1834E-01
330	8.0037E-10	1.7502E-10	-9.10	6.2535E-10	0.0000E+00	2.0417E-01
331	3.0561E-08	1.4650E-09	-7.51	2.9096E-08	0.0000E+00	1.2484E+00
332	7.2597E-08	1.3820E-08	-7.14	5.8777E-08	0.0000E+00	2.9163E-01
333	6.7306E-07	1.9527E-07	-6.17	4.7779E-07	0.0000E+00	1.6778E-01
334	6.2482E-06	5.5143E-07	-5.20	1.8346E-06	3.8622E-06	2.2813E-01
335	1.1596E-05	5.7749E-07	-4.94	2.8744E-06	8.1443E-06	3.4130E-01
336	6.6591E-06	5.4768E-07	-5.18	1.7247E-06	4.3867E-06	2.1594E-01
337	7.8175E-06	5.5120E-07	-5.11	1.8592E-06	5.4071E-06	2.3128E-01
338	9.7847E-06	5.6054E-07	-5.01	2.2215E-06	7.0027E-06	2.7176E-01
339	5.2388E-06	5.4128E-07	-5.28	1.5329E-06	3.1646E-06	1.9420E-01
340	8.7103E-06	5.5663E-07	-5.06	2.0718E-06	6.0818E-06	2.5523E-01
341	9.3128E-06	5.6012E-07	-5.03	2.2084E-06	6.5443E-06	2.7036E-01
342	4.7945E-06	5.4065E-07	-5.32	1.5135E-06	2.7404E-06	1.9196E-01
343	-1.8830E-15	3.8535E-33	-32.00	6.1465E-33	0.0000E+00	9.1143E-02
344	9.8769E-15	3.8059E-15	-14.01	6.0710E-15	0.0000E+00	9.1152E-02
345	4.7012E-14	1.8078E-14	-13.33	2.8934E-14	0.0000E+00	9.1460E-02
346	4.1994E-12	1.5703E-12	-11.38	2.6291E-12	0.0000E+00	9.5673E-02
347	2.7938E-11	9.7601E-12	-10.55	1.8178E-11	0.0000E+00	1.0643E-01
348	4.0354E-10	1.1257E-10	-9.39	2.9097E-10	0.0000E+00	1.4770E-01
349	2.7230E-09	3.7846E-10	-8.56	2.3446E-09	0.0000E+00	3.8940E-01
350	7.1414E-08	9.1649E-09	-7.15	6.2249E-08	0.0000E+00	4.6574E-01

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
351	1.9034E-07	4.6160E-08	-6.72	1.4418E-07	0.0000E+00	2.1419E-01
352	1.9573E-05	7.8915E-07	-4.71	7.0149E-06	1.1769E-05	6.0954E-01
353	2.8697E-05	1.9966E-06	-4.54	9.3439E-06	1.7357E-05	3.2091E-01
354	1.4482E-06	4.1352E-07	-5.84	1.0347E-06	0.0000E+00	1.7158E-01
355	2.5848E-05	1.3125E-06	-4.59	8.8124E-06	1.5723E-05	4.6039E-01
356	2.8607E-05	1.8753E-06	-4.54	9.2867E-06	1.7445E-05	3.3957E-01
357	8.5645E-07	2.3524E-07	-6.07	6.2122E-07	0.0000E+00	1.8109E-01
358	2.6715E-05	1.5669E-06	-4.57	9.0853E-06	1.6062E-05	3.9759E-01
359	2.7418E-05	1.7284E-06	-4.56	9.2027E-06	1.6487E-05	3.6510E-01
360	6.4977E-07	1.7411E-07	-6.19	4.7566E-07	0.0000E+00	1.8734E-01
361	1.2585E-15	4.8496E-16	-14.90	7.7350E-16	0.0000E+00	9.1143E-02
362	-2.1912E-15	3.8534E-33	-32.00	6.1466E-33	0.0000E+00	9.1143E-02
363	5.8816E-14	2.2652E-14	-13.23	3.6164E-14	0.0000E+00	9.1230E-02
364	1.4178E-12	5.3773E-13	-11.85	8.8011E-13	0.0000E+00	9.3526E-02
365	1.9214E-11	6.9339E-12	-10.72	1.2280E-11	0.0000E+00	1.0120E-01

366	6.9422E-11	2.1347E-11	-10.16	4.8075E-11	0.0000E+00	1.2869E-01
367	1.9731E-09	3.4309E-10	-8.70	1.6300E-09	0.0000E+00	2.9864E-01
368	1.1847E-08	9.0265E-10	-7.93	1.0944E-08	0.0000E+00	8.3140E-01
369	1.5059E-07	3.1622E-08	-6.82	1.1896E-07	0.0000E+00	2.5797E-01
370	5.7178E-07	1.4081E-07	-6.24	4.3097E-07	0.0000E+00	2.0987E-01
371	9.0326E-07	2.4083E-07	-6.04	6.6242E-07	0.0000E+00	1.8861E-01
372	1.3780E-06	3.8064E-07	-5.86	9.9740E-07	0.0000E+00	1.7968E-01
373	9.7237E-07	2.6235E-07	-6.01	7.1002E-07	0.0000E+00	1.8558E-01
374	1.0924E-06	2.9156E-07	-5.96	8.0081E-07	0.0000E+00	1.8834E-01
375	1.1367E-06	2.9968E-07	-5.94	8.3704E-07	0.0000E+00	1.9153E-01
376	1.0375E-06	2.6968E-07	-5.98	7.6785E-07	0.0000E+00	1.9524E-01
377	1.1148E-06	2.8890E-07	-5.95	8.2591E-07	0.0000E+00	1.9603E-01
378	1.0565E-06	2.7263E-07	-5.98	7.8384E-07	0.0000E+00	1.9715E-01
379	-4.7211E-16	3.8536E-33	-32.00	6.1464E-33	0.0000E+00	9.1143E-02
380	2.2857E-15	8.8079E-16	-14.64	1.4049E-15	0.0000E+00	9.1145E-02
381	-2.7276E-15	3.8531E-33	-32.00	6.1469E-33	0.0000E+00	9.1143E-02
382	6.4160E-13	2.4570E-13	-12.19	3.9590E-13	0.0000E+00	9.2073E-02
383	6.3792E-12	2.3684E-12	-11.20	4.0108E-12	0.0000E+00	9.6767E-02
384	7.1389E-11	2.3270E-11	-10.15	4.8119E-11	0.0000E+00	1.1817E-01
385	2.4477E-10	4.9316E-11	-9.61	1.9545E-10	0.0000E+00	2.9441E-01
386	8.8183E-09	5.8253E-10	-8.05	8.2358E-09	0.0000E+00	1.2926E+00
387	2.3363E-08	5.1572E-09	-7.63	1.8206E-08	0.0000E+00	3.2276E-01
388	7.0536E-08	1.7909E-08	-7.15	5.2627E-08	0.0000E+00	2.6867E-01
389	1.5260E-07	3.9860E-08	-6.82	1.1274E-07	0.0000E+00	2.5859E-01
390	1.9287E-07	4.9977E-08	-6.71	1.4290E-07	0.0000E+00	2.6142E-01
391	2.1117E-07	5.3679E-08	-6.68	1.5749E-07	0.0000E+00	2.6825E-01
392	1.8138E-07	4.5174E-08	-6.74	1.3621E-07	0.0000E+00	2.7567E-01
393	1.8678E-07	4.5832E-08	-6.73	1.4095E-07	0.0000E+00	2.8118E-01
394	1.8448E-07	4.4819E-08	-6.73	1.3966E-07	0.0000E+00	2.8490E-01
395	1.7939E-07	4.3331E-08	-6.75	1.3606E-07	0.0000E+00	2.8708E-01
396	1.8289E-07	4.4088E-08	-6.74	1.3880E-07	0.0000E+00	2.8785E-01
397	6.2521E-16	2.4093E-16	-15.20	3.8428E-16	0.0000E+00	9.1143E-02
398	-7.3135E-16	3.8535E-33	-32.00	6.1465E-33	0.0000E+00	9.1143E-02
399	7.9882E-15	3.0783E-15	-14.10	4.9099E-15	0.0000E+00	9.1143E-02
400	7.6353E-14	2.9381E-14	-13.12	4.6972E-14	0.0000E+00	9.1355E-02

OUTPUT TABLE 14..CONCEN. (M/L**3) AT TIME = 6.0000E+01, (DELT = 5.0000E-01)

*** ITIME = 120 ITER = 1 --- CHEMICAL NO. 3 (URANIUM) --- ***

NP	TOTAL C	DISSOL C	XLOG	SORBED C	PRECIP C	KD
401	2.4381E-12	9.2770E-13	-11.61	1.5104E-12	0.0000E+00	9.3035E-02
402	2.8492E-11	1.0071E-11	-10.55	1.8421E-11	0.0000E+00	1.0453E-01
403	2.5903E-10	5.6796E-11	-9.59	2.0223E-10	0.0000E+00	2.5433E-01
404	2.1583E-09	1.4847E-10	-8.67	2.0099E-09	0.0000E+00	1.1604E+00
405	8.1712E-09	1.0383E-09	-8.09	7.1328E-09	0.0000E+00	5.8882E-01
406	2.0111E-08	2.9557E-09	-7.70	1.7156E-08	0.0000E+00	4.9750E-01
407	3.5357E-08	5.2209E-09	-7.45	3.0136E-08	0.0000E+00	4.9476E-01
408	4.7201E-08	6.8138E-09	-7.33	4.0387E-08	0.0000E+00	5.0806E-01
409	4.9229E-08	6.9043E-09	-7.31	4.2325E-08	0.0000E+00	5.2545E-01
410	4.6864E-08	6.4090E-09	-7.33	4.0455E-08	0.0000E+00	5.4105E-01
411	4.3961E-08	5.9056E-09	-7.36	3.8056E-08	0.0000E+00	5.5234E-01
412	4.3259E-08	5.7526E-09	-7.36	3.7506E-08	0.0000E+00	5.5885E-01
413	4.2314E-08	5.6012E-09	-7.37	3.6713E-08	0.0000E+00	5.6182E-01

414	4.1795E-08	5.5092E-09	-7.38	3.6286E-08	0.0000E+00	5.6455E-01
415	-3.3547E-16	3.8536E-33	-32.00	6.1464E-33	0.0000E+00	9.1143E-02
416	1.6561E-15	6.3817E-16	-14.78	1.0179E-15	0.0000E+00	9.1145E-02
417	-2.7292E-15	3.8537E-33	-32.00	6.1463E-33	0.0000E+00	9.1143E-02
418	6.7514E-14	2.5999E-14	-13.17	4.1514E-14	0.0000E+00	9.1242E-02
419	6.4734E-13	2.4853E-13	-12.19	3.9881E-13	0.0000E+00	9.1694E-02
420	2.0884E-11	7.5577E-12	-10.68	1.3326E-11	0.0000E+00	1.0076E-01
421	1.5916E-10	4.4898E-11	-9.80	1.1426E-10	0.0000E+00	1.4542E-01
422	7.4211E-10	1.6529E-10	-9.13	5.7682E-10	0.0000E+00	1.9941E-01
423	1.7156E-09	3.5580E-10	-8.77	1.3598E-09	0.0000E+00	2.1840E-01
424	3.0420E-09	6.3708E-10	-8.52	2.4050E-09	0.0000E+00	2.1571E-01
425	4.1507E-09	8.9633E-10	-8.38	3.2543E-09	0.0000E+00	2.0747E-01
426	4.6048E-09	1.0273E-09	-8.34	3.5776E-09	0.0000E+00	1.9900E-01
427	4.4176E-09	1.0138E-09	-8.35	3.4038E-09	0.0000E+00	1.9186E-01
428	3.9181E-09	9.2119E-10	-8.41	2.9969E-09	0.0000E+00	1.8591E-01
429	3.4746E-09	8.3362E-10	-8.46	2.6410E-09	0.0000E+00	1.8104E-01
430	3.1577E-09	7.7068E-10	-8.50	2.3870E-09	0.0000E+00	1.7699E-01
431	2.9261E-09	7.2444E-10	-8.53	2.2017E-09	0.0000E+00	1.7366E-01
432	2.7111E-09	6.8915E-10	-8.57	2.0219E-09	0.0000E+00	1.6765E-01
433	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
434	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
435	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
436	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
437	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
438	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
439	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
440	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
441	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
442	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
443	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
444	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
445	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
446	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
447	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
448	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
449	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02
450	1.0000E-20	3.8536E-21	-20.00	6.1464E-21	0.0000E+00	9.1143E-02

NP	PH	EH
1	7.3268E+00	0.0000E+00
2	7.3268E+00	0.0000E+00
3	7.3268E+00	0.0000E+00
4	7.3269E+00	0.0000E+00
5	7.3269E+00	0.0000E+00
6	7.3269E+00	0.0000E+00
7	7.3270E+00	0.0000E+00
8	7.3270E+00	0.0000E+00
9	7.3271E+00	0.0000E+00
10	7.3271E+00	0.0000E+00
11	7.3271E+00	0.0000E+00
12	7.3271E+00	0.0000E+00
13	7.3271E+00	0.0000E+00

14	7.3271E+00	0.0000E+00
15	7.3271E+00	0.0000E+00
16	7.3271E+00	0.0000E+00
17	7.3271E+00	0.0000E+00
18	7.3271E+00	0.0000E+00
19	7.3268E+00	0.0000E+00
20	7.3268E+00	0.0000E+00
21	7.3269E+00	0.0000E+00
22	7.3270E+00	0.0000E+00
23	7.3271E+00	0.0000E+00
24	7.3273E+00	0.0000E+00
25	7.3274E+00	0.0000E+00
26	7.3276E+00	0.0000E+00
27	7.3277E+00	0.0000E+00
28	7.3277E+00	0.0000E+00
29	7.3278E+00	0.0000E+00
30	7.3278E+00	0.0000E+00
31	7.3278E+00	0.0000E+00
32	7.3278E+00	0.0000E+00
33	7.3278E+00	0.0000E+00
34	7.3278E+00	0.0000E+00
35	7.3278E+00	0.0000E+00
36	7.3278E+00	0.0000E+00
37	7.3269E+00	0.0000E+00
38	7.3270E+00	0.0000E+00
39	7.3273E+00	0.0000E+00
40	7.3280E+00	0.0000E+00
41	7.3289E+00	0.0000E+00
42	7.3299E+00	0.0000E+00
43	7.3308E+00	0.0000E+00
44	7.3317E+00	0.0000E+00
45	7.3324E+00	0.0000E+00
46	7.3329E+00	0.0000E+00
47	7.3332E+00	0.0000E+00
48	7.3333E+00	0.0000E+00
49	7.3333E+00	0.0000E+00
50	7.3332E+00	0.0000E+00
51	7.3332E+00	0.0000E+00
52	7.3331E+00	0.0000E+00
53	7.3331E+00	0.0000E+00
54	7.3331E+00	0.0000E+00
55	7.3271E+00	0.0000E+00
56	7.3274E+00	0.0000E+00
57	7.3286E+00	0.0000E+00
58	7.3312E+00	0.0000E+00
59	7.3345E+00	0.0000E+00
60	7.3383E+00	0.0000E+00
61	7.3420E+00	0.0000E+00
62	7.3454E+00	0.0000E+00
63	7.3480E+00	0.0000E+00
64	7.3498E+00	0.0000E+00
65	7.3507E+00	0.0000E+00
66	7.3510E+00	0.0000E+00
67	7.3510E+00	0.0000E+00
68	7.3508E+00	0.0000E+00

69	7.3505E+00	0.0000E+00
70	7.3504E+00	0.0000E+00
71	7.3502E+00	0.0000E+00
72	7.3502E+00	0.0000E+00
73	7.3275E+00	0.0000E+00
74	7.3285E+00	0.0000E+00
75	7.3322E+00	0.0000E+00
76	7.3406E+00	0.0000E+00
77	7.3517E+00	0.0000E+00
78	7.3642E+00	0.0000E+00
79	7.3770E+00	0.0000E+00
80	7.3885E+00	0.0000E+00
81	7.3974E+00	0.0000E+00
82	7.4033E+00	0.0000E+00
83	7.4062E+00	0.0000E+00
84	7.4071E+00	0.0000E+00
85	7.4067E+00	0.0000E+00
86	7.4059E+00	0.0000E+00
87	7.4051E+00	0.0000E+00
88	7.4044E+00	0.0000E+00
89	7.4040E+00	0.0000E+00
90	7.4039E+00	0.0000E+00
91	7.3281E+00	0.0000E+00
92	7.3304E+00	0.0000E+00
93	7.3400E+00	0.0000E+00
94	7.3636E+00	0.0000E+00
95	7.3952E+00	0.0000E+00
96	7.4326E+00	0.0000E+00
97	7.4721E+00	0.0000E+00
98	7.5088E+00	0.0000E+00
99	7.5378E+00	0.0000E+00
100	7.5566E+00	0.0000E+00
101	7.5656E+00	0.0000E+00
102	7.5677E+00	0.0000E+00
103	7.5660E+00	0.0000E+00
104	7.5631E+00	0.0000E+00
105	7.5602E+00	0.0000E+00
106	7.5581E+00	0.0000E+00
107	7.5568E+00	0.0000E+00
108	7.5564E+00	0.0000E+00
109	7.3288E+00	0.0000E+00
110	7.3336E+00	0.0000E+00
111	7.3559E+00	0.0000E+00
112	7.4177E+00	0.0000E+00
113	7.5062E+00	0.0000E+00
114	7.6222E+00	0.0000E+00
115	7.7596E+00	0.0000E+00
116	7.8972E+00	0.0000E+00
117	8.0043E+00	0.0000E+00
118	8.0661E+00	0.0000E+00
119	8.0932E+00	0.0000E+00
120	8.0975E+00	0.0000E+00
121	8.0906E+00	0.0000E+00
122	8.0805E+00	0.0000E+00
123	8.0712E+00	0.0000E+00

124	8.0644E+00	0.0000E+00
125	8.0603E+00	0.0000E+00
126	8.0590E+00	0.0000E+00
127	7.3291E+00	0.0000E+00
128	7.3375E+00	0.0000E+00
129	7.3829E+00	0.0000E+00
130	7.5352E+00	0.0000E+00
131	7.7916E+00	0.0000E+00
132	8.1493E+00	0.0000E+00
133	8.4520E+00	0.0000E+00
134	8.6396E+00	0.0000E+00
135	8.7450E+00	0.0000E+00
136	8.7976E+00	0.0000E+00
137	8.8177E+00	0.0000E+00
138	8.8196E+00	0.0000E+00
139	8.8136E+00	0.0000E+00
140	8.8056E+00	0.0000E+00
141	8.7985E+00	0.0000E+00
142	8.7934E+00	0.0000E+00
143	8.7903E+00	0.0000E+00
144	8.7893E+00	0.0000E+00
145	7.3285E+00	0.0000E+00
146	7.3397E+00	0.0000E+00
147	7.4185E+00	0.0000E+00
148	7.7736E+00	0.0000E+00
149	8.3529E+00	0.0000E+00
150	8.7557E+00	0.0000E+00
151	8.9803E+00	0.0000E+00
152	9.1115E+00	0.0000E+00
153	9.1861E+00	0.0000E+00
154	9.2234E+00	0.0000E+00
155	9.2373E+00	0.0000E+00
156	9.2385E+00	0.0000E+00
157	9.2346E+00	0.0000E+00
158	9.2297E+00	0.0000E+00
159	9.2255E+00	0.0000E+00
160	9.2225E+00	0.0000E+00
161	9.2207E+00	0.0000E+00
162	9.2201E+00	0.0000E+00
163	7.3276E+00	0.0000E+00
164	7.3384E+00	0.0000E+00
165	7.4363E+00	0.0000E+00
166	8.0117E+00	0.0000E+00
167	8.6514E+00	0.0000E+00
168	8.9879E+00	0.0000E+00
169	9.1773E+00	0.0000E+00
170	9.2917E+00	0.0000E+00
171	9.3588E+00	0.0000E+00
172	9.3933E+00	0.0000E+00
173	9.4068E+00	0.0000E+00
174	9.4089E+00	0.0000E+00
175	9.4067E+00	0.0000E+00
176	9.4035E+00	0.0000E+00
177	9.4008E+00	0.0000E+00
178	9.3987E+00	0.0000E+00

179	9.3975E+00	0.0000E+00
180	9.3971E+00	0.0000E+00
181	7.3272E+00	0.0000E+00
182	7.3359E+00	0.0000E+00
183	7.4397E+00	0.0000E+00
184	8.1613E+00	0.0000E+00
185	8.7921E+00	0.0000E+00
186	9.0975E+00	0.0000E+00
187	9.2716E+00	0.0000E+00
188	9.3792E+00	0.0000E+00
189	9.4443E+00	0.0000E+00
190	9.4786E+00	0.0000E+00
191	9.4926E+00	0.0000E+00
192	9.4958E+00	0.0000E+00
193	9.4949E+00	0.0000E+00
194	9.4930E+00	0.0000E+00
195	9.4912E+00	0.0000E+00
196	9.4899E+00	0.0000E+00
197	9.4890E+00	0.0000E+00
198	9.4887E+00	0.0000E+00
199	7.3271E+00	0.0000E+00
200	7.3328E+00	0.0000E+00
201	7.4300E+00	0.0000E+00
202	8.2431E+00	0.0000E+00
203	8.8706E+00	0.0000E+00
204	9.1597E+00	0.0000E+00
205	9.3238E+00	0.0000E+00
206	9.4283E+00	0.0000E+00
207	9.4943E+00	0.0000E+00
208	9.5301E+00	0.0000E+00
209	9.5452E+00	0.0000E+00
210	9.5497E+00	0.0000E+00
211	9.5502E+00	0.0000E+00
212	9.5496E+00	0.0000E+00
213	9.5487E+00	0.0000E+00
214	9.5478E+00	0.0000E+00
215	9.5473E+00	0.0000E+00
216	9.5471E+00	0.0000E+00
217	7.3271E+00	0.0000E+00
218	7.3302E+00	0.0000E+00
219	7.4099E+00	0.0000E+00
220	8.2504E+00	0.0000E+00
221	8.9060E+00	0.0000E+00
222	9.1897E+00	0.0000E+00
223	9.3466E+00	0.0000E+00
224	9.4509E+00	0.0000E+00
225	9.5214E+00	0.0000E+00
226	9.5598E+00	0.0000E+00
227	9.5763E+00	0.0000E+00
228	9.5824E+00	0.0000E+00
229	9.5844E+00	0.0000E+00
230	9.5848E+00	0.0000E+00
231	9.5847E+00	0.0000E+00
232	9.5843E+00	0.0000E+00
233	9.5841E+00	0.0000E+00

234	9.5840E+00	0.0000E+00
235	7.3271E+00	0.0000E+00
236	7.3288E+00	0.0000E+00
237	7.3851E+00	0.0000E+00
238	8.1637E+00	0.0000E+00
239	8.8961E+00	0.0000E+00
240	9.1931E+00	0.0000E+00
241	9.3440E+00	0.0000E+00
242	9.4536E+00	0.0000E+00
243	9.5333E+00	0.0000E+00
244	9.5735E+00	0.0000E+00
245	9.5915E+00	0.0000E+00
246	9.5996E+00	0.0000E+00
247	9.6029E+00	0.0000E+00
248	9.6043E+00	0.0000E+00
249	9.6047E+00	0.0000E+00
250	9.6047E+00	0.0000E+00
251	9.6046E+00	0.0000E+00
252	9.6046E+00	0.0000E+00
253	7.3270E+00	0.0000E+00
254	7.3283E+00	0.0000E+00
255	7.3632E+00	0.0000E+00
256	7.9745E+00	0.0000E+00
257	8.8100E+00	0.0000E+00
258	9.1604E+00	0.0000E+00
259	9.3192E+00	0.0000E+00
260	9.4466E+00	0.0000E+00
261	9.5378E+00	0.0000E+00
262	9.5743E+00	0.0000E+00
263	9.5949E+00	0.0000E+00
264	9.6060E+00	0.0000E+00
265	9.6106E+00	0.0000E+00
266	9.6125E+00	0.0000E+00
267	9.6133E+00	0.0000E+00
268	9.6134E+00	0.0000E+00
269	9.6134E+00	0.0000E+00
270	9.6134E+00	0.0000E+00
271	7.3268E+00	0.0000E+00
272	7.3282E+00	0.0000E+00
273	7.3428E+00	0.0000E+00
274	7.6277E+00	0.0000E+00
275	8.4024E+00	0.0000E+00
276	8.9600E+00	0.0000E+00
277	9.1949E+00	0.0000E+00
278	9.4094E+00	0.0000E+00
279	9.5374E+00	0.0000E+00
280	9.5581E+00	0.0000E+00
281	9.5818E+00	0.0000E+00
282	9.6068E+00	0.0000E+00
283	9.6102E+00	0.0000E+00
284	9.6122E+00	0.0000E+00
285	9.6137E+00	0.0000E+00
286	9.6134E+00	0.0000E+00
287	9.6134E+00	0.0000E+00
288	9.6140E+00	0.0000E+00

289	7.3268E+00	0.0000E+00
290	7.3274E+00	0.0000E+00
291	7.3365E+00	0.0000E+00
292	7.4516E+00	0.0000E+00
293	7.8128E+00	0.0000E+00
294	8.5468E+00	0.0000E+00
295	8.9655E+00	0.0000E+00
296	9.3249E+00	0.0000E+00
297	9.4657E+00	0.0000E+00
298	9.3232E+00	0.0000E+00
299	9.2954E+00	0.0000E+00
300	9.4296E+00	0.0000E+00
301	9.3939E+00	0.0000E+00
302	9.3770E+00	0.0000E+00
303	9.4558E+00	0.0000E+00
304	9.3938E+00	0.0000E+00
305	9.3852E+00	0.0000E+00
306	9.4574E+00	0.0000E+00
307	7.3268E+00	0.0000E+00
308	7.3271E+00	0.0000E+00
309	7.3324E+00	0.0000E+00
310	7.3851E+00	0.0000E+00
311	7.5122E+00	0.0000E+00
312	7.9738E+00	0.0000E+00
313	8.6583E+00	0.0000E+00
314	9.1801E+00	0.0000E+00
315	9.3370E+00	0.0000E+00
316	7.5599E+00	0.0000E+00
317	7.2269E+00	0.0000E+00
318	9.3120E+00	0.0000E+00
319	7.4173E+00	0.0000E+00
320	7.2480E+00	0.0000E+00
321	9.3271E+00	0.0000E+00
322	7.3332E+00	0.0000E+00
323	7.2770E+00	0.0000E+00
324	9.3227E+00	0.0000E+00
325	7.3268E+00	0.0000E+00
326	7.3269E+00	0.0000E+00
327	7.3298E+00	0.0000E+00
328	7.3572E+00	0.0000E+00
329	7.4183E+00	0.0000E+00
330	7.6216E+00	0.0000E+00
331	8.2106E+00	0.0000E+00
332	9.0073E+00	0.0000E+00
333	9.2325E+00	0.0000E+00
334	9.0297E+00	0.0000E+00
335	8.7851E+00	0.0000E+00
336	9.0606E+00	0.0000E+00
337	9.0229E+00	0.0000E+00
338	8.9300E+00	0.0000E+00
339	9.1185E+00	0.0000E+00
340	8.9670E+00	0.0000E+00
341	8.9332E+00	0.0000E+00
342	9.1246E+00	0.0000E+00
343	7.3268E+00	0.0000E+00

344	7.3268E+00	0.0000E+00
345	7.3281E+00	0.0000E+00
346	7.3442E+00	0.0000E+00
347	7.3826E+00	0.0000E+00
348	7.4923E+00	0.0000E+00
349	7.8879E+00	0.0000E+00
350	8.8003E+00	0.0000E+00
351	9.1388E+00	0.0000E+00
352	8.0296E+00	0.0000E+00
353	7.2439E+00	0.0000E+00
354	9.1980E+00	0.0000E+00
355	7.5296E+00	0.0000E+00
356	7.2834E+00	0.0000E+00
357	9.1935E+00	0.0000E+00
358	7.4021E+00	0.0000E+00
359	7.3362E+00	0.0000E+00
360	9.1848E+00	0.0000E+00
361	7.3268E+00	0.0000E+00
362	7.3268E+00	0.0000E+00
363	7.3271E+00	0.0000E+00
364	7.3361E+00	0.0000E+00
365	7.3641E+00	0.0000E+00
366	7.4501E+00	0.0000E+00
367	7.7032E+00	0.0000E+00
368	8.5371E+00	0.0000E+00
369	9.0585E+00	0.0000E+00
370	9.1363E+00	0.0000E+00
371	9.1733E+00	0.0000E+00
372	9.1793E+00	0.0000E+00
373	9.1785E+00	0.0000E+00
374	9.1679E+00	0.0000E+00
375	9.1589E+00	0.0000E+00
376	9.1536E+00	0.0000E+00
377	9.1491E+00	0.0000E+00
378	9.1486E+00	0.0000E+00
379	7.3268E+00	0.0000E+00
380	7.3268E+00	0.0000E+00
381	7.3269E+00	0.0000E+00
382	7.3305E+00	0.0000E+00
383	7.3483E+00	0.0000E+00
384	7.4188E+00	0.0000E+00
385	7.6372E+00	0.0000E+00
386	8.4619E+00	0.0000E+00
387	9.0903E+00	0.0000E+00
388	9.1690E+00	0.0000E+00
389	9.1834E+00	0.0000E+00
390	9.1776E+00	0.0000E+00
391	9.1658E+00	0.0000E+00
392	9.1547E+00	0.0000E+00
393	9.1459E+00	0.0000E+00
394	9.1402E+00	0.0000E+00
395	9.1370E+00	0.0000E+00
396	9.1357E+00	0.0000E+00
397	7.3268E+00	0.0000E+00
398	7.3268E+00	0.0000E+00

399	7.3268E+00	0.0000E+00
400	7.3276E+00	0.0000E+00
401	7.3342E+00	0.0000E+00
402	7.3757E+00	0.0000E+00
403	7.6057E+00	0.0000E+00
404	8.4839E+00	0.0000E+00
405	8.7976E+00	0.0000E+00
406	8.8721E+00	0.0000E+00
407	8.8740E+00	0.0000E+00
408	8.8618E+00	0.0000E+00
409	8.8468E+00	0.0000E+00
410	8.8339E+00	0.0000E+00
411	8.8248E+00	0.0000E+00
412	8.8196E+00	0.0000E+00
413	8.8173E+00	0.0000E+00
414	8.8151E+00	0.0000E+00
415	7.3268E+00	0.0000E+00
416	7.3268E+00	0.0000E+00
417	7.3268E+00	0.0000E+00
418	7.3272E+00	0.0000E+00
419	7.3290E+00	0.0000E+00
420	7.3626E+00	0.0000E+00
421	7.4909E+00	0.0000E+00
422	7.6298E+00	0.0000E+00
423	7.6830E+00	0.0000E+00
424	7.6956E+00	0.0000E+00
425	7.6801E+00	0.0000E+00
426	7.6595E+00	0.0000E+00
427	7.6411E+00	0.0000E+00
428	7.6256E+00	0.0000E+00
429	7.6131E+00	0.0000E+00
430	7.6028E+00	0.0000E+00
431	7.5945E+00	0.0000E+00
432	7.5800E+00	0.0000E+00
433	7.3268E+00	0.0000E+00
434	7.3268E+00	0.0000E+00
435	7.3268E+00	0.0000E+00
436	7.3268E+00	0.0000E+00
437	7.3268E+00	0.0000E+00
438	7.3268E+00	0.0000E+00
439	7.3268E+00	0.0000E+00
440	7.3268E+00	0.0000E+00
441	7.3268E+00	0.0000E+00
442	7.3268E+00	0.0000E+00
443	7.3268E+00	0.0000E+00
444	7.3268E+00	0.0000E+00
445	7.3268E+00	0.0000E+00
446	7.3268E+00	0.0000E+00
447	7.3268E+00	0.0000E+00
448	7.3268E+00	0.0000E+00
449	7.3268E+00	0.0000E+00
450	7.3268E+00	0.0000E+00

B.4.1 BLT-EC Chemistry Output File for the Two-Dimensional Reactive Transport Problem

The chemistry output file is:

```
_____ PART 1 of OUTPUT FILE _____
2D EXAMPLE PROBLEM
SAME MESH AS PROB 5 IN NUREG 6305

---
 Temperature (Celsius):  25.00
 Units of concentration: MOLAL
 Ionic strength:  0.000 molal; FIXED
 If specified, carbonate concentration represents total inorganic carbon.
 Do not automatically terminate if charge imbalance exceeds 30%
 Precipitation is allowed for all solids in the thermodynamic database and
   the print option for solids is set to: 1
 The maximum number of iterations is: 200
 The method used to compute activity coefficients is: Davies equation
 Abbreviated output file
 Adsorption model: Activity Langmuir
 Number of adsorbing surfaces: 1

---
81
0.000E+00   0.00 0.000 0.000
0.000E+00   0.00 0.000 0.000
0.000E+00   0.00 0.000 0.000
0.000E+00   0.00 0.000 0.000
0.000E+00   0.00 0.000 0.000


COMPONENTS AND REACTIONS SPECIFIED IN THE CHEMISTRY INPUT FILE


   811  0.000E+00   0.00 y
   330  0.000E+00   0.00 y
   150  0.000E+00   0.00 y
   140  0.000E+00   0.00 y
   460  0.000E+00   0.00 y
   580  0.000E+00   0.00 y
   732  0.000E+00   0.00
   950  0.000E+00   0.00 y
   893  0.000E+00   0.00 y
8118930 sohm1
  0.000000000000000      3.00000000000000          3   1.00000
     811   1.00000        893  -1.00000        330       0
  0.000000000000000      0.000000000000000         0       0
  0.000000000000000      0.000000000000000         0       0
  0.000000000000000      0.000000000000000         0       0
  0.000000000000000      0.000000000000000         0       0
8113300 so
  0.000000000000000     -10.3000000000000          2   1.00000
     811  -1.00000        330       0  0.000000000000000
  0.000000000000000          0       0  0.000000000000000
```

```
 0.000000000000000          0        0  0.000000000000000
 0.000000000000000          0        0  0.000000000000000
 0.000000000000000          0        0
8113301 sohh
 0.000000000000000   5.40000000000000          2   1.00000
    811   1.00000        330        0  0.000000000000000
 0.000000000000000          0        0  0.000000000000000
 0.000000000000000          0        0  0.000000000000000
 0.000000000000000          0        0  0.000000000000000
 0.000000000000000          0        0
```

****
****

CHEMICAL CONDITIONS AT NODE 234
TIME = 0.000000E+00

```
 ---------------------------------------
| IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION: |
|    CO3-2     Log activity guess:  -12.77    |
|    PO4-3     Log activity guess:  -17.94    |
|    SO4-2     Log activity guess:   -4.53    |
|                                     |
 ---------------------------------------
```

1

PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
0	UO2+2	1.000E-20	9.124E-19	-20.00000	9.124E-19
1	UO2+2	1.000E-20	1.558E-18	-21.00000	1.558E-18
2	UO2+2	1.000E-20	5.317E-18	-22.00000	5.317E-18
3	UO2+2	1.000E-20	6.012E-18	-23.00000	6.012E-18
4	UO2+2	1.000E-20	1.514E-18	-24.00000	1.514E-18
5	UO2+2	1.000E-20	2.798E-17	-23.24833	2.798E-17
6	UO2+2	1.000E-20	4.336E-18	-23.05192	4.336E-18
7	UO2+2	1.000E-20	1.260E-18	-23.44567	1.260E-18
8	UO2+2	1.000E-20	4.897E-20	-24.76318	4.897E-20
9	UO2+2	1.000E-20	1.371E-22	-25.52670	1.371E-22

ID	NAME	ANAL MOL	CALC MOL	LOG ACTVTY	GAMMA	DIFF FXN
811	ADS1TYP1	1.000E-05	9.873E-06	-5.00557	1.000000	8.470E-21
330	H+1	1.100E-04	4.712E-08	-7.32681	1.000000	1.274E-18
150	Ca+2	1.700E-04	1.688E-04	-3.77258	1.000000	-1.355E-19
140	CO3-2	1.000E-04	8.948E-08	-7.04829	1.000000	-3.158E-18
460	Mg+2	1.200E-04	1.192E-04	-3.92360	1.000000	-1.220E-19
580	PO4-3	5.000E-07	2.446E-12	-11.61159	1.000000	-2.824E-18

```
 732 SO4-2      3.000E-05 2.842E-05  -4.54645   1.000000  3.727E-20
 950 Zn+2       7.600E-07 7.142E-07  -6.14617   1.000000  3.282E-20
 893 UO2+2       1.000E-20 2.933E-26 -25.53262   1.000000 -3.952E-28
   2 H2O        1.000E-32 -2.430E-07   0.00000   1.000000  0.000E+00
1
```

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

```
+ADS1TYP1
+          98.7   PERCENT BOUND IN SPECIES #   811  ADS1TYP1

+           1.2   PERCENT BOUND IN SPECIES #8113301  sohh


+H+1
+          81.9   PERCENT BOUND IN SPECIES #3301400  HCO3 -

+          17.3   PERCENT BOUND IN SPECIES #3301401  H2CO3 AQ


+Ca+2
+          99.3   PERCENT BOUND IN SPECIES #   150  Ca+2


+CO3-2
+          90.0   PERCENT BOUND IN SPECIES #3301400  HCO3 -

+           9.5   PERCENT BOUND IN SPECIES #3301401  H2CO3 AQ


+Mg+2
+          99.4   PERCENT BOUND IN SPECIES #   460  Mg+2


+PO4-3
+           4.6   PERCENT BOUND IN SPECIES #4605802  MgHPO4 AQ

+           4.7   PERCENT BOUND IN SPECIES #1505800  CaHPO4 AQ

+          51.1   PERCENT BOUND IN SPECIES #3305800  HPO4 -2

+          38.8   PERCENT BOUND IN SPECIES #3305801  H2PO4 -


+SO4-2
+          94.7   PERCENT BOUND IN SPECIES #   732  SO4-2

+           2.0   PERCENT BOUND IN SPECIES #4607320  MgSO4 AQ

+           3.3   PERCENT BOUND IN SPECIES #1507320  CaSO4 AQ


+Zn+2
```

```
+          94.0   PERCENT BOUND IN SPECIES #   950  Zn+2

+           2.2   PERCENT BOUND IN SPECIES #9503300  ZnOH +

+           1.7   PERCENT BOUND IN SPECIES #9501401  ZnCO3 AQ


+UO2+2
+          37.9   PERCENT BOUND IN SPECIES #8935801  UO2HPO4)2

+          61.5   PERCENT BOUND IN SPECIES #8118930  sohm1


+H2O
+          87.7   PERCENT BOUND IN SPECIES #3300020  OH-

+           1.7   PERCENT BOUND IN SPECIES #4603300  MgOH +

+           6.8   PERCENT BOUND IN SPECIES #9503300  ZnOH +

+           3.3   PERCENT BOUND IN SPECIES #9503301  Zn(OH)2 AQ

1
```

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
330	H+1	1.099E-04	99.9	1.063E-07	0.1	0.000E+00	0.0
150	Ca+2	1.700E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.000E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.200E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	5.000E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	3.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	7.600E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
893	UO2+2	3.854E-21	38.5	6.146E-21	61.5	0.000E+00	0.0
2	H2O	2.430E-07	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 5.779E-04 Sum of ANIONS 1.480E-04
PERCENT DIFFERENCE = 5.923E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 0.000E+00
EQUILIBRIUM pH = 7.327

****
****

CHEMICAL CONDITIONS AT NODE 320
TIME = 0.000000E+00

```
 ------------------------------------------
| IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION: |
|    CO3-2     Log activity guess:  -11.89    |
|    PO4-3     Log activity guess:  -17.06    |
|    SO4-2     Log activity guess:   -4.52    |
|                                  |
 ------------------------------------------
```

1

PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
0	UO2+2	1.000E-20	2.517E-18	-20.00000	2.517E-18
1	UO2+2	1.000E-20	9.671E-18	-21.00000	9.671E-18
2	UO2+2	1.000E-20	3.312E-17	-22.00000	3.312E-17
3	UO2+2	1.000E-20	2.652E-17	-23.00000	2.652E-17
4	UO2+2	1.000E-20	9.659E-18	-24.00000	9.659E-18
5	UO2+2	1.000E-20	1.522E-18	-25.00000	1.522E-18
6	UO2+2	1.000E-20	6.472E-19	-26.00000	6.472E-19
7	UO2+2	1.000E-20	7.027E-20	-26.88853	7.027E-20
8	UO2+2	1.000E-20	6.632E-21	-27.52601	6.632E-21
9	UO2+2	1.000E-20	1.051E-23	-27.74583	1.050E-23

1

PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
10	UO2+2	1.000E-20	-9.266E-24	-27.74628	9.256E-24
11	Zn+2	7.600E-07	-2.897E-11	-8.36293	2.821E-11

ID	NAME	ANAL MOL	CALC MOL	LOG ACTVTY	GAMMA	DIFF FXN
811	ADS1TYP1	1.000E-05	8.466E-06	-5.07235	1.000000	2.421E-15
330	H+1	4.000E-05	2.766E-10	-9.55813	1.000000	-7.475E-14
150	Ca+2	2.450E-04	2.378E-04	-3.62375	1.000000	3.049E-16
140	CO3-2	1.000E-04	1.354E-05	-4.86836	1.000000	-1.920E-14
460	Mg+2	1.200E-04	1.171E-04	-3.93145	1.000000	1.085E-15
893	UO2+2	1.000E-20	1.810E-28	-27.74232	1.000000	-8.994E-30
732	SO4-2	3.000E-05	2.806E-05	-4.55197	1.000000	-4.405E-20
950	Zn+2	7.600E-07	4.336E-09	-8.36288	1.000000	-3.295E-15
580	PO4-3	5.000E-07	1.320E-12	-11.87946	1.000000	-6.776E-21
2	H2O	1.000E-32	-3.887E-05	0.00000	1.000000	0.000E+00

1

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

```
+ADS1TYP1
+          84.7   PERCENT BOUND IN SPECIES #   811  ADS1TYP1

+          15.3   PERCENT BOUND IN SPECIES #8113300  so


+H+1
+         199.2   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Ca+2
+          97.4   PERCENT BOUND IN SPECIES #   150  Ca+2

+           1.9   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ


+CO3-2
+          13.5   PERCENT BOUND IN SPECIES #   140  CO3-2

+           1.5   PERCENT BOUND IN SPECIES #4601400  MgCO3 AQ

+           4.6   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ

+          80.0   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Mg+2
+          97.6   PERCENT BOUND IN SPECIES #   460  Mg+2

+           1.3   PERCENT BOUND IN SPECIES #4601400  MgCO3 AQ


+UO2+2
+          33.4   PERCENT BOUND IN SPECIES #8931401  UO2CO3)2-2

+          10.9   PERCENT BOUND IN SPECIES #8931402  UO2CO3)3-4

+          55.4   PERCENT BOUND IN SPECIES #8118930  sohm1


+SO4-2
+          93.5   PERCENT BOUND IN SPECIES #   732  SO4-2

+           1.9   PERCENT BOUND IN SPECIES #4607320  MgSO4 AQ

+           4.5   PERCENT BOUND IN SPECIES #1507320  CaSO4 AQ


+Zn+2
+           2.3   PERCENT BOUND IN SPECIES #9503300  ZnOH +

+          94.1   PERCENT BOUND IN SPECIES #9503301  Zn(OH)2 AQ

+           1.1   PERCENT BOUND IN SPECIES #9503302  Zn(OH)3 -

+           1.5   PERCENT BOUND IN SPECIES #9501401  ZnCO3 AQ
```

+PO4-3
+ 24.0 PERCENT BOUND IN SPECIES #4605800 MgPO4 -

+ 2.8 PERCENT BOUND IN SPECIES #4605802 MgHPO4 AQ

+ 4.2 PERCENT BOUND IN SPECIES #1505800 CaHPO4 AQ

+ 36.2 PERCENT BOUND IN SPECIES #1505801 CaPO4 -

+ 32.5 PERCENT BOUND IN SPECIES #3305800 HPO4 -2

+H2O
+ 93.8 PERCENT BOUND IN SPECIES #3300020 OH-

+ 1.8 PERCENT BOUND IN SPECIES #4603300 MgOH +

+ 3.7 PERCENT BOUND IN SPECIES #9503301 Zn(OH)2 AQ

1

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
330	H+1	4.170E-05	103.8	-1.533E-06	-3.8	0.000E+00	0.0
150	Ca+2	2.442E-04	99.7	0.000E+00	0.0	8.292E-07	0.3
140	CO3-2	1.000E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.200E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
893	UO2+2	4.461E-21	44.6	5.539E-21	55.4	0.000E+00	0.0
732	SO4-2	3.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	7.600E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	2.494E-09	0.5	0.000E+00	0.0	4.975E-07	99.5
2	H2O	3.870E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 7.111E-04 Sum of ANIONS 1.995E-04
PERCENT DIFFERENCE = 5.618E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 0.000E+00
EQUILIBRIUM pH = 9.558

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CHEMICAL CONDITIONS AT NODE 321
TIME = 0.000000E+00

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| IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION: |
|    CO3-2     Log activity guess:  -11.89    |
|    PO4-3     Log activity guess:  -17.06    |
|    SO4-2     Log activity guess:  -4.52     |
|                                             |
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PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
0	UO2+2	1.000E-20	2.517E-18	-20.00000	2.517E-18
1	UO2+2	1.000E-20	9.671E-18	-21.00000	9.671E-18
2	UO2+2	1.000E-20	3.312E-17	-22.00000	3.312E-17
3	UO2+2	1.000E-20	2.652E-17	-23.00000	2.652E-17
4	UO2+2	1.000E-20	9.659E-18	-24.00000	9.659E-18
5	UO2+2	1.000E-20	1.522E-18	-25.00000	1.522E-18
6	UO2+2	1.000E-20	6.472E-19	-26.00000	6.472E-19
7	UO2+2	1.000E-20	7.027E-20	-26.88853	7.027E-20
8	UO2+2	1.000E-20	6.632E-21	-27.52601	6.632E-21
9	UO2+2	1.000E-20	1.051E-23	-27.74583	1.050E-23

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PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
10	UO2+2	1.000E-20	-9.266E-24	-27.74628	9.256E-24
11	Zn+2	7.600E-07	-2.897E-11	-8.36293	2.821E-11

ID	NAME	ANAL MOL	CALC MOL	LOG ACTVTY	GAMMA	DIFF FXN
811	ADS1TYP1	1.000E-05	8.466E-06	-5.07235	1.000000	2.421E-15
330	H+1	4.000E-05	2.766E-10	-9.55813	1.000000	-7.475E-14
150	Ca+2	2.450E-04	2.378E-04	-3.62375	1.000000	3.049E-16
140	CO3-2	1.000E-04	1.354E-05	-4.86836	1.000000	-1.920E-14
460	Mg+2	1.200E-04	1.171E-04	-3.93145	1.000000	1.085E-15
893	UO2+2	1.000E-20	1.810E-28	-27.74232	1.000000	-8.994E-30
732	SO4-2	3.000E-05	2.806E-05	-4.55197	1.000000	-4.405E-20
950	Zn+2	7.600E-07	4.336E-09	-8.36288	1.000000	-3.295E-15
580	PO4-3	5.000E-07	1.320E-12	-11.87946	1.000000	-6.776E-21
2	H2O	1.000E-32	-3.887E-05	0.00000	1.000000	0.000E+00

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PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

+ADS1TYP1

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+          84.7   PERCENT BOUND IN SPECIES #   811  ADS1TYP1

+          15.3   PERCENT BOUND IN SPECIES #8113300  so


+H+1
+         199.2   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Ca+2
+          97.4   PERCENT BOUND IN SPECIES #   150  Ca+2

+           1.9   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ


+CO3-2
+          13.5   PERCENT BOUND IN SPECIES #   140  CO3-2

+           1.5   PERCENT BOUND IN SPECIES #4601400  MgCO3 AQ

+           4.6   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ

+          80.0   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Mg+2
+          97.6   PERCENT BOUND IN SPECIES #   460  Mg+2

+           1.3   PERCENT BOUND IN SPECIES #4601400  MgCO3 AQ


+UO2+2
+          33.4   PERCENT BOUND IN SPECIES #8931401  UO2CO3)2-2

+          10.9   PERCENT BOUND IN SPECIES #8931402  UO2CO3)3-4

+          55.4   PERCENT BOUND IN SPECIES #8118930  sohm1


+SO4-2
+          93.5   PERCENT BOUND IN SPECIES #   732  SO4-2

+           1.9   PERCENT BOUND IN SPECIES #4607320  MgSO4 AQ

+           4.5   PERCENT BOUND IN SPECIES #1507320  CaSO4 AQ


+Zn+2
+           2.3   PERCENT BOUND IN SPECIES #9503300  ZnOH +

+          94.1   PERCENT BOUND IN SPECIES #9503301  Zn(OH)2 AQ

+           1.1   PERCENT BOUND IN SPECIES #9503302  Zn(OH)3 -

+           1.5   PERCENT BOUND IN SPECIES #9501401  ZnCO3 AQ


+PO4-3
+          24.0   PERCENT BOUND IN SPECIES #4605800  MgPO4 -
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+          2.8   PERCENT BOUND IN SPECIES #4605802  MgHPO4 AQ

+          4.2   PERCENT BOUND IN SPECIES #1505800  CaHPO4 AQ

+         36.2   PERCENT BOUND IN SPECIES #1505801  CaPO4 -

+         32.5   PERCENT BOUND IN SPECIES #3305800  HPO4 -2


+H2O
+         93.8   PERCENT BOUND IN SPECIES #3300020  OH-

+          1.8   PERCENT BOUND IN SPECIES #4603300  MgOH +

+          3.7   PERCENT BOUND IN SPECIES #9503301  Zn(OH)2 AQ

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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
330	H+1	4.170E-05	103.8	-1.533E-06	-3.8	0.000E+00	0.0
150	Ca+2	2.442E-04	99.7	0.000E+00	0.0	8.292E-07	0.3
140	CO3-2	1.000E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.200E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
893	UO2+2	4.461E-21	44.6	5.539E-21	55.4	0.000E+00	0.0
732	SO4-2	3.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	7.600E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	2.494E-09	0.5	0.000E+00	0.0	4.975E-07	99.5
2	H2O	3.870E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 7.111E-04 Sum of ANIONS 1.995E-04
PERCENT DIFFERENCE = 5.618E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 0.000E+00
EQUILIBRIUM pH = 9.558

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CHEMICAL CONDITIONS AT NODE 234
TIME = 0.189346E+10

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
CO3-2 Log activity guess: -11.77
PO4-3 Log activity guess: -17.25
SO4-2 Log activity guess: -4.52

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PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
0	UO2+2	4.553E-07	1.321E-04	-6.34173	1.321E-04
1	UO2+2	4.553E-07	5.236E-04	-7.34173	5.236E-04
2	UO2+2	4.553E-07	1.721E-03	-8.34173	1.721E-03
3	UO2+2	4.553E-07	1.343E-03	-9.34173	1.343E-03
4	UO2+2	4.553E-07	1.104E-03	-10.34173	1.104E-03
5	UO2+2	4.553E-07	1.571E-02	-11.34173	1.571E-02
6	UO2+2	4.553E-07	4.671E-03	-11.50953	4.671E-03
7	UO2+2	4.553E-07	4.791E-04	-12.02270	4.791E-04
8	UO2+2	4.553E-07	1.095E-04	-12.31190	1.095E-04
9	UO2+2	4.553E-07	3.243E-05	-12.53098	3.243E-05
10	UO2+2	4.553E-07	1.058E-05	-12.77731	1.058E-05
11	UO2+2	4.553E-07	3.003E-06	-13.19177	3.003E-06
12	UO2+2	4.553E-07	-8.712E-09	-14.10485	8.712E-09
13	UO2+2	4.553E-07	1.587E-11	-14.10170	1.541E-11

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PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
14	UO2+2	4.553E-07	-9.270E-11	-14.10171	9.224E-11
15	Zn+2	7.600E-07	-6.135E-12	-8.41324	5.375E-12

ID	NAME	ANAL MOL	CALC MOL	LOG ACTVTY	GAMMA	DIFF FXN
811	ADS1TYP1	1.000E-05	8.178E-06	-5.08737	1.000000	9.952E-17
330	H+1	3.456E-05	2.606E-10	-9.58397	1.000000	-3.401E-15
150	Ca+2	2.329E-04	2.264E-04	-3.64515	1.000000	1.347E-17
140	CO3-2	9.772E-05	1.384E-05	-4.85873	1.000000	-8.554E-16
460	Mg+2	1.200E-04	1.170E-04	-3.93172	1.000000	5.008E-17
893	UO2+2	4.553E-07	7.943E-15	-14.10000	1.000000	-1.625E-17
732	SO4-2	3.000E-05	2.812E-05	-4.55101	1.000000	-2.033E-20
950	Zn+2	7.600E-07	3.862E-09	-8.41323	1.000000	-1.458E-16
580	PO4-3	2.414E-07	1.405E-12	-11.85240	1.000000	0.000E+00
2	H2O	1.000E-32	-4.106E-05	0.00000	1.000000	0.000E+00

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PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

```
+ADS1TYP1
+          81.8   PERCENT BOUND IN SPECIES #   811  ADS1TYP1

+           2.5   PERCENT BOUND IN SPECIES #8118930  sohm1

+          15.7   PERCENT BOUND IN SPECIES #8113300  so


+H+1
+         222.5   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Ca+2
+          97.4   PERCENT BOUND IN SPECIES #   150  Ca+2

+           1.9   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ


+CO3-2
+          14.2   PERCENT BOUND IN SPECIES #   140  CO3-2

+           1.6   PERCENT BOUND IN SPECIES #4601400  MgCO3 AQ

+           4.6   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ

+          78.9   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Mg+2
+          97.5   PERCENT BOUND IN SPECIES #   460  Mg+2

+           1.3   PERCENT BOUND IN SPECIES #4601400  MgCO3 AQ


+UO2+2
+          33.6   PERCENT BOUND IN SPECIES #8931401  UO2CO3)2-2

+          11.2   PERCENT BOUND IN SPECIES #8931402  UO2CO3)3-4

+          54.7   PERCENT BOUND IN SPECIES #8118930  sohm1


+SO4-2
+          93.7   PERCENT BOUND IN SPECIES #   732  SO4-2

+           2.0   PERCENT BOUND IN SPECIES #4607320  MgSO4 AQ

+           4.3   PERCENT BOUND IN SPECIES #1507320  CaSO4 AQ


+Zn+2
+           2.1   PERCENT BOUND IN SPECIES #9503300  ZnOH +

+          94.4   PERCENT BOUND IN SPECIES #9503301  Zn(OH)2 AQ

+           1.1   PERCENT BOUND IN SPECIES #9503302  Zn(OH)3 -

+           1.4   PERCENT BOUND IN SPECIES #9501401  ZnCO3 AQ
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+PO4-3
+ 25.1 PERCENT BOUND IN SPECIES #4605800 MgPO4 -

+ 2.8 PERCENT BOUND IN SPECIES #4605802 MgHPO4 AQ

+ 4.0 PERCENT BOUND IN SPECIES #1505800 CaHPO4 AQ

+ 36.0 PERCENT BOUND IN SPECIES #1505801 CaPO4 -

+ 31.9 PERCENT BOUND IN SPECIES #3305800 HPO4 -2

+H2O
+ 94.1 PERCENT BOUND IN SPECIES #3300020 OH-

+ 1.8 PERCENT BOUND IN SPECIES #4603300 MgOH +

+ 3.5 PERCENT BOUND IN SPECIES #9503301 Zn(OH)2 AQ

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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
330	H+1	3.646E-05	105.3	-1.821E-06	-5.3	0.000E+00	0.0
150	Ca+2	2.325E-04	99.8	0.000E+00	0.0	3.982E-07	0.2
140	CO3-2	9.772E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.200E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
893	UO2+2	2.060E-07	45.3	2.492E-07	54.7	0.000E+00	0.0
732	SO4-2	3.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	7.600E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	2.542E-09	1.1	0.000E+00	0.0	2.389E-07	98.9
2	H2O	4.098E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 6.881E-04 Sum of ANIONS 2.001E-04
PERCENT DIFFERENCE = 5.495E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 0.000E+00
EQUILIBRIUM pH = 9.584

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CHEMICAL CONDITIONS AT NODE 320
TIME = 0.189346E+10

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| IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION: |
|    CO3-2     Log activity guess:  -12.15    |
|    PO4-3     Log activity guess:  -19.09    |
|    SO4-2     Log activity guess:  -4.53     |
|                                  |
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PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
0	UO2+2	3.355E-05	6.220E-03	-4.47433	6.220E-03
1	UO2+2	3.355E-05	4.716E-03	-5.47433	4.716E-03
2	UO2+2	3.355E-05	1.015E-02	-6.47433	1.015E-02
3	UO2+2	3.355E-05	9.224E-02	-7.47433	9.224E-02
4	UO2+2	3.355E-05	4.506E-03	-8.47433	4.506E-03
5	UO2+2	3.355E-05	1.060E-03	-8.51377	1.060E-03
6	UO2+2	3.355E-05	1.558E-04	-8.97044	1.558E-04
7	UO2+2	3.355E-05	1.823E-05	-9.27795	1.823E-05
8	UO2+2	3.355E-05	4.793E-07	-9.32579	4.793E-07
9	UO2+2	3.355E-05	3.435E-10	-9.32349	3.099E-10

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PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
10	PO4-3	8.482E-09	-4.443E-09	-13.43035	4.443E-09
11	Zn+2	7.600E-07	7.550E-08	-6.09443	7.550E-08
12	Zn+2	7.600E-07	1.730E-10	-6.14193	1.722E-10
13	Zn+2	7.600E-07	1.358E-10	-6.14209	1.350E-10
14	Zn+2	7.600E-07	8.920E-13	-6.14227	1.320E-13
15	PO4-3	8.482E-09	9.903E-13	-13.98397	9.818E-13

ID	NAME	ANAL MOL	CALC MOL	LOG ACTVTY	GAMMA	DIFF FXN
811	ADS1TYP1	1.000E-05	6.521E-07	-6.18571	1.000000	3.388E-21
330	H+1	5.400E-05	5.649E-08	-7.24804	1.000000	5.498E-17
150	Ca+2	2.072E-04	2.058E-04	-3.68654	1.000000	-8.132E-20
140	CO3-2	9.989E-05	7.200E-08	-7.14269	1.000000	-1.355E-20
460	Mg+2	1.200E-04	1.193E-04	-3.92347	1.000000	1.355E-20
580	PO4-3	8.482E-09	1.038E-14	-13.98400	1.000000	2.750E-17
732	SO4-2	3.000E-05	2.821E-05	-4.54954	1.000000	-1.355E-20
950	Zn+2	7.600E-07	7.207E-07	-6.14227	1.000000	4.235E-22
893	UO2+2	3.355E-05	8.090E-10	-9.09206	1.000000	-1.323E-22
2	H2O	1.000E-32	-6.818E-05	0.00000	1.000000	0.000E+00

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PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

+ADS1TYP1
+ 6.5 PERCENT BOUND IN SPECIES # 811 ADS1TYP1

+ 93.4 PERCENT BOUND IN SPECIES #8118930 sohm1

+H+1
+ 88.2 PERCENT BOUND IN SPECIES #3301400 HCO3 -

+ 22.4 PERCENT BOUND IN SPECIES #3301401 H2CO3 AQ

+Ca+2
+ 99.3 PERCENT BOUND IN SPECIES # 150 Ca+2

+CO3-2
+ 87.0 PERCENT BOUND IN SPECIES #3301400 HCO3 -

+ 11.0 PERCENT BOUND IN SPECIES #3301401 H2CO3 AQ

+Mg+2
+ 99.4 PERCENT BOUND IN SPECIES # 460 Mg+2

+PO4-3
+ 1.4 PERCENT BOUND IN SPECIES #4605802 MgHPO4 AQ

+ 1.7 PERCENT BOUND IN SPECIES #1505800 CaHPO4 AQ

+ 15.3 PERCENT BOUND IN SPECIES #3305800 HPO4 -2

+ 13.9 PERCENT BOUND IN SPECIES #3305801 H2PO4 -

+ 3.6 PERCENT BOUND IN SPECIES #8935800 UO2HPO4 AQ

+ 63.7 PERCENT BOUND IN SPECIES #8935801 UO2HPO4)2

+SO4-2
+ 94.0 PERCENT BOUND IN SPECIES # 732 SO4-2

+ 2.0 PERCENT BOUND IN SPECIES #4607320 MgSO4 AQ

+ 3.9 PERCENT BOUND IN SPECIES #1507320 CaSO4 AQ

+Zn+2
+ 94.8 PERCENT BOUND IN SPECIES # 950 Zn+2

+ 1.8 PERCENT BOUND IN SPECIES #9503300 ZnOH +

+ 1.4 PERCENT BOUND IN SPECIES #9501401 ZnCO3 AQ

+UO2+2
+ 1.0 PERCENT BOUND IN SPECIES #8933300 UO2OH +1

+ 6.2 PERCENT BOUND IN SPECIES #8933302 UO2)3OH5+1

+ 6.5 PERCENT BOUND IN SPECIES #8931400 UO2CO3 AQ

+ 3.7 PERCENT BOUND IN SPECIES #8931401 UO2CO3)2-2

+ 82.5 PERCENT BOUND IN SPECIES #8118930 sohm1

+H2O
+ 11.9 PERCENT BOUND IN SPECIES #3300020 OH-

+ 7.8 PERCENT BOUND IN SPECIES #8933300 UO2OH +1

+ 78.6 PERCENT BOUND IN SPECIES #8933302 UO2)3OH5+1

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PART 5 of OUTPUT FILE

-------- EQUILIBRATED MASS DISTRIBUTION --------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
330	H+1	1.078E-04	109.5	-9.329E-06	-9.5	0.000E+00	0.0
150	Ca+2	2.072E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	9.989E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.200E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	8.482E-09	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	3.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	7.600E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
893	UO2+2	1.981E-06	5.9	9.338E-06	27.8	2.223E-05	66.3
2	H2O	1.494E-06	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 6.523E-04 Sum of ANIONS 1.445E-04
PERCENT DIFFERENCE = 6.374E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 0.000E+00
EQUILIBRIUM pH = 7.248

****
****

CHEMICAL CONDITIONS AT NODE 321
TIME = 0.189346E+10

```
 ---------------------------------------------
| IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION: |
|    CO3-2     Log activity guess:  -12.26    |
|    PO4-3     Log activity guess:  -17.42    |
|    SO4-2     Log activity guess:   -4.53    |
|                                             |
 ---------------------------------------------
1
```

PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
0	UO2+2	1.375E-06	2.241E-04	-5.86185	2.241E-04
1	UO2+2	1.375E-06	5.694E-04	-6.86185	5.694E-04
2	UO2+2	1.375E-06	2.249E-03	-7.86185	2.249E-03
3	UO2+2	1.375E-06	2.147E-03	-8.86185	2.147E-03
4	UO2+2	1.375E-06	1.615E-03	-9.86185	1.615E-03
5	UO2+2	1.375E-06	2.359E-02	-10.86185	2.359E-02
6	UO2+2	1.375E-06	6.960E-03	-11.03528	6.960E-03
7	UO2+2	1.375E-06	8.037E-04	-11.51578	8.037E-04
8	UO2+2	1.375E-06	1.656E-04	-11.83673	1.656E-04
9	UO2+2	1.375E-06	4.713E-05	-12.06044	4.713E-05
10	UO2+2	1.375E-06	1.495E-05	-12.29054	1.495E-05
11	UO2+2	1.375E-06	4.523E-06	-12.62156	4.523E-06
12	UO2+2	1.375E-06	1.628E-07	-13.23157	1.628E-07
13	UO2+2	1.375E-06	-9.222E-09	-13.29922	9.220E-09

1

PART 3 of OUTPUT FILE

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL MOL	DIFF FXN	LOG ACTVTY	RESIDUAL
14	UO2+2	1.375E-06	-5.180E-09	-13.29634	5.178E-09
15	Zn+2	7.600E-07	-1.087E-10	-7.91649	1.079E-10

ID	NAME	ANAL MOL	CALC MOL	LOG ACTVTY	GAMMA	DIFF FXN
811	ADS1TYP1	1.000E-05	8.222E-06	-5.08500	1.000000	4.924E-15
330	H+1	6.164E-05	4.708E-10	-9.32713	1.000000	-7.391E-13
150	Ca+2	2.081E-04	2.033E-04	-3.69176	1.000000	2.683E-15
140	CO3-2	9.986E-05	8.591E-06	-5.06596	1.000000	-2.168E-13
460	Mg+2	1.200E-04	1.179E-04	-3.92845	1.000000	1.154E-14
893	UO2+2	1.375E-06	5.161E-14	-13.28727	1.000000	-2.533E-14
732	SO4-2	3.000E-05	2.824E-05	-4.54916	1.000000	1.694E-20
950	Zn+2	7.600E-07	1.213E-08	-7.91629	1.000000	-5.021E-14
580	PO4-3	5.161E-07	2.046E-12	-11.68911	1.000000	3.388E-21
2	H2O	1.000E-32	-2.346E-05	0.00000	1.000000	0.000E+00

1

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

```
+ADS1TYP1
+        82.2   PERCENT BOUND IN SPECIES #   811  ADS1TYP1

+         9.0   PERCENT BOUND IN SPECIES #8118930  sohm1

+         8.8   PERCENT BOUND IN SPECIES #8113300  so


+H+1
+       139.8   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Ca+2
+        98.1   PERCENT BOUND IN SPECIES #   150  Ca+2

+         1.2   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ


+CO3-2
+         8.6   PERCENT BOUND IN SPECIES #   140  CO3-2

+         2.5   PERCENT BOUND IN SPECIES #1501401  CaCO3 AQ

+        86.5   PERCENT BOUND IN SPECIES #3301400  HCO3 -


+Mg+2
+        98.3   PERCENT BOUND IN SPECIES #   460  Mg+2


+UO2+2
+        27.9   PERCENT BOUND IN SPECIES #8931401  UO2CO3)2-2

+         5.8   PERCENT BOUND IN SPECIES #8931402  UO2CO3)3-4

+        65.6   PERCENT BOUND IN SPECIES #8118930  sohm1


+SO4-2
+        94.1   PERCENT BOUND IN SPECIES #   732  SO4-2

+         2.0   PERCENT BOUND IN SPECIES #4607320  MgSO4 AQ

+         3.9   PERCENT BOUND IN SPECIES #1507320  CaSO4 AQ


+Zn+2
+         1.6   PERCENT BOUND IN SPECIES #   950  Zn+2

+         3.7   PERCENT BOUND IN SPECIES #9503300  ZnOH +

+        90.8   PERCENT BOUND IN SPECIES #9503301  Zn(OH)2 AQ

+         2.7   PERCENT BOUND IN SPECIES #9501401  ZnCO3 AQ
```

```
+PO4-3
+          19.9   PERCENT BOUND IN SPECIES #4605800  MgPO4 -

+          4.0    PERCENT BOUND IN SPECIES #4605802  MgHPO4 AQ

+          5.1    PERCENT BOUND IN SPECIES #1505800  CaHPO4 AQ

+          25.4   PERCENT BOUND IN SPECIES #1505801  CaPO4 -

+          45.3   PERCENT BOUND IN SPECIES #3305800  HPO4 -2


+H2O
+          91.6   PERCENT BOUND IN SPECIES #3300020  OH-

+          1.8    PERCENT BOUND IN SPECIES #4603300  MgOH +

+          5.9    PERCENT BOUND IN SPECIES #9503301  Zn(OH)2 AQ

1
```

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
330	H+1	6.359E-05	102.9	-1.776E-06	-2.9	0.000E+00	0.0
150	Ca+2	2.073E-04	99.6	0.000E+00	0.0	8.523E-07	0.4
140	CO3-2	9.986E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.200E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
893	UO2+2	4.732E-07	34.4	9.013E-07	65.6	0.000E+00	0.0
732	SO4-2	3.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	7.600E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	4.716E-09	0.9	0.000E+00	0.0	5.114E-07	99.1
2	H2O	2.329E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 6.434E-04 Sum of ANIONS 1.825E-04
PERCENT DIFFERENCE = 5.581E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 0.000E+00
EQUILIBRIUM pH = 9.327

APPENDIX C
CHEMICAL AND MATHEMATICAL CONCEPTS

This appendix provides a brief review of the important concepts used to solve the general chemical equilibrium problem. After developing some definitions, we provide the relevant mass action and mole balance equations and describe their solution using an example problem first without, then with a solid phase. Other equations and algorithms used in BLT-EC for correcting equilibrium constants, computing total dissolved carbonate concentration from alkalinity, and obtaining other values are also presented. The material presented in this appendix is taken directly from the MINTEQA2 user's manual and modified to be consistent with this report. This material also applies to adsorption reactions, but the additional concepts that distinguish adsorption algorithms are presented in Appendix D.

Component and Species Definitions

Components - These are the basis entities or building - blocks from which all species in the system can be built. BLT-EC has an associated component database file containing more than 100 components (see Appendix E) from which the user selects only those needed in the specific problem of interest. The components used in BLT-EC form a pre-defined set, e.g., the component for calcium is Ca^{+2} and not some other species such as $CaOH^{+}$. The thermodynamic database, written in terms of these components, is searched automatically to retrieve only those species relevant to a specific problem. Components represent an accounting system and, while it is not required that they be actual chemical species, nearly all BLT-EC components except certain of those used to represent electrostatic terms in adsorption models are physically realizable species.

Type I Components as Species in Solution - These are the components themselves defined as actual chemical species. As mentioned above, in the general case, a component need not be an actual chemical species. The set of available components in BLT-EC happens to include components that are all bona fide chemical species (excepting the electrostatic components). Thus, all (non-electrostatic) components in a BLT-EC problem will also be defined as Type I species.

Type II Other Species in Solution or Adsorbed - These are all dissolved species other than those that are Type I. These may be complexes or free ions, for example, Cr^{3+} (the component for Cr^{3+} is $Cr(OH)_2^{+}$). Insofar as components may be thought of as reactants, TYPE II species may be considered aqueous and adsorption reaction products.

Type III Species with Fixed Activity - Generally, these are either species that are present at fixed equilibrium activity or are mock species that define a fixed equilibrium activity relationship between two real species. In earlier MINTEQ documentation, Type III species were referred to as Fixed Solids because all TYPE III species are treated mathematically in the same way as solids that are explicitly constrained to be present at equilibrium (not subject to complete dissolution; an infinite solid), any components whose activities are explicitly constrained to a given equilibrium value (e.g. fixed pH or pe), any gases whose partial pressures are explicitly constrained to a given equilibrium pressure, or any mock species whose equilibrium activity; is explicitly constrained to an equilibrium value (such as a redox couple that fixes the equilibrium activity ratio of two components that form a redox pair.)

Type IV Finite Solids - These are solid phases that are presumed present initially or precipitate from the solution. In the latter case, the appropriate components are depleted in the aqueous phase to "create" the precipitated solids. With BLT-EC, it is also possible to specify one or mor precipitated solids as present initially at some given amount (per liter basis). For those Type IV solids that are specified as present initially, the entire amount may dissolve if equilibrium demands it and the concentrations of the appropriate components will then be supplemented in the aqueous phase. The reader should realize that, in theory, it doesn't matter to BLT-EC whether the system totals for various components are specified at the outset as all dissolved or all bound precipitated solid(s) of given amount(s). In practice, it helps to avoid phase rule violations (discussed later) if Type IV solids are entered with a concentration of zero. In that case, the total dissolved concentrations of the components of the solid represent total system concentrations. BLT-EC will shift mass from the dissolved to precipitated phases or vice versa as required by equilibrium.

Type V Possible (Undersaturated) Solids - These are solid phases that are defined in BLT-EC; however, they are not

oversaturated, do not physically exist, and thus have no direct impact on the chemical equilibrium problem. When the solution becomes oversaturated with respect to a particular possible solid, and if that solid is more oversaturated than any other possible solid composed of the same components, BLT-EC will precipitate that solid depleting the aqueous phase concentrations of the appropriate components. The newly precipitated solid is then re-assigned as a Type IV species. If any Type IV solid dissolves completely so that its entire mass is shifted to the aqueous phase, that solid is re-assigned as Type V. Note that in ECIN and in the listing of input data that BLT-EC includes in its output file, Type V solids are referred to as POSSIBLE solids. In the listing if equilibrated results however, Type V species are referred to as UNDERSATURATED solids.

Type VI Excluded Species - These are species that would ordinarily be Type I, II, III, or V but are assigned as Type VI to exclude them from mass balance calculations. Reasons for wanting to impose such exclusions are varied. For example, the mass of the component representing the electron (e-) is entered as zero in the database. For obvious reasons, one would not want to impose the condition of mass balance on e-. Therefore, unless an equilibrium pe is imposed, e- is excluded from mass balance calculations by designating it as Type VI. When BLT-EC reads the input file for a specific problem, it searches the database to find all species that can be reaction products of the specified reactants (components). Of these possible species, all gases and redox couples are entered as Type VI unless they are explicitly designated in the input file as Type III. Unless a flag in the input file directs otherwise, all solid phases are treated as Type VI by default. All electrostatic components used in adsorption reactions are entered as Type VI in the input file because they are not real chemical entities; they have no mass. Finally, any species that the user wishes to explicitly exclude may be so designated in the input file. For example, a solid phase that is suspected to be unrealistic for kinetic reasons, but which would otherwise precipitate may be explicitly excluded. ECIN has the logic to properly assign species to the TYPE VI category as necessary and provides for explicitly assigning any species to Type VI as desired by the user.

The Pre-Defined Set of Components

The pre-defined set of components available in BLT-EC (see Appendix E) includes naked ions such as Na^+ and neutral and charged complexes (e.g. H_4Si0_4, $CR(OH)_2^+$). In general, the species chosen to serve as components are those that are expected to be the dominant dissolved species in natural waters, i.e., H_4Si0_4 as opposed to some other species of dissolved silica. Of course, for a specific problem, the species which represents the component may not always be the dominant equilibriums species. Whatever components are selected, it is only necessary that they linearly combine to produce every species in the system and that it be impossible to produce any component through another combination of components (multiple oxidation states of the same chemical element being exempted form this latter requirement; i.e, the fact that component Fe^{3+} can be produced from a combination of components Fe^{2+} and e^- is acceptable).

Oxidation/Reduction Reactions

Redox reactions are represented in either of two ways in BLT-EC. One way is the designation of separate components to represent the oxidation states of interest. For example, in the current database, there are separate components for Fe^{2+} and Fe^{3+}. Thus, separate reactions can be written for each of these components; in fact, this has been done and those reactions are available in the thermodynamic database. Also, as mentioned earlier in defining Type III Species with Fixed Activity, mock species are defined to represent the activity ratio between two members of a redox couple. When such a species is assigned as Type III and the equilibrium pe is also specified, mass is shifted from one member of the couple to the other in such a way as to cause their activity ratio to honor the Nernst Equation at the equilibrium pe specified. The other way to represent different oxidation states requires only on oxidation state to be defined as a component. Then any reaction that would involve a different oxidation state of that same component is written to include the gain or loss of electrons and the log K for the formation of the product is adjusted accordingly. Had the scheme been used for the iron system, Fe^{3+} might have been chosen as a component and Fe^{2+} would have been a Type II species with Fe^{3+} and e^- as reactants. While most of the redox chemistry in BLT-EC is represented by the components of separately defined oxidation states, the electron appears in many reactions as well.

General Problem Formulation

Two general approaches are commonly used to formulate and solve multiple-component chemical equilibrium problems: 1) minimization of the system free energy under mass balance constraints or 2) simultaneous solution of the nonlinear mass action expressions and linear mass balance relationships. BLT-EC uses the latter approach, frequently referred to as the "equilibrium constant method".

To solve the chemical equilibrium problem, BLT-EC uses an initial guess for the activity of each component to calculate the concentration of each species according to mass action expressions written in terms of component activities. The total mass of each component is then calculated from the concentrations of every species containing that component. The calculated total mass for each component is then compared with the known input total mass for each component. If the calculated total mass and the known input total mass for any component differ by more than a pre-set tolerance level, a new estimate of the component activity is made and the entire procedure is repeated. The aqueous phase equilibrium composition is that set of species concentrations which gives a mass imbalance less than the tolerance level for every component.

After equilibrating the aqueous phase, BLT-EC computes the saturation index (SI) for each possible solid with respect to the solution. The solid with the most positive SI is allowed to precipitate by depleting the dissolved concentrations of those components comprising the solid in accordance with the known stoichiometry of each component. The reverse process occurs if an existing solid is found to be undersaturated with respect to the solution. In either case, it is necessary to re-equilibrate the solution after mass has been added to or depleted from the aqueous phase. Thus the aqueous solution is re-equilibrated just as before except with one less degree of freedom if precipitation has occurred or one more if dissolution has occurred. The entire computational loop of iterating to equilibrium, checking for precipitation or dissolution, and shifting mass from the aqueous to the solid phase or vice versa is repeated until equilibrium is achieved and there are no oversaturated possible solids and no undersaturated existing solids.

The number of degrees of freedom of the system is the number of independent variables. These would ordinarily include temperature, pressure, and all the component activities that can be independently varied. Several constraints are used in BLT-EC that modify the usual phase rule relationship. Because temperature and pressure are both specified to be invariant by the user, the phase rule expression that applies to BLT-EC calculations is

$$f = C - P \qquad \textbf{(C-1)}$$

where:

f = the number of degrees of freedom

C = the number of components

P = NN(III) + NN(IV)

NN(III) = the number of Type III Species with Fixed Activity

NN(IV) = the number of Type IV Finite Solid Species

BLT-EC calculates f at the outset of each problem and if f is greater than zero, proceeds with the calculations. One additional degree of freedom is lost for each new solid phase that forms, that is, each species that is reassigned from Type V to type IV. Conversely, each existing solid that dissolves (Type IV species reassigned to Type V) adds one degree of freedom. Examples of constraints that result in reducing the number of degrees of freedom, that is, that contribute to P in Eqn. C-1, are the fixed activity of the component H_2O or of other components with fixed activities. As is evident above, each solid phase present (Type III or IV) also contributes to P. This follows from the solubility product constraint imposed by the presence of a solid phase. To see why the precipitation of a solid results in the loss of one degree of freedom, consider the example

$$AG^{+} + Cl^{-} \rightleftarrows AgCl(s) \quad \log K = 9.75 \tag{C-2}$$

By convention, the activity of the pure precipitated AgCl(s) is 1.0. Thus,

$$K = 10^{9.75} = \{AgCl(s)\}/\{Ag^{+}\}\{Cl^{-}\} \tag{C-3}$$

or

$$\{Ag\} = 10^{-9.75}\{Cl^{-}\}^{-1} \tag{C-4}$$

Thus, when pure AgCl(s) exists{Ag^+} and {Cl^-} are no longer independent variables.

A system of n independent components that can combine to form species is represented by a set of mass action expressions of the form

$$K_i = \{S_i\}\prod_j X_j^{-a_{ij}} \tag{C-5}$$

where:

K_i = equilibrium constant for the formation of species i

$\{S_i\}$ = activity of species i

X_j = activity of component j

a_{ij} = stoichiometric coefficient of component j in species i

$\prod$ = indicates the product over all components in species i

The concentration of species i, $[S_i]$, is related to the activity $\{S_i\}$ by the activity coefficient, γ_i

$$\{S_i\} = \gamma_i[S_i] \tag{C-6}$$

Substituting this expression for $\{S_i\}$ in Eqn. C-5 and rearranging gives

$$[S_i] = K_i/\gamma_i \prod_j X_j^{a_{ij}} \tag{C-7}$$

Now, if we define K'_i such that

$$K_i' = K_i / \gamma_i \quad \textbf{(C-8)}$$

then

$$C_i = [S_i] = K_i' \prod_j X_j^{a_{ij}} \quad \textbf{(C-9)}$$

For notational convenience, we will use C_i and $[S_i]$ interchangeably; both mean the concentration of species i. In Eqn. C-9, the activity coefficient term is incorporated into the equilibrium constant K'_i and ideal conditions (ionic strength = 0; activity coefficients = 1) correspond to the condition $K'_i = K_i$.

In logarithmic form, Eqn. C-9 becomes

$$\log C_i = \log K_i' + \sum_j a_{ij} \log X_j \quad \textbf{(C-10)}$$

In addition to the mass action expressions, the set of n independent components is governed by n mass balance equations of the form

$$Y_j = \sum_i a_{ij} C_i - T_j \quad \textbf{(C-11)}$$

where:

T_j = total dissolved concentration of component j (also referred to as the total analytical concentration because T_j is generally a known measured input parameter)

Y_j = the difference between the *calculated* total dissolved concentration of component j and the *known analytical* total dissolved concentration of component j

The solution (in the mathematical sense) is that set of component activities X (using matrix notation for brevity) which results in the set of concentrations C such that each individual of the set of mass balance differences Y is equal to zero. In practice, it is only necessary to find X such that each individual of Y is made less than some tolerance value. The general procedure is to first guess X (ECIN makes this guess and puts it in the input file), then calculate C and Y. If any individual of Y exceeds (in absolute terms) its prescribed tolerance value, a new guess is made for X, C and Y are recalculated, and the test is repeated. This iterative procedure is continued until all the individuals of Y are less than the tolerance value. Like MINTEQA2, BLT-EC uses the Newton-Raphson approximation method to estimate the new X at each iteration. The tolerance value or convergence criteria for BLT-EC is pre-set to 10^{-4} times T_j for each component j.

Example Problem without a Solid Phase

To illustrate the generalized mathematical formalisms used to solve chemical equilibrium problems, it is instructive to consider a simple problem in detail. The example problem formulation that follows is based on a simple calcium carbonate ($CaCO_3$) solution. A 0.001 molar solution of $CaCO_3$ that has no access to atmospheric gases is considered. No solid phases are considered. Furthermore, no absorbent phases are present, no redox reactions occur, and no Type III species

are included.

The $CaCO_3$ solution at equilibrium will contain ten soluble species: Ca^{2+}, $CaOH^+$, $CaCO_3°$, $CaHCO_3^+$, H_2CO_3, HCO_3^-, CO_3^{2-}, H^+, OH^-, and H_2O. (Note $CaCO_3°$ refers to the soluble complex, not the solid which is designated $CaCO_3(s)$.) The set of 6 independent reactions involving these species is shown in Table C.1. The choice of components to represent a given solution, in general, is not unique; however, the component set used in BLT-EC is pre-set (see Appendix E).

The required number of components is equal to the number of species minus the number of independent reactions. Thus, for this problem we need four components. Some general guidelines for choosing components are:

1) Always choose H_2O as a component; this is required in BLT-EC and, in fact, H_2O is chosen automatically.

2) Always choose H^+ as a component; this is not required but, except for certain problems of academic interest, H^+ should always be a component.

3) If redox transformations are involved in this problem, include the electron as a component. Remember that those database reactions that involve the electron as a component, such as $CH_4(g)$, will not be brought into the problem if e^- is not a component. Even so, do not include e^- unless it is necessary.

4) For all other components, the choices are obvious; ECIN can provide a listing of all available components but there is only one that can represent As^{3+}, one that can represent Ca^{2+}, etc.

The four components that are applicable to the $CaCO_3$ solution are H_2O, H^+, Ca^{2+}, and CO_3^{2-}. H_20 is presumed to exist at constant activity. This is a good assumption for all dilute solutions because the mass of H_2O present is several orders of magnitude greater than the other components. The small mass of water consumed (or generated) by reactions with other components is justifiably neglected; there is no mole balance on H_2O.

Table C.1. Reactions and log equilibrium constants for soluble species in a 0.001 M solution of $CaCO_3$ at 25°C

Reactions	log K
$H_2O - H^+ \rightleftharpoons OH^-$	-14.0
$CO_3^{2-} + H^+ \rightleftharpoons HCO_3^-$	10.2
$CO_3^{2-} + 2H^+ \rightleftharpoons H_2CO_3$	16.5
$Ca^{2+} + H_2O - H^+ \rightleftharpoons CaOH^+$	-12.2
$Ca^{2+} + CO_3^{2-} + H^+ \rightleftharpoons CaHCO_3^+$	11.6
$Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO3°$	3.0

For any species, the stoichiometric coefficients for each component are given by the corresponding reaction written with the components all on the left side of the reaction and the species as the sole reaction product on the right side. For example,

$$Ca^{2+} + H_2O - H^+ \rightleftharpoons CaOH^+$$

Thus, the stoichiometric coefficient for the component H^+ in the species $CaOH^+$ is -1. Similarly for H_2CO_3

$$CO_3^{2-} + 2H^+ \rightleftharpoons H_2CO_3$$

the stoichiometric coefficient for the component H^+ in the species H_2CO_3 is +2. If BLT-EC's component list had been chosen differently (we have already observed that the selection of components in our pre-defined list is arbitrary) so that 0^{2-} were a component, then the reaction for H_2CO_2 in the data base would have been:

$$CO_3^{2-} + H_2O - O_2 \leftrightarrow H_2CO_3$$

In that case, the components CO_3^{2-}, H_2O, and 0^{2-} would have stoichiometries 1, 1, and -1 respectively. Of course, the equilibrium constant for this reaction would be different from that of the former H_2CO_3 reaction.

The stoichiometric coefficients and log equilibrium constants for all species in the $CaCO_3$ problem are shown in Table C.2. Note that the equilibrium constants are for the formation of the species from the components with the corresponding stoichiometries and that these are thermodynamic database constants. Before they are used in BLT-EC, they will each be corrected by the species activity coefficient as in Eqn. C-8.

Table C.2 Stoichiometric matrix representing the 0.001 M $CaCO_3$ solution.

Species	Components				
	H_2O	H^+	Ca^{2+}	CO_3^{2-}	K
H_2O	1	0	0	0	K_1
H^+	0	1	0	0	K_2
Ca^{2+}	0	0	1	0	K_3
CO_3^{2-}	0	0	0	1	K_4
OH^-	1	-1	0	0	K_5
HCO_3^-	0	1	0	1	K_6
H_2CO_3	0	2	0	1	K_7
$CaOH^+$	1	-1	1	0	K_8
$CaHCO_3^+$	0	1	1	1	K_9
CaCO3°	0	0	1	1	K_{10}

Note that Table C.2 includes several identity relationships. The generalized nature of the computational algorithm is such that to make the species H^+ for example, requires that the stoichiometry of the component H^+ be one and that of all other components be zero.

The set of mass action constraints that apply to the reactions in Table C.2 are given in Table C.3. Note that because we are expressing species concentrations in terms of component activities, we must use the mixed equilibrium constants as given by Eqn. C-8.

Table C.3. Mass action expressions applicable to the $CaCO_3$ solution using mixed equilibrium constants.

(1)	$[H_2O] = \{H_2O\}\, K'_1$
(2)	$[H^+] = \{H^+\}\, K'_2$
(3)	$[Ca^{2+}] = \{Ca^{2+}\}\, K'_3$
(4)	$[CO_3^{2-}] = \{CO_3^{2-}\}\, K'_4$
(5)	$[OH^-] = \{H_2O\}\, \{H^+\}^{-1}\, K'_5$
(6)	$[HCO_3^1] = \{CO_3^{2-}\}\, \{H^+\}\, K'_6$
(7)	$[H_2CO_3] = \{CO_3^{2-}\}\, \{H^+\}^2\, K'_7$
(8)	$[CaOH^+] = \{Ca^{2+}\}\, \{H_2O\}\, \{H^+\}^{-1}\, K'_8$
(9)	$[CaHCO_3^+] = \{Ca^{+2}\}\, \{CO_3^{2-}\}\, \{H^+\}\, K'_9$
(10)	$[CaCO_3^\circ] = \{Ca^{+2}\}\, \{CO_3^{2-}\}\, K'_{10}$

Three mole balance expressions are required to complete the set of equations that define the $CaCO_3$ system (recall that mass balance is neglected on H_2O). The mole balance expressions corresponding to Eqn. C.11 are generated by summing the concentrations of all species involving a particular component and subtracting the respective analytical input concentration for that component. The resulting expressions are:

$$Y_{Ca}^{2+} = [Ca^{2+}] + [CaOH^+] + [CaHCO_3^+] + [CaCO_3^\circ] - T_{Ca}^{2+} \qquad \textbf{(C-12)}$$

$$Y_{CO_3^{2-}} = [CO_3^{2-}] + [HCO_3^-] + [H_2CO_3] + [CaHCO_3^+] + [CaCO_3^\circ] - T_{CO_3^{2-}} \qquad \textbf{(C-13)}$$

$$Y_H^+ = [H^+] + [HCO_3^-] + 2[H_2CO_3] + [CaHCO_3^+] - [CaOH^+] - [OH^-] - T_{H^+} \qquad \textbf{(C-14)}$$

The ultimate goal is to solve these mole balance equations under the constraints of the mass action expressions in Table C.3. To do this, the species concentration terms in those equations are replaced with their corresponding mass action expressions from the table. The final set of mole balance equations then becomes:

$$Y_{Ca^{2+}} = K'_3\{Ca^{2+}\} + K'_8\{Ca^{2+}\}\{H_2O\}\{H^+\}^{-1} + K'_9\{Ca^{2+}\}\{H^+\}\{CO_3^{2-}\} + K'_{10}\{Ca^{2+}\}\{CO_3^{2-}\} - T_{Ca^{2+}} \qquad \textbf{(C-15)}$$

$$Y_{H^+} = K'_2\{H^+\} + K'_6\{H^+\}\{CO_3^{2-}\} + 2K'_7\{H^+\}^2\{CO_3^{2-}\} + K'_9\{Ca^{2+}\}H^+\{CO_3^{2-}\} - K'_8\{H_2O\}\{Ca^{2+}\}\{H^+\}^{-1} - K'_5\{H_2O\}\{H^+\}^{-1} - T_{H^+} \qquad \textbf{(C-16)}$$

$$Y_{CO_3^{2-}} = K'_4\{CO_3^{2-}\} + K'_6\{H^+\}\{CO_3^{2-}\} + K'_7\{H^+\}^2\{CO_3^{2-}\} + K'_9\{Ca^{2+}\}\{H^+\}\{CO_3^{2-}\} + K'_{10}\{Ca^{2+}\}\{CO_3^{2-}\} - T_{CO}^{2-} \quad \textbf{(C-17)}$$

These three equations are now expressed in terms of three unknowns, $\{H^+\}$, $\{Ca^{2+}\}$, and $\{CO_3^{2-}\}$. The adjusted equilibrium constants, analytical component total dissolved concentrations, and the activity of H_2O are known. (Recall that the analytical input concentrations (T_{Ca}^{2+}, T_{CO3}^{2-}, and T_H^+) are supplied by the user when the problem is specified and H_2O always has activity fixed at approximately 1.0). The mathematical solution is that set of component activities which gives Y_{CA}^{2+}, Y_{CO3}^{2-}, and Y_H^+ all equal to zero, or more practically, all less than some acceptably small error (convergence criteria). From final component activities, the equilibrium concentrations of all species can be calculated using the mass action expressions in Table C.3.

Example Problem with a Solid Phase and with a Gas Phase

Let us consider the same calcium carbonate system as before except with a solid phase, calcite, present at equilibrium. In that case, we would add the following reaction to Table C.1

$$Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3\,(s) \qquad K_{11}$$

and the stoichiometric coefficients for $CaCO_3$(s) in Table C.2 would be the same as for the dissolved species $CaCO_3°$. The appropriate mass action expression (Eqn. C-9) that would be added to Table C.3 is

$$[CaCO_3°] = \{Ca^{+2}\}\{CO_3^{2-}\}\ K'_{11} \quad \textbf{(C-18)}$$

Now, because $CaCO_3$ (s) is a pure phase,

$$[CaCO_3°] = \{CaCO_3\,(s)\} = 1$$

and we can solve Eqn. C-18 for either $\{Ca^{2+}\}$ or $\{CO_3^{2-}\}$; let us choose $\{CO_3^{2-}\}$. Then,

$$\{CO_3^{2-}\} = \frac{1}{K'_{11}\{Ca^{2+}\}} \quad \textbf{(C-19)}$$

Thus, the three unknowns of Eqn.s C-15 thru C-17 have been reduced to only two by making use of the fact that a pure phase has activity of 1. If we make this substitution (Eqn. C-19) in the three mole balance equations, we obtain

$$Y_{Ca^{2+}} = K'_3\{Ca^{2+}\} + K'_8\{Ca^{2+}\}\{H_2O\}\{H^+\}^{-1} + K'_9\{H^+\}(K'_{11})^{-1} + K'_{10}(K'_{11})^{-1} - T_{Ca^{2+}} \quad \textbf{(C-20)}$$

$$Y_{H+} = K'_2\{H^+\} + K'_6\{H^+\}(K'_{11}\{Ca^{2+}\})^{-1} + 2K'_7\{H^+\}^2(K'_{11}\{Ca^{2+}\})^{-1} + K'_9\{H^+\}(K'_{11})^{-1} - K'_8\{H_2O\}\{Ca^{2+}\}\{H^+\}^{-1} - K'_5\{H_2O\}\{H^+\}^{-1} - T_{H^+} \quad \textbf{(C-21)}$$

$$Y_{CO_3^{2-}} = K'_4(K'_{11}\{Ca^{2+}\})^{-1} + K'_6\{H^+\}(K'_{11}\{Ca^{2+}\})^{-1} + K'_7\{H^+\}^2(K'_{11}\{Ca^{2+}\})^{-1} + K'_9\{H^+\}(K'_{11})^{-1} + K'_{10}(K'_{11})^{-1} - T_{CO_3^{2-}} \quad \textbf{(C-22)}$$

Note that Eqn.s C-20 through C-22 now contain only $\{Ca^{2+}\}$ and $\{H^+\}$ as unknowns. Carbonate ion activity has been eliminated as a component and the dimensions of the Jacobian matrix that must be calculated to estimate new component activities at each succeeding iteration during the Newton-Raphson iteration sequence have been reduced.

For more complicated systems that may contain a number of solids (Types III or IV), the process of eliminating variables is more complicated. A priority order of thermodynamic stabilities of each solid is established by comparing the appropriate ion activity products (IAP) with the corresponding formation constant after the aqueous phase has been equilibrated. The logarithmic ratio of these terms (saturation index) is calculated and used to establish the stability order for precipitation or dissolution of solids.

$$Saturation\ Index = \log \frac{IAP}{K} \quad \textbf{(C-23)}$$

If the saturation index for a particular mineral is negative, the system is undersaturated with respect to that mineral. If the index is positive, the solution is supersaturated and, if the user has selected the appropriate precipitation option, BLT-EC will precipitate the solid in question until the equilibrium condition is satisfied, i.e., until:

$$\log \frac{IAP}{K} = 0 \quad \textbf{(C-24)}$$

Undersaturation for a given mineral can arise from three situations: a) a less soluble mineral phase could be controlling the activities of one or more common ions, b) the component input concentrations are insufficient to exceed the formation constant, or c) free solution ion activities are limited by sorption reactions.

BLT-EC re-evaluates the saturation indices for each solid each time the aqueous phase is equilibrated. The user may choose to:

1) Allow no solids to precipitate regardless of saturation state,

2) Allow the precipitation of explicitly designated solids but only if they become oversaturated,

3) Allow all oversaturated solids to precipitate, or

4) Allow all oversaturated solids to precipitate except for those explicitly designated as excluded (Type VI).

In cases where precipitation is allowed, the entire computational loop of iterating to equilibrium, checking for precipitation or dissolution, and shifting mass from the aqueous to the solid phase or vice versa is repeated until equilibrium is achieved with no oversaturated Type V Possible Solids and no undersaturated Type IV Finite Solids.

Because the formation of solid phases changes the equilibrium species distributions, the inclusion of a large number of Type IV or V solids in BLT-EC executions requires that the species distribution equilibria problem be resolved several times during the iteration sequence for precipitating solids. The difficulty of obtaining convergence is increased accordingly. For this reason, model systems should be spared unnecessary detail. The user should note that usually only a small number

of solids control the free solution activities of species representing a given metal. It may be useful to perform a run with all solids prohibited from precipitating; examination of the saturation indices will provide information as to the dominant solids. The initial rule is, "If in doubt leave it out." The saturation index listings can be used to detect first-pass mistakes. All unprecipitated (supersaturated) solids will be represented by a positive saturation index. If any positive values are found, the user may then add the omitted solid and repeat the execution. In the final analysis, all controlling solids (those that actually precipitate) will be identified with saturation indices equal to zero.

Specifying a gas phase at a fixed partial pressure in the example $CaCO_3$ system would have much the same effect mathematically as did the solid calcite phase. When a $CO_2(g)$ gas phase is present, the following reaction would apply

$$CO_3^{2-} + 2H^+ - H_2O \rightleftarrows CO_2(g) \quad K'_{12} \tag{C-25}$$

The corresponding mass action expression would be represented by

$$P_{CO_2} = \{CO_3^{2-}\}\{H^+\}^2\{H_2O\}^{-1} \; K'_{12} \tag{C-26}$$

where P_{CO2} = the partial pressure of CO_2 in atmospheres. For systems open to the atmosphere, P_{CO2} is fixed at $10^{-3.5}$ atmospheres. The new equilibrium constant would be:

$$K''_{12} = K'_{12}/P_{CO_2} \tag{C-27}$$

Then,

$$\{H^+\} = [\{CO_3^{2-}\}\; K''_{12}]^{-½} \tag{C-28}$$

If the solid phase is present as before, the expression for $\{CO_3^{2-}\}$ (Eqn. C-19) can be substituted in Eqn. C-28 to give

$$\{H^+\} = [\{Ca^{2+}\}K'_{11}(K''_{12})^{-1}]^{½} \tag{C-29}$$

This expression for $\{H^+\}$ can be substituted into the mole balance Eqn.s (C-20 through C-22) which are then expressed in terms of the only remaining unknown, namely $\{Ca^{2+}\}$.

Note that ECIN computes the adjusted equilibrium constant from the user-specified partial pressure. The database log K is 18.16 and if $P_{CO2} = 10^{-3.5}$atm, then the adjusted log K is computed from

$$\log K''_{12} = 18.16 - (-3.5) = 21.66 \tag{C-30}$$

It is possible to over-constrain a system (eliminate all degrees of freedom) by entering too many fixed species. If, for instance, a user simultaneously fixed P_{CO2} and $\{H^+\}$ in the $CaCO_3$ problem above and then if a solid phase is precipitated (by BLT-EC in computing the equilibrium or by the user specifying an initial solid), there would be no remaining variables in the mole balance equations and the system would be over-constrained. BLT-EC would report a phase rule violation and

execution would end with an error.

In introducing the $CaCO_3$ problem originally, the gas phase reactions were excluded. If this problem had been executed using BLT-EC, the user would have been reminded of this exclusion in the output listing for Type VI Excluded Species.

Adjustments to Equilibrium Constants

The equilibrium constants in Eqn.s C-15 through C-17 are functions of the system temperature and ionic strength. The values supplied in BLT-EC's thermodynamic database are referenced to 25°C and an ionic strength of zero. If the temperature is not at 25°C, a new set of equilibrium constants must be calculated before solving the equations. The ionic strength affects activity coefficients which in turn affect the adjusted equilibrium constants (Eqn. C-8). BLT-EC allows the option of specifying a fixed ionic strength or of recalculating the ionic strength from the new estimates of species concentrations at each iteration.

Temperature Corrections of Equilibrium Constants

BLT-EC incorporates two schemes for adjusting the equilibrium constants for temperature. If the necessary data are available in the thermodynamic database, BLT-EC uses a power function of the form

$$K_T = A + BT + C/T + D\ Log(T) + ET^2 + F/T^2 + GT^{1/2} \qquad \textbf{(C-31)}$$

where:

T = temperature (K°)

A, B,..., G = empirical constants stored in the thermodynamic database

Only 25 of the more than 1000 species in the database have these constants available.

For any species that does not have the constants needed for Eqn. C-31, the equilibrium constant is corrected for temperature variations from 25°C by the van't Hoff equation

$$\log K_T = \log K_{T_r} - \frac{\Delta H_r^\circ}{2.303R}\left(\frac{1}{T} - \frac{1}{T_r}\right) \qquad \textbf{(C-32)}$$

where:

T_r = reference temperature, 298.16°K

$\log K_{tr}$ = logarithm of the equilibrium constant at the reference temperature

R = molar gas constant

T = temperature of the system to be modeled (Kelvin)

Δh_r° = standard enthalpy change of the reaction

Caution should be used in attempting to apply BLT-EC to high temperature systems. The van't Hoff equation

implicitly assumes the enthalpies of reaction to be independent of temperature. This assumption is not always valid and significant errors can result at temperatures far above 25°C. For this reason, BLT-EC calculations should be restricted to a temperature range below 100°C. Applications to high temperature geothermal systems should definitely not be attempted unless empirical temperature correction data are available.

If the standard enthalpy change is not available in the database, BLT-EC uses the uncorrected log K's (25°C). Users are encouraged to become familiar with the database and to evaluate the impacts of these limitations on their systems. Missing enthalpy data can be permanently added to the database or, alternatively, temporarily entered into a given model execution using instructions provided by ECIN. The latter option is convenient for testing a given system's sensitivity for individual reaction enthalpies.

Activity Coefficient Corrections of Equilibrium Constants

Activity coefficients for all species are functions of solution ionic strength (I) and vary as species distributions alter the ionic strength. Unless a fixed ionic strength is specified, successive sets of activity coefficients are calculated for all solution species with each iteration. These are used to generate corrected values of the equilibrium constants (see Eqn. C-8) that appear in the mole balance expressions (Eqn. C-11). Initial activity guesses for the input components are provided in the input file for a given problem. These initial component activity guesses are used to"crudely" estimate the concentrations of each dissolved species so that the solution ionic strength can be calculated. Each succeeding iteration provides improved estimates of species concentrations and activity corrections. The solution ionic strength is used in either the modified Debye-Hückel equation or the Davies equation to calculate activity coefficients (γ) for all charged species. If the user selects the modified Debye-Hückel equation, it will be used for those species that have the necessary parameters in the database. For any species lacking the necessary parameters, the Davies equation will be used to estimate the activity coefficient for that species. If the user selects the Davies equation at the outset, it will be used throughout the problem because it requires no species-specific data other than charge. The activity coefficients are used in Eqn. C-8 to compute adjusted equilibrium constants.

The modified Debye-Hückel expression used to calculate the activity coefficients is

$$\gamma_i = \frac{-A_d Z_i^2 I^{1/2}}{1 + B_d a_i I^{1/2}} + b_i I \qquad \textbf{(C-33)}$$

where:

A_d and B_d = constants that depend on the dielectric constant and temperature

Z_i = the charge on each species i

a_i = ion size parameter

b_i = ion specific parameter that accounts for the decrease in solvent concentration in concentrated solutions

I = solution ionic strength

the ionic strength (I) is calculated from

$$I = \tfrac{1}{2} \sum_{i=1}^{m} Z_i^2 C_i \qquad \textbf{(C-34)}$$

where:

C_i = concentration of ion species i

m = number of charged species present in the solution

Z_i = charge on species i

The modified Debye-Hückel relation above is used only when the parameters a_i and b_i are available in the database. The current database contains a_i and b_i parameters for many major inorganic ion species and a few important trace metals. The values used were taken largely from the WATEQ3 data compilation. Where data are not available or if the user selects it, the Davies equation will be used.

The Davies equation as implemented in BLT-EC is

$$\log \gamma_i = -AZ_i^2 \left(\frac{I^{1/2}}{1+I^{1/2}} - 0.24I \right) \qquad \textbf{(C-35)}$$

in which the variables are defined as in Eqn. C-33.

With the exception of H_2O, activity coefficients of neutral species are calculated using

$$\log \gamma_i = \alpha_1 I \qquad \textbf{(C-36)}$$

where the constant α_1 is set equal to 0.1 in BLT-EC.

Users are cautioned that the activity correction models presented here are generally not intended for use at ionic strengths greater than 0.5. At higher ionic strengths, as in marine conditions (ionic strength = 0.7 m), these correction equations may still provide usable results; this should be verified for the specific system to be modeled. Alternatively, one should consider adding expanded versions of the Debye-Hückel equation, which include terms to account for ion interactions occurring in more concentrated solutions.

Successive sets of log K values that reflect the temperature corrections (van't Hoff) and activity coefficient corrections (Debye-Hückel or Davies) above are computed and substituted into the mole balance expressions. If no solids are specified, the Jacobian matrix relating changes in mass balance to changes in component activities is used to calculate that set of component activities that will simultaneously minimize the mass imbalance for all species. The procedure used is an iterative Gaussian elimination and back substitution with a convergence test following each iteration.

Activity of H_2O

The activity of water is estimated from

$$H_2O\} = 1 - 0.017 \sum_{i=1}^{n} C_i \qquad \textbf{(C-37)}$$

where the C_i's represent the concentrations of individual ion species. Eqn. C-37 is applicable only in dilute solutions and is based on a derivation using Raoult's law. The proportionality constant (0.017) is derived from a plot of H_2O activity versus the number of solute ions.

Obtaining Total Dissolved Carbonate from Alkalinity

Most geochemical equilibria of the natural environment are in some way dependent upon the total dissolved carbonate concentration, T_{CO3}^{2-}. Water analyses frequently provide an alkalinity measurement rather than an analytical measurement of dissolved carbonate. BLT-EC can compute T_{CO3}^{2-} from alkalinity. Implicit in the method used to compute T_{CO3}^{2-} are the assumptions that the titration used to determine alkalinity was to the CO_2 equivalence point and that there exists no solid phase in the titrated solution possessing additional acid-neutralizing capacity, all solids having been dissolved. This last assumption means that no solids should be allowed in a BLT-EC run that uses alkalinity. If modeling of solid phases is desired, do a preliminary model run without solids solely for calculating T_{CO3}^{2-}, then use that calculated value in further modeling with solids rather than alkalinity.

Alkalinity as used here means that the value supplied represents the acid-neutralizing capacity of the solution as determined by titrating the solution to the CO_2 equivalence point. This corresponds to an operational definition implemented in BLT-EC which is: the alkalinity is given by the negative of the TOTH expression when the components are the principal components at the CO_2 equivalence point. Beyond this, the exact definition of alkalinity as used in a particular problem depends upon the content of the database file, ALK.DBS. The content of that file is entirely the responsibility of the user; it is not to be thought of as a database file, but rather as an auxiliary input file. The definition of alkalinity as the negative of the equation for TOTH and the use of ALK.DBS are illustrated below.

In general, the principal components of an aqueous solution at the CO_2 equivalence point are H_2O, H^+, and the most abundant soluble species of each chemical entity. BLT-EC has a pre-defined set of components not all of which are the principal components at the CO_2 equivalence point, but this does not invalidate the applicability of the operational definition of alkalinity. It simply means that the alkalinity expression will incorporate species that may also be components. Practically, the procedure for determining the alkalinity factors needed for carbonate containing species in THERMO.DBS and for entries in ALK.DBS is to write (outside of BLT-EC) the TOTH expression derived using the principal components at the CO_2 equivalence point. The negative of the coefficient for each species as it occurs in the TOTH equation is the alkalinity factor for that species. Stated differently, the contribution of each species in solution to the alkalinity is given by the negative of the stoichiometry of H^+ in that species times the species concentration. The only species that are implicitly included as contributors to the entered alkalinity is the Type I species (CO_3^{2-}) and those Type 2 species for which there is a non-zero entry for the alkalinity factor in THERMO.DBS (such as for HCO_3^-). For these species, it is not necessary for the user to know the alkalinity factor; the appropriate factor is already in THERMO.DBS. If other species are to be included as contributors to alkalinity, the ID number and the proper alkalinity factor, as given by the TOTH expression derived using the principal components at the CO_2 equivalence point, must be entered in ALK.DBS. Entries for species containing CO_3^{2-} MUST NOT be included in that file. Suppose for example that the sample you wish to model and for which you have measured the alkalinity contains appreciable dissolved phosphate. You may wish to account for the phosphate contribution to the measured alkalinity so as to arrive at a more correct value for total dissolved carbonate. The procedure for doing this is:

1) Determine the principal components at CO_2 equivalence point:

$$H^+, H_2CO_3, H_2PO_4^-$$

2) Write out a mole balance equation for H^+ including all species for which the stoichiometry of the component H^+ is non-zero. This is done by first writing the reactions to produce all the species using the components above as reactants. For example,

$$H_2PO_4^- + H^+ \rightleftharpoons H_3PO_4$$

and

$$H_2CO_3 - H^+ \rightleftharpoons HCO_3^-$$

The stoichiometries of H^+ in HCO_3^- and H_3PO_4, respectively, are 1 and -1. The complete TOTH expression then is

$$TOTH = [H^+] - [OH^-] - [HCO_3^-] - 2[CO_3^{2-}] + [H_3PO_4] - [HPO_4^{2-}] - 2[PO_4^{3-}] \quad \textbf{(C-38)}$$

3) Noting that the pK_1 for H_3PO_4 is 2.2, we might choose to omit that species altogether due to its negligible concentration above pH 4. Retaining it here for illustration, entries in ALK.DBS would be:

3305802	-1.00
3305800	1.00
580	2.00
3300020	1.00
330	-1.00

where the 7-digit and 3-digit numbers are species ID numbers and the rightmost digit in each ID number is in column 7 and the first line in the file holds the first entry. The ID numbers correspond to species:

3305802	$= H_3PO_4$
3305800	$= HPO_4^{2-}$
580	$= PO_4^{3-}$
3300020	$= OH^-$
330	$= H^+$

The alkalinity equation to which the value input for alkalinity corresponds is alk = -TOTH or:

$$alk = -[H^+] + [OH^-] + [HCO_3^-] + 2[CO_3^{2-}] - [H_3PO_4] + [HPO_4^{2-}] + 2[PO_4^{3-}] \quad \textbf{(C-39)}$$

In most natural systems, the phosphate species are at much lesser concentration than the carbonate and can be neglected. In any case, the user controls the alkalinity equation by preparing ALK.DBS.

If this same file is used in a BLT-EC run for which component ID # 580 (PO_4^{3-})is not included, then those entries in ALK.DBS that involve component 580 are simply ignored and the alkalinity equation that would be used is:

$$alk = -[H^+] + [OH^-] + [HCO_3^-] + 2[CO_3^{2-}] \quad \textbf{(C-40)}$$

Let the contribution of non-carbonate containing species to the input alkalinity be called non-carbonate alkalinity.

Then, the dissolved total inorganic carbon T_{CO3}^{2-} is given by

$$T_{CO_3^{2-}} = alk - excrb - noncrb + [H_2CO_3] \qquad \textbf{(C-41)}$$

where

alk = input alkalinity value converted to eq/L.

excrb = total number of excess equivalents of acid consumed per mole of carbonate containing species, (summed over all such species). For each carbonate species, the alkalinity factor gives the total number of equivalents of acid consumed per mole. Therefore, the excess equivalents for each such species is given by the difference between the alkalinity factor and the stoichiometry of CO_3^{2-} in that species times the number of moles, that is, times the concentration (per liter basis).

noncrb = total number of equivalents of non-carbonate alkalinity (summed over all species contributing to non-carbonate alkalinity). For each non-carbonate species, the alkalinity factor is the number of equivalents of acid consumed per mole. Therefore, the number of equivalents of non-carbonate alkalinity for each such species is the alkalinity factor times the species concentration (per liter basis).

Since the alkalinity as given by Eqn. C-41 is a function of the speciation and thus, so is T_{CO3}^{2-}, BLT-EC re-computes the T_{CO3}^{2-} with each iteration. The user is reminded that the measured alkalinity assumes that there is no additional acid-neutralizing capacity in the form of solids. The measured alkalinity value cannot be used to compute an accurate value of T_{CO3}^{2-} if solid phases are specified or allowed to precipitate. If the problem being modeling involves solids, use the alkalinity value in a preliminary run with no solid phases present or allowed. Then, in subsequent runs with solid phases, use the computed total dissolved carbonate concentration (T_{CO3}^{2-}) from that preliminary run rather than the measured alkalinity.

APPENDIX D
ADSORPTION MODELS

Seven options are currently available in BLT-EC for modeling surface reactions. These include: 1) the activity K_d model, 2) the activity Langmuir model, 3) the activity Freundlich model, 4) the ion exchange model, 5) the constant capacitance model, 6) the triple-layer model, and 7) the diffuse-layer model. Thermodynamic database files of surface reactions are generally not provided for these models as is done for aqueous and solid species; the user must provide the set of surface reactions and their equilibrium constants. An exception is a database of several surface reactions relevant to the diffuse-layer model for trace metal adsorption onto an iron oxide surface. Mathematical formalisms and input data requirements of the individual adsorption models are discussed in separate sections below.

To accomodate different materials with different sorption properties, up to five different materials may be specified (see DATA SET 23B in BLT-EC's main input file) in the transport domain. In the implementation of adsorption models in BLT-EC, five different surfaces may be simultaneously defined for each material. Each surface may have up to two types of sites. Only one adsorption model may be specified in a single execution - e.g., it is not possible to define one surface undergoing adsorption in accordance with the Freundlich model and another surface undergoing Langmuir adsorption in the same BLT-EC run. However, each material may have different surface properties (i.e., solid concentration, specific surface area, and capacitances) and reaction data (log K and stoichiometries). The general modeling approach is to create a component to represent a particular type of site on a particular surface and then to write reactions between other components and that site. The reactions are introduced to BLT-EC through its input file and the solution is equilibrated with the surface species treated mathematically as aqueous species except with certain peculiarities pertinent to the adsorption model specified. When the equilibrium composition is determined, the equilibrated mass distribution between the dissolved, sorbed, and solid phases is computed and reported. When comparing BLT-EC equilibrated results with experimental K_d values, the BLT-EC adsorbed and precipitated species should be grouped together because these two phases are not experimentally distinguishable. There is no intrinsic difference within BLT-EC that distinguishes one surface from another nor one site on a surface from another. The user establishes the difference between any two surfaces and between the two sites on a surface by specifying the surface concentration and other surface specific parameters, such as specific surface area and by specifying the reactions that each site may undergo.

Naming and Numbering Surface Species

Developing a coherent notational scheme for the naming of surface sites and the species that pertain to them is a difficult task. The notation frequently used in the literature for the electrostatic models seems to be primarily applicable to oxide surfaces. Nevertheless, it does provide a coherent system and we have used "SOH" to designate a surface site throughout this Appendix. Within BLT-EC, a more elaborate but generic scheme is used both for naming and numbering surface species. The explanation that follows is not intended as a guide on how to name or number surface reactions. In fact, ECIN is aware of the rules described below so that specifying surfaces, sites, the parameters that define them, and the reactions in which they are involved is rather automatic. BLT-EC does not really care about the names; they are for the benefit of the user in organizing the problem and interpreting the results. ID numbers do have significance within BLT-EC. The cardinal rule is: do not change the component or species ID numbers assigned by ECIN.

As for all BLT-EC components, the pre-defined adsorption components have 3 digits - they span the range 811 through 859. The middle digit designates the surface number (1-5) and the meaning of the rightmost digit is:

1 = surface site 1
2 = surface site 2
3 = electrostatic component for the o-plane
4 = electrostatic component for the β-plane
5 = electrostatic component for the d-plane
6 = not used
7 = not used

8 = not used
9 = not used

thus, component 834 represents the electrostatic component for the β-plane for the surface number 3, etc. It is not really necessary to have defined surfaces 1 and 2 in order to have a surface with the number 3 although ECIN, which would ordinarily be used to design the input file, will define the surfaces beginning with number 1. Also, as will be seen below, the electrostatic component for the β-plane is relevant to the triple-layer model only; this component would never be used for any of the other models.) The 3-digit ID number of a site and the 3-digit ID number of another component that reacts with that site are combined by suffixing the former with the latter and then an arbitrary digit is suffixed to that result to give a 7-digit number to represent the reaction product. For example, 8123301 would represent a surface species resulting from a reaction between site 2 on surface 1 and H^+ (whose 3-digit number is 330). The rightmost digit (1) is arbitrary and is there to insure that the 7-digit number is unique (there could be other reactions between this site and H^+).

The names assigned to those surface species that are reaction products are left to the discretion of the user (ECIN will query for the name). However, the names of the surface components themselves are pre-determined. These names are of the form ADSnTYP1, ADSnTYP2, ADSnPSIO, ADSnPSIB, ADSnPSID where n refers to surface number. For example, ADS1TYP1 corresponds to site 1 on surface 1 (component ID number 811), ADS4PSID corresponds to the electrostatic component representing the d-plane on surface number 4.

For the explanation and discussion of the adsorption models that follows, we have used the simpler notation of SOH to designate a surface site and electrostatic terms are referred to in accepted notation of σ and ψ to represent surface charge and potential, respectively.

Non-Electrostatic Adsorption Models

The seven adsorption models in BLT-EC are conveniently grouped into those that involve electrostatic terms and those that do not. The non-electrostatic models have been in common use and certain conventions as to their use have become accepted [Morel, 1983]. The specifics of each model and departures from accepted model conventions in BLT-EC are explained below.

Activity K_d Adsorption Model

The activity K_d adsorption model implemented in BLT-EC differs in two respects from the usual definition of the K_d model. For an adsorbing metal M, K_d is conventionally defined as the ratio of the concentration of metal bound on the surface to total dissolved metal concentration at equilibrium. That is,

$$K_d = \frac{[SOH{\cdot}M]}{[M]_T} \qquad \textbf{(D-1)}$$

where [SOH· M] represents the concentration of adsorption sites occupied by an ion M or surface-bound metal and $[M]_T$ is the total dissolved equilibrium concentration of M.

In the BLT-EC activity K_d model,

$$K_d^{act} = \frac{\{SOH{\cdot}M\}}{\{M\}} \qquad \textbf{(D-2)}$$

where {M} is the free activity of M in the equilibrium solution. Following convention and because there is no generally

accepted method of computing activity coefficients for unreacted or reacted adsorption sites, we define those coefficients as unity so that {SOH·M} = [SOH·M]. Then in terms of concentrations, Eqn. D-2 becomes

$$K_d^{act} = \frac{[SOH \cdot M]}{\gamma_m [M]} \qquad \textbf{(D-3)}$$

where γ_m is the activity coefficient of dissolved species M and K_d^{act} may be thought of as the equilibrium constant of the surface reaction

$$SOH + M \rightleftarrows SOH \cdot M \qquad \textbf{(D-4)}$$

SOH represents unreacted surface sites and is present at a fixed activity (or fixed concentration if we insist that the activity coefficient pertaining to SOH is unity). Taking the activity of SOH as 1.0 Eqn. D-3 may be thought of as a mass action expression for reaction D-4. This is implemented in BLT-EC by assigning the component representing unreacted sites, SOH, as a Type III species. The constraint is that there is an unlimited supply of fresh unreacted sites; the surface cannot approach saturation no matter how much M adsorbs. The reader will note that this constraint also renders competition between different metals (M_1, M_2,...) meaningless. Eqn. D-2 defines the equilibrium constant actually used for an activity K_d reaction in BLT-EC; the reader will observe that this is a unitless ratio. However, ECIN calculates this value from the more common expression of K_d in 1/kg and solid concentration in kg/l (e.g., the number of kg of soil with which one liter of solution is equilibrated).

Activity Langmuir Adsorption Model

In the Langmuir adsorption model, the number of surface sites available for adsorption must be specified at the outset. The surface reaction can be written identically as for the activity K_d model

$$SOH + M \rightleftarrows SOH \cdot M \quad K_L^{act} \qquad \textbf{(D-5)}$$

and where we again express the equilibrium constant in terms of activities

$$K_L^{act} = \frac{\{SOH \cdot M\}}{\{M\}\{SOH\}} \qquad \textbf{(D-6)}$$

If, as is the case for every adsorption model in BLT-EC, we arbitrarily assign the value of unity to the activity coefficients pertaining to unreacted and reacted surface sites, we can rewrite the mass action Eqn. D-6 as

$$K_L^{act} = \frac{[SOH \cdot M]}{\gamma_m [M][SOH]} \qquad \textbf{(D-7)}$$

To see the correspondence between this implementation of the Langmuir model and the defining equation to which that model is commonly ascribed, we note that the mass balance equation written for the surface sites is

$$[SOH]_T = [SOH{\cdot}M] + [SOH] \qquad \textbf{(D-8)}$$

where $[SOH]_T$ = total concentration of surface sites available. The combined mass balance and mass action expressions yield the Langmuir relationship in terms of activities

$$[SOH{\cdot}M] = \frac{K_L^{act}[SOH]_T \gamma_m [M]}{1 + K_L^{act} \gamma_m [M]} \qquad \textbf{(D-9)}$$

To express D-9 in terms of concentrations, replace K_L^{act} with K_L and let $\gamma_m = 1$.

The so-called competitive Langmuir model for the competing metals M_1, M_2,... is derived in a similar manner with additional reactions defined:

$$SOH + M_1 \rightleftarrows SOH{\cdot}M_1 \quad K_{L1}^{act}$$
$$SOH + M_2 \rightleftarrows SOH{\cdot}M_2 \quad K_{L2}^{act}$$
$$\vdots$$
$$SOH + M_n \rightleftarrows SOH{\cdot}M_n \quad K_{Ln}^{act}$$

$$\vdots$$

$$SOH + M_n \rightleftarrows SOH{\cdot}M_n \quad K_{Ln}^{act}$$

All that is required to model such competition in BLT-EC is to define these separate reactions on the surface.

The only difference between the Langmuir and activity K_d treatments is that the Langmuir equation accounts for the finite concentration of surface sites. It is also important to remember that the K_L used is an "activity" K_L rather than the conventional concentration-based constant.

A meaningful way to employ commonly available "concentration" K_L data is to model the experimental supernatant solution in which the K_L was determined and replot the data in terms of the BLT-EC activities of the sorbate. To do this, the Langmuir isotherm is first rewritten in the linear form.

$$\frac{[M]}{[SOH{\cdot}M]} = \frac{1}{K_L[SOH]_T} + \frac{[M]}{[SOH]_T} \qquad \textbf{(D-10)}$$

If the Langmuir isotherm accurately describes the system, a plot of [M]/[SOH·M] will yield a straight line of slope $1/[SOH_T]$ and intercept $1/K_L[SOH_T]$. Conventionally, the constant K_L is obtained by dividing the slope by the intercept. The K_i^{act} can be derived from an analogous plot in which the BLT-EC sorbate activities {M} are plotted in place of the sorbate concentration terms [M].

Activity Freundlich Model

The mass action equation representing the Freundlich model can be written

$$SOH + (1/n)M \rightleftarrows SOH{\cdot}M \quad K_f^{act} \tag{D-11}$$

$$K_f^{act} = \frac{\{SOH{\cdot}M\}}{\{M\}^{1/n}\{SOH\}} \tag{D-12}$$

Like the activity K_d model, an unlimited supply of unreacted sites is assumed and the activity and concentration of surface species are considered to be equal. Imposing the condition {SOH} = 1.0.

$$[SOH{\cdot}M] = K_f^{act}\{M^{m+}\}^{1/n} \tag{D-13}$$

[SOH·M] = equilibrium concentration of reacted sites or surface-bound metal

{M} = equilibrium activity of the free metal species M

1/n = mass action stoichiometric coefficient pertaining to M

This is similar to the activity K_d relationship except that the stoichiometric coefficient of the reacting species M is 1/n. For the special case where n = 1, the Freundlich and activity K_d mass action equations are identical. Note that the mass balance stoichiometry for M is 1.0, just as it is for the activity K_d model. It is only the mass action stoichiometry that is 1/n.

K_f^{act} may be derived from conventional concentration K_f data in a manner similar to obtaining K_d^{act} from conventional K_d data. The logarithmic form of the Freundlich mass action Eqn. (D-13) is

$$\log [SOH{\cdot}M] = \log K_f^{act} + 1/n \log \{M\} \tag{D-14}$$

If the Freundlich model is applicable to a given system, a plot of log [SOH·M] versus log {M} will yield a straight line of slope 1/n and intercept log K_f^{act}. Experimental isotherms usually involve concentration rather than activity plots. The K_f values from these plots can be converted to K_f^{act}'s by using BLT-EC to speciate the equilibrium solution at each point along the adsorption isotherm and re-plotting the isotherm in terms of log {M} rather than log [M]. The resulting intercept will be the K_f^{act} required by BLT-EC. Alternatively, one can simply guess the activity coefficient of the adsorbing metal M for each concentration along the curve.

Ion-Exchange Adsorption Model

Ion-exchange sorption is defined as the process by which an ion from solution is exchanged for one on the solid surface. The relative abilities of solute ion species to compete for surface sites is governed by intrinsic factors and their solution activities. The ion-exchange model assumes that the surface site is initially occupied by an exchangeable ion that is released into solution during the exchange process. The ion-exchange reaction and its corresponding mass action equation can be expressed as

$$SOH{\cdot}M_1 - M_1 + M_2 \rightleftharpoons SOH{\cdot}M_2 \qquad \textbf{(D-15)}$$

$$K_{ex} = \frac{\{M_1\}\{SOH{\cdot}M_2\}}{\{M_2\}\{SOH{\cdot}M_1\}} \qquad \textbf{(D-16)}$$

where M_1 is the ion initially occupying the exchange site, M_2 is the replacing ion to be adsorbed, and $SOH{\cdot}M_1$, $SOH{\cdot}M_2$ are surface sites occupied by the respective ions. As for the previous models, no attempt is made to calculate activity coefficients for the occupied sites; they are arbitrarily taken as unity and K_{ex} is written in terms of concentrations by replacing activity of each species in Eqn. D-16 with the product of concentration and activity coefficient.

Earlier versions of MINTEQ implemented the ion exchange model in such a way as to require an infinite supply of solid of constant composition. This condition implied a fixed solution phase activity ratio between the two exchanging ions. Also, there was no mass balance on the ion that initially occupied the surface and was expelled during the exchange reaction. Beginning with MINTEQA2 version 3.00, these features are no longer model constraints; the model conforms to conventional and accepted usage as given by Eqns. D-15 and D-16.

Selectivity coefficients (K_{ex}'s) can be derived from the literature for most common ions such as Na^+, K^+,Ca^{2+}, Mg^{2+}, etc., but are seldom available for trace metals. In using the ion exchange algorithm, users must supply the reaction stoichiometries and selectivity constants and specify the ion that initially occupies the exchange sites. Note also that reaction stoichiometries may be related to ion charge. For example, a single Ca^{2+} ion may replace two Na^+ ions and thus occupy two sites.

Electrostatic Adsorption Models

All four adsorption models discussed thus far neglect the electrostatic influences of charged surfaces on the solution and the counter influences of changes in surface charge due to solution composition. Many colloidal particles carry a significant surface charge that creates electrostatic potentials extending into the suspending solutions. Solution ions with charge of the same polarity as the surface are repelled and ions of opposite charge are attracted. Because of this, the electrostatic potentials associated with charged surfaces may greatly influence the adsorptive behavior of charged species. This influence is incorporated in electrostatic adsorption models by including terms in the mass action equations that modify the activities of sorbate ions approaching charged surfaces by the electrical work necessary to penetrate the zone of electrostatic potentials (ψ's) extending away from the surface.

Several models are available to account for these effects in various degrees of detail. Readers are referred to Westall and Hohl's excellent review [Westall and Hohl. 1980] for clear comparisons of the presently available surface complexation/electrosatic models. The discussion that follows will be limited to brief descriptions of the three surface complexation model options provided in BLT-EC: the constant capacitance, diffuse-layer, and triple-layer models. These three models are closely related in many ways. Each treats adsorption as a surface complexation reaction (that is, the reaction is treated as analogous to a solution phase complexation reaction governed by a mass action equation) and each accounts for the electrostatic potentials at the charged surface. They differ primarily in the types of surface species that are allowed within specific physical locations or layers extending away from the surface and in the parameters of the electrostatic model that each employs.

The surface complexation models available in BLT-EC were developed to describe surface reactions in amorphous metal oxide systems [Davis and Leckie, 1978] and have also been applied to clay systems [James and Parks, 1982]. The large body of experimental evidence that has accumulated from laboratory bench studies of pure oxide systems indicates that surface complexation models can predict adsorption behavior [Dzombak, 1986]. Few data exist for applying these models to natural systems where complex mixtures of impure amorphous oxides, clays, and humic materials provide the reactive surfaces. Recent work [Loux et. al., 1989] has demonstrated good model agreement with experimental results on an aquifer

material spiked with trace metal cations. The adsorbing surface was modeled as amorphous iron oxide using MINTEQ with the diffuse-layer model using surface reactions and their associated stability constants as given by Dzombak [1986]. In general, freshly prepared laboratory oxide systems often behave differently from the aged, impure mixtures found in the environment. The interactions are such that properties of the mixture as a whole are not necessarily those obtained by summing the properties of the individual components. Care must be used in selecting input parameters for natural systems using BLT-EC's surface complexation models.

The constant capacitance, diffuse-layer, and triple-layer models all treat trace metal surface reactions as complexation reactions analogous to the formation of complexes in solution. Surface sites are represented as SOH groups where S's are metals associated with the solid structure and located at the solid-liquid interface. Some ions, such as H^+, OH^-, and a variety of trace metal ions are presumed to be specifically adsorbed at the surface via complexation with the surface sites. In all three models, a charge (σ) associated with the surface is assumed to be balanced by a charge (σ_d) associated with a diffuse layer of counterions. These charges are such that $\sigma + \sigma_d = 0$. In the constant capacitance and diffuse-layer models, all specifically adsorbed ions contribute to the surface charge (σ). However, in the triple-layer model, the net charge due to adsorption is the sum of the charges associated with two adsorbing planes rather than one. The innermost of the two planes (the o-plane) specifically adsorbs H^+ and OH^- and is characterized by charge σ_o. The other plane (β-plane) has charge σ_β resulting from the adsorption of other ions. The net surface charge is given by $\sigma = \sigma_o + \sigma_\beta$ and is balanced by the charge in the diffuse layer such that $\sigma + \sigma_d = 0$. Because the electrical potential gradients extending away from the surface are the direct result of the surface charge, the specifically adsorbed potential determining ions also govern distributions of counterions in the diffuse layer.

Activities of ions in solution and near the surface are influenced by the presence of electrostatic potentials arising from the surface charge. The activity difference between ions near the surface and those far away is the result of electrical work in moving the ions across the potential gradient between the charged surface and the bulk solution. The activity change between these zones is related to the ion charge (z) and the electrical potential (ψ) near the surface and can be expressed using the exponential Boltzmann expression,

$$\{X_s^z\} = \{X^z\}[e^{-\psi F/RT}]^z \qquad \textbf{(D-17)}$$

where:

Z = charge of ion X

$\{X_s^z\}$ = activity of an ion X of charge z near the surface

$\{X^{z)}$ = corresponding activity of X in bulk solution outside the influence of the charged surface

$e^{-\psi F/RT}$ = Boltzmann factor

F = Faraday constant

R = ideal gas constant

T = absolute temperature

General Implementation of Electrostatic Models in BLT-EC

The general algorithm is similar for all three of the electrostatic models. Specific details for each model are discussed separately below. As mentioned above, for the constant capacitance and diffuse-layer models, there is only one layer or plane within which specifically adsorbed ions define the surface charge σ. Accordingly, that plane is commonly referred to as the o-plane and the surface charge and potential are denoted σ_o and ψ_o. We will retain that notation here as

well as the notation σ_d and ψ_d for their counterparts in the diffuse layer. We point out, however, that the o-plane is defined differently in the triple-layer model and those parameters subscripted with "o" in that model should not be regarded as equivalent to the o-plane parameters of the former two models. Also, with regard to the constant capacitance and diffuse-layer models, we may refer to σ_o and ψ_o as "surface" charge and "surface"potential. This is not true of the triple-layer model because there are two planes ("o" and "β") associated with the surface. Thus, the charge at the beginning of the diffuse layer is defined in terms of $\sigma_o + \sigma_\beta$.

The Boltzmann factor of Eqn. D-17 (with the potential ψ subscripted to indicate the layer to which it applies) is incorporated as a scaling factor by assigning it a component ID number and writing the surface reaction so as to include it as a reactant of appropriate stoichiometry. The reader should realize that this is only a mathematical way to incorporate the parameters of the desired model into an existing computational scheme. The mass action equations for surface reactions will contain those fake components (which we shall refer to as electrostatic components) that are really the Boltzmann factors. Also, because they are not real chemical entities, there is no analytical total to ascribe as input for the electrostatic components, rather the total charge is calculated via expressions that are unique to each model and are mathematically related to the potential. Still, we will refer below to T_σ referenced to a specific plane as the total charge for that plane but note that we do not imply a measured input value as was the case with earlier references to T. Also, BLT-EC will seek to perform mass balance calculations on all components. It is necessary, therefore, to direct otherwise for the electrostatic components by designating them as Type VI (excluded from mass balance). Charge balance equations that are analogous to mass balance (see Eqn. C-10) are defined for the electrostatic components and have the form

$$Y_\sigma = \sum_i a_{i\sigma} C_i - T_\sigma \qquad \textbf{(D-18)}$$

where $a_{i\sigma}$ is the stoichiometry of the electrostatic component pertaining to σ in species i.

The overall sense of the electrostatic calculations for a given plane is this:

1) Calculate the total charge T_σ from the potential on the plane by using a functional relationship appropriate for the model (see below). Initial guesses for the potential of each plane are provided in the input file.

2) Calculate the total charge on the plane by a different method, namely, by summing the charges of all species specifically adsorbed on that plane. Operationally, this becomes a summation of the charge contribution from all species in which the stoichiometry of the component representing the plane is non-zero.

$$\sum_i a_{i\sigma} C_i$$

3) Obtain the difference in the total charge pertaining to the plane as in Eqn. D-18. Test whether the difference is less than some small tolerance value. If not, adjust the potential for that plane and repeat. Of course, the potentials are adjusted simultaneously with the activities of other components.

Calculations involving the surface sites themselves are exactly as described for other real chemical entities by the mass action Eqns. (C-8) and mass balance Eqns. (C-10).

As for all BLT-EC adsorption models, the activity coefficients of both the reacted and unreacted surface sites are always taken as unity. The artificial contrivance whereby we have created components to represent the Boltzmann factors demands that we create activity coefficients for them as well. Imaginary though they be, we make them innocuous by setting them to unity.

All surface reactions in BLT-EC are written in terms of the neutral surface site SOH (components 8nl or 8n2; n

= 1,2,...,5) and the equilibrium constants appropriate for BLT-EC are formation constants. The constants from any reactions found in the literature are intrinsic constants, which sometimes are referenced to the protonated surface site SOH_2^+ (for adsorbing anions) and to the deprotonated site SO^- (for adsorbing cations). Such reactions must be rewritten in terms of BLT-EC components and their equilibrium constants adjusted accordingly before use in BLT-EC. The surface reactions, which are generally model specific, must be provided to BLT-EC through its chemistry input file; there is no permanent database of adsorption reactions. BLT-EC includes a separate file containing surface reactions that are applicable to the diffuse-layer model for an iron oxide surface. To be used, that file (FEO-DLM.DBS) must be appended to a previously prepared input file. Instructions for doing this are provided in ECIN. For other surface reactions that the user may wish to create for an input file, ECIN is capable of computing the correct stoichiometry for the electrostatic components. In fact, this is done automatically without user intervention. The user may be asked to supply an initial activity guess for the electrostatic components (for use in item 1 above). Specifically, a seed value representing the negative of the exponent in the Boltzmann factor of Eqn. D-17 is requested and a guess of zero will usually work.

The analytical input concentration for the surface site, T_{SOH}, is expressed in moles of sites per liter and is calculated from

$$T_{SOH} = \frac{N_s S_A C_s}{N_A} \qquad \textbf{(D-19)}$$

where:

N_s - the analytically determined surface site density (number of sites/m^2)

S_A = specific surface area of the solid (m^2/g)

C_s = concentration of solid in the suspension (g/L)

N_A = Avogadro's number (6.02×10^{23})

N_s, S_A, and C_s are requested from the user by ECIN. From these parameters, T_{SOH} is calculated.

Constant Capacitance and Diffuse-Layer Models

The constant capacitance and diffuse-layer models have many similarities. Both define specific adsorption of all ions on the "o" plane. Also, their mass action and charge balance equations are identical (except for the numerical value of the equilibrium constants). The difference in these two models is in the function relating total surface charge σ_o to surface potential ψ_o. For the diffuse-layer model,

$$T_{\sigma_o} = 0.1174\ I^{1/2} \sinh(Z\psi_o F/2RT) \qquad \textbf{(D-20)}$$

where Z is the valency of the symmetrical electrolyte (which we take as unity), I is ionic strength, and all other parameters are defined as in Eqn. D-17. This expression is used in evaluating Eqn. D-18.

The constant capacitance model is a special case of the diffuse-layer model for solutions of high ionic strength and surfaces of flow potential. In such systems, Eqn. D-20 can be approximated by

$$T_{\sigma_o} \approx C\psi_o \qquad \textbf{(D-21)}$$

where C is a constant capacitance term. Eqn. D-21 is used to evaluate Eqn. D-18 for the constant capacitance model. Although the models are similar in implementation, the capacitance term C is often treated as a fitting parameter rather than as a measured characteristic of the system and the constant capacitance model can be applied to systems of all ionic strengths. Outside the range of ionic strength where the approximation of Eqn. D-21 is valid, the constant capacitance and diffuse-layer models are not the same.

As mentioned, the assignment of specifically adsorbed species to the o-plane, the mass action equations, and the charge balance equations for the constant capacitance and diffuse-layer models are the same. The discussion of surface reactions that follows applies to either model.

Surface reactions are represented by mass action expressions with Boltzmann factors represented as components (see Eqn. D-17). Stoichiometries of those components are included in the definition of surface reactions provided to BLT-EC. Several examples of such reactions and their corresponding mass action expressions are given below to illustrate the use of Boltzmann factors. Consider the protonation reaction

$$SOH + H_s^+ \rightleftarrows SOH_2^+ \qquad \textbf{(D-22)}$$

where H_s^+ denotes a hydronium ion near the surface. The corresponding mass action expression is

$$K = \frac{\{SOH_2^+\}}{\{SOH\}\ \{H_s^+\}} \qquad \textbf{(D-23)}$$

As mentioned previously, the surface species are presumed to have activity coefficients equal to unity and the terms $\{SOH_2^+\}$ and $\{SOH\}$ need no further conversion; however, the activity of the surface hydronium ions must be corrected for the energy expended in moving them to the charged surface where the reaction occurs. This is accomplished by expressing $\{H_s^+\}$ in terms of the bulk solution hydronium ion activity $\{H^+\}$. In this case, z = 1 and Eqn. D-17 is written

$$\{H_s^+\} = \{H^+\} e^{-\psi_o F/RT} \qquad \textbf{(D-24)}$$

The mass action expression used in BLT-EC is obtained by substituting this expression into Eqn. D-23.

$$K = \frac{\{SOH_2^+\}}{\{SOH\}\ \{H^+\}\ [e^{-\psi_o F/RT}]} \qquad \textbf{(D-25)}$$

With the Boltzmann factor incorporated as a component, the stoichiometry for this reaction in BLT-EC corresponds to:

$$SOH + H^+ + e^{-\psi_o F/RT} \rightleftarrows SOH_2^+ \qquad \textbf{(D-26)}$$

For the corresponding deprotonation reaction

$$SOH - H_s^+ \rightleftarrows SO^- \tag{D-27}$$

and its mass action expression

$$K = \frac{\{SO^-\}\ \{H^+\}\ [e^{-\psi_o F/RT}]}{\{SOH\}} \tag{D-28}$$

The stoichiometry in BLT-EC corresponds to:

$$SOH - H^+ - e^{-\psi_o F/RT} \rightleftarrows SO^- \tag{D-29}$$

For multivalent species, both charge and stoichiometry of the adsorbing ion must be considered in writing the mass action expression. Consider the surface reaction involving the divalent cation M^{2+}

$$SOH + M_s^{2+} - H_s^+ \rightleftarrows SO{\cdot}M^+ \tag{D-30}$$

The corresponding mass action expression is

$$\begin{aligned} K &= \frac{\{SO{\cdot}M^+\}\ \{H_s^+\}}{\{SOH\}\ \{M_s^{2+}\}} \\ &= \frac{\{SO{\cdot}M^+\}\ \{H^+\}[e^{-\psi_o F/RT}]}{\{SOH\}\ \{M^{2+}\}[e^{-\psi_o F/RT}]^2} \\ &= \frac{\{SO{\cdot}M^+\}\ \{H^+\}}{\{SOH\}\ \{M^{2+}\}[e^{-\psi_o F/RT}]} \end{aligned} \tag{D-31}$$

In this case, the Boltzmann factor in the numerator can be canceled and the stoichiometry in BLT-EC corresponds to:

$$SOH + M^{2+} - H^+ + e^{-\psi_o F/RT} \rightleftarrows SO{\cdot}M^+ \tag{D-32}$$

Mass action expressions for other surface reactions are formulated in a similar manner.

In addition to the surface reactions with their equilibrium constants and the parameters of Eqn. D-19, the constant capacitance model requires an input value for the capacitance, C. This is the capacitance (farads/m^2) between the o-plane and the diffuse layer of counterions.

Triple-Layer Model

The triple-layer model is generally more complex than the constant capacitance and diffuse-layer models. In the BLT-EC implementation of the triple-layer model, only protonation and deprotonation of surface sites are assigned to the

o-plane. Other specifically adsorbed ions are assigned to the β-plane and determine the charge σ_β and potential ψ_β in that zone. Non-specifically adsorbed ions are envisioned as residing in the diffuse layer or 'd' plane and are influenced by ψ_d potentials. The capacitance between the o-plane and the β-plane is denoted C_1 and between the β-plane and d-plane, C_2. Both are treated as user-supplied constants in BLT-EC. Background electrolytes are allowed to adsorb. Also, note that the potential gradients in the inner and outer zones are linear, but potentials decay exponentially in the diffuse layer zone.

The input parameters for the triple-layer model are similar to those for the constant capacitance model except that two capacitance terms and three electrostatic components are required. As with the other electrostatic models, the first of these components (id number 8n3) pertains to the charge and potential on the o-plane. The second (id number 8n4) pertains to the charge and potential on the β-plane and the third (id number 8n5) to the d-plane.

Total charges associated with the triple-layer model o-, β-, and d-planes are related to the potential differences between planes.

$$T_{\sigma o} = C_1 (\psi_o - \psi_\beta) \quad \textbf{(D-33)}$$

$$T_{\sigma\beta} = C_1 (\psi_\beta - \psi_o) + C_2 (\psi_\beta - \psi_d) \quad \textbf{(D-34)}$$

$$T_{\sigma d} = C_2 (\psi_d - \psi_\beta) \quad \textbf{(D-35)}$$

Where:

$T_{\sigma o}$, $T_{\sigma\beta}$, and $T_{\sigma d}$ = total charges associated with the o-, β-, and d-planes

C_1 and C_2 = capacitances associated with the zones between the o- and β-planes and β- and d-planes, respectively

ψ_o, ψ_β, and ψ_d = electrostatic potentials at the o-, β-, and d-planes

The total charge on the o- and β-planes are used in Eqn. D-18 along with the summation of species that are specifically adsorbed on each plane and have non-zero stoichiometry in the appropriate electrostatic component.

Recalling that the d-plane has no specifically adsorbed ions and thus has zero stoichiometry in all species, we replace Eqn. D-18 for that plane only with

$$Y_{\sigma_d} = \sigma_d - T_{\sigma_d} \quad \textbf{(D-36)}$$

where the diffuse layer charge (σ_d) for a monovalent symmetric electrolyte is given by the Gouy-Chapman relationship

$$\sigma_d = -(\varepsilon\varepsilon_o RIT)^{1/2} \sinh(F\psi_d/2RT) \quad \textbf{(D-37)}$$

where:

ϵ = dielectric constant

ϵ_o = permittivity in free space (8.85×10^{-12} (coulombs)^2/joule-m)

I = ionic strength

BLT-EC also uses Eqn. D-37 as an approximation for non-symmetric electrolytes.

Surface reactions in the triple-layer model are represented in a manner similar to the other two electrostatic models except that mass action expressions must have the proper stoichiometry for the electrostatic component representing the β-plane as well as the o-plane. No stoichiometry is needed for the d-plane because no specific adsorption occurs on that plane.

The following surface reactions and mass action expressions illustrate the determination of stoichiometric coefficients for those components. For the surface protonation and de-protonation reactions, the triple-layer model results are identical to those obtained for the constant capacitance and diffuse-layer models in Eqns. D-26 and D-29 (although one could expect the numerical value of the equilibrium constants to be different). For the monovalent metal ion M+

$$SOH - H_s^+ + M_s^+ \rightleftarrows (SO{\cdot}M) \qquad \textbf{(D-38)}$$

With the substitution for H_s^+

$$\{H_s^+\} = \{H^+\}\ [e^{-\psi_o F/RT}] \qquad \textbf{(D-39)}$$

(see Eqn. D-17) and a similar substitution for the metal ion near the surface (except the effective potential refers to the β-plane because that is where M^+ is specifically adsorbed)

$$\{M_s^+\} = \{M^+\}\ [e^{-\psi_\beta F/RT}] \qquad \textbf{(D-40)}$$

the mass action expression is

$$K = \frac{\{SO{\cdot}M\}\ \{H^+\}\ [e^{-\psi_o F/RT}]}{\{SOH\}\ \{M^+\}\ [e^{-\psi_\beta F/RT}]} \qquad \textbf{(D-41)}$$

The reaction written in terms of BLT-EC components and including the electrostatic components is

$$SOH - H^+ - e^{-\psi_o F/RT} + M^+ + e^{-\psi_\beta F/RT} \rightleftarrows SO{\cdot}M \qquad \textbf{(D-42)}$$

For a surface reaction involving a divalent metal, M^{2+}

$$SOH - H_s^+ + M_s^{2+} \rightleftarrows (SO{\cdot}M)^+ \qquad \textbf{(D-43)}$$

the substitution of Eqn. D-39 together with

$$\{M^{2+}\} = \{M_s^{2+}\}\ [e^{-\psi_\beta F/RT}]^2 \qquad \textbf{(D-44)}$$

provides the mass action expression

$$K = \frac{\{SO{\cdot}M^{+}\}\ \{H^{+}\}[e^{-\psi_o F/RT}]}{\{SOH\}\ \{M^{2+}\}[e^{-\psi_o F/RT}]^2} \quad \textbf{(D-45)}$$

The corresponding BLT-EC reaction is

$$SOH - H^{+} - e^{-\psi_o F/RT} + M^{2+} + 2e^{-\psi_\beta F/RT} \rightleftarrows SO{\cdot}M^{+} \quad \textbf{(D-46)}$$

The combined hydrolysis/sorption reaction for an M^{2+} ion is expressed

$$SOH + M_s^{2+} + H_2O - 2H_s^{+} \rightleftarrows SO{\cdot}MOH \quad \textbf{(D-47)}$$

and the corresponding mass action expression is written

$$K = \frac{\{SO{\cdot}MOH\}\ \{H^{+}\}^2\ [e^{-\psi_o F/RT}]^2}{\{SOH\}\ \{M^{2+}\}\{H_2O\}\ [e^{-\psi_o F/RT}]^2} \quad \textbf{(D-48)}$$

The corresponding BLT-EC reaction is

$$SOH + M^{2+} + 2e^{-\psi_\beta F/RT} + H_2O - 2H^{+} - 2e^{-\psi_o F/RT} \rightleftarrows SO{\cdot}M^{+} \quad \textbf{(D-49)}$$

For the reaction of a monovalent anion (A^-), a neutral surface species can result

$$SOH + A_s^{-} + H_s^{+} \rightleftarrows SOH_2{\cdot}A \quad \textbf{(D-50)}$$

With the substitution

$$\{A_s^{-}\} = \{A^{-}\}\ [e^{-\psi_\beta F/RT}]^{-1} \quad \textbf{(D-51)}$$

the mass action expression is

$$K = \frac{\{SOH_2{\cdot}A\}\ [e^{-\psi_\beta F/RT}]}{\{SOH\}\ \{A^{-}\}\{H^{+}\}\ [e^{-\psi_o F/RT}]} \quad \textbf{(D-52)}$$

and the BLT-EC reaction is written

$$SOH + A^- - e^{-\psi_\beta F/RT} + H^+ + e^{-\psi_\sigma F/RT} \rightleftarrows SOH_2 \cdot A \qquad \textbf{(D-53)}$$

Finally, for a divalent anion,

$$SOH + A_s^{2-} + H_s^+ \rightleftarrows SOH_2 \cdot A^- \qquad \textbf{(D-54)}$$

the mass action expression is

$$K = \frac{\{SOH_2 \cdot A^-\}[e^{-\psi_\beta F/RT}]^2}{\{SOH\}\ \{A^{2-}\}\{H^+\}[e^{-\psi_\sigma F/RT}]} \qquad \textbf{(D-55)}$$

the BLT-EC reaction is written

$$SOH + A^{2-} - 2e^{-\psi_\beta F/RT} + H^+ + e^{-\psi_\sigma F/RT} \rightleftarrows SOH_2 \cdot A^- \qquad \textbf{(D-56)}$$

The reader is reminded to write adsorption reactions in terms of BLT-EC components and to adjust the equilibrium constants accordingly before entering the reaction through ECIN. The electrostatic components are of no concern in this procedure. ECIN will add the appropriate electrostatic components at the correct stoichiometry when the reaction is entered.

APPENDIX E
THE THERMODYNAMIC DATABASE USED BY BLT-EC

The thermodynamic database used by BLT-EC contains over 1000 species. The best way to search the database for a species of interest is to use ECIN or an editor with a search/find utility. If the latter option is used, you must know how the species ID number or names are derived and expressed. Because FORTRAN does not support the use of super - or subscripts, the customary method of writing chemical formulas cannot be accommodated without modification. The following naming rules are used in BLT-EC.

1) Stoichiometric coefficients are written with parentheses and brackets enclosing the elements in the formula to which the stoichiometry applies.

2) Species charge numbers will always be preceded with a sign (+/-). The one (1) in (+1) and (-1) may be omitted. If a species name ends with an unsigned number, that number represents stoichiometry.

3) Species names involving organics may be shortened by leaving out letters.

Examples:

H2O means H_2O
CR(OH)2+ means $CR(OH)_2^+$
HG(OH)2 means $Hg(OH)_2$
S04-2 means SO_4^{2-}
TARTRAT mean Tartrate

The following is an explanation of BLT-EC's thermodynamic database files. This information is useful for adding new reactions to any of the four database files: THERMO.DBS, TYPE6.DBS, REDOX.DBS or GASES.DBS. Before attempting to add to or modify these files, note the following.

- You should make a backup copy of the file you are going to modify before you start. Give the copy a name such as TYPE6.SAV. This is just in case things do not go as planned.

- When adding to or modifying the thermodynamic database, if the reaction is an Aqueous species, you need only edit THERMO.DBS. If the reaction is a SOLID (mineral), REDOX couple, or GAS, you must edit two files as explained below. The main file, THERMO.DBS, is divided into several sections delineated by blank lines and lines that contain a zero in column 7. The first section is for AQUEOUS species and is followed by three lines with zeroes separated by blank lines. After these separator lines, the next section is for SOLIDS and that section is followed with one blank line and one line with a zero. The next section is for REDOX couples and is followed immediately by the GAS section. The file is terminated with a blank line then a line with a zero. YOU MUST HONOR THE SECTIONAL DIVISIONS WHEN MAKING ADDITIONS- - DO NOT DELETE OR CHANGE THE SEPARATOR LINES. The arrangement of these sections serves to signal BLT-EC as to the nature of the species (AQUEOUS species, SOLID, etc.).

- To add a new AQUEOUS species, it need only be entered in THERMO.DBS. The other files remain unchanged.

- To add a new SOLID (MINERAL), it must be entered in THERMO.DBS and in TYPE6.DBS.

- To add a new REDOX couple, it must be entered in THERMO.DBS and in REDOX.DBS.

- After all desired changes are made to THERMO.DBS and TYPE6.DBS, new versions of the corresponding files that are actually used by BLT-EC and ECIN must be created. This is easily accomplished by executing

the program UNFRMT.EXE (included on the distribution media). Before executing UNFRMT, rename the current THERMO.UNF and TYPE6.UNF to something else for safe keeping. UNFRMT creates unformatted versions of THERMO and TYPE6 that can be read faster than their formatted counterparts. The unformatted files cannot be edited directly because they are unintelligible. The program FRMT.EXE does exactly the inverse of UNFRMT so that THERMO.DBS and TYPE6.DBS can be recreated from the unformatted files if desired.

- To add a new GAS, it must be entered in THERMO.DBS and in GASES.DBS.

- Constants for all entries are referenced to a temperature of 25 degrees C. AQEUOUS species constants are for ionic strength of zero, REDOX couple constants are for zero potential, and GAS constants are for a partial pressure of one atmosphere.

The Component Database File

The component database file is shown below. The 3-digit ID number, BLT-EC name, and real chemical name are shown for each component. Note that ID numbers 240 through 259 are reserved and should not be used for newly created components. Also, note the adsorption components are numbered 811 through 859.

001 E-1	e^-	030 A1+3	Al^{+3}
002 H2O	H_2O	060 H3ASO3	H^3AsO_3
020 AG+1	AG^{+1}	061 H3AsO4	H^3AsO_4
090 H3BO3	H_3BO_3	815 ADS1PSID	Adsorbant 1, electrostatic d layer
100 BA+2	Ba^{+2}	821 ADS2TYP1	Adsorbant 2, type 1
130 BR-1	Br^{-1}	822 ADS2TYP2	Adsorbant 2, type 2
140 CO3-2	CO_3^{-2}	823 ADS2PSI0	Adsorbant 2, electrostatic surface layer
143 CN-	CN^-	824 ADS2PSIB	Adsorbant 2, electrostatic layer
144 OCN-	OCN^-	825ADS2PSIB	Adsorbant 2 electrostatic d layer
150 Ca+2	Ca^{+2}	831ADS3TYP1	Adsorbant 3, type 1
160 Cd+2	Cd^{+2}	832 ADS3TYP2	Adsorbant 3, type 2
180 Cl-1	Cl^{-1}	833 ADS3PSI0	Adsorbant 3, electrostatic surface layer
210 Cr+2	Cr^{+2}	834 ADS3PSIB	Adsorbant 3, electrostatic layer
211 Cr(OH)2+	$Cr(OH)_2^+$	835 ADS3PSID	Asorbant 3, electrostatic d layer

212 Cr04-2	$Cr0_4^{-2}$	841 ADS4TYP1	Adsorbant 4, type 1
230 Cu+1	Cu^{+1}	842 ADSTYP2	Adsorbant 4, type2
231 Cu+2	Cu^{+2}	843 ADS4PSI0	Adsorbant 4, electrostatic surface layer
240-259	RESERVED	844 ADS4PSIB	Adsorbant 4, electrostatic layer
270 F-1	F^{-1}	845 ADS4PSID	Adsorbant 4, electrostatic d layer
280 Fe+2	Fe^{+2}	851 ADS5TYP1	Adsorbant 5, type 1
281 Fe+3	Fe^{+3}	852 ADS5TYP2	Adsorbant 5, type 2
330 H+1	H^{+1}	853 ADS5PSI0	Adsorbant 5, electrostatic surface layer
360 Hg2+2	Hg_2^{+2}	854 ADS5PSIB	Adsorbant 5, electrostatic layer
361 Hg(OH)2	$Hg(OH)_2$	855 ADS5PSID	Adsorbant 5, electrostatic d layer
380 I-1	I^{-1}	870 Tl+1	Tl^{+1}
410 K+1	K^{+1}	871 Tl(OH)3	$Tl(OH)_3$
440 Li+1	Li^{+1}	891 U+4	U^{+4}
460 Mg+2	Mg^{+2}	890 U+3	U^{+3}
470 Mn+2	Mn^{+2}	892 UO2+1	UO_2^{+1}
471 Mn+3	Mn^{+3}	893 UO2+2	UO_2^{+2}
490 NH4+1	NH_4^{+1}	900 V+2	V^{+2}
491 NO2-1	NO_2^{-1}	901 V+3	V^{+3}
492 NO3-1	NO_3^{-1}	902 VO+2	VO^{+2}
500 Na+1	Na^{+1}	903 VO2+1	VO_2^{+1}
540 Ni+2	Ni^{+2}	950 Zn+2	Zn^{+2}
580 PO4-3	PO_4^{-3}	955 Dietham	diethylamine
600 Pb+2	Pb^{+2}	956 Nbutyam	n-butylamine
680 Rb+1	Rb^{+1}	958 Metham	methylamine
730 HS-1	HS^{-1}	959 Dimetham	dimethylamine
731 S	S	960 Trbuth	tributylphosphate

732 SO4-2	SO_4^{-2}	961 Hexam	hexylamine
740 Sb(OH)3	$Sb(OH)^3$	963 EN	ethylenediamine
741 Sb(OH)6-	$Sb(OH)_6^-$	964 Npropam	n-propylamine
760 HSe-1	HSe^{-1}	965 Ipropam	iso-propylamine
761 HSeO3-1	$HSeO_3^{-1}$	966 Tmetham	tri-methylamine
762 SeO4-2	SeO_4^{-2}	967 Citrate	citrate
770 H4Sio4	H_4Sio_4	968 NTA-3	nitrilotriacetate $^{-3}$
800 Sr+2	Sr^{+2}	969 EDTA-4	$EDTA^{-4}$
811 ADS1TYP1	Adsorbant 1, type 1	971 Prpanot	propanoate
812 ADS1TYP2	Adsorbant 1, type 2	972 Butanot	bbutyrate
813 ADS1PSI0	Adsorbant 1, electrostatic surface layer	973 Isobuty	iso-butyrate
814 ADS1PSIB	Adsorbant 1, electrostatic layer	980 2Metpyr	2-methyl pyridine
981 3Metpyr	3-methyl pyridine	982 4Metpyr	4-methyl pyridine
983 Formate	formate	984 Isvaler	iso-valerate
985 Valerat	valerate	990 Fulvate	fulvate
991 Humate	humate	992 Acetate	acetate
993 Tartrat	tartrate	994 Glycine	glyscine
995 Salicyl	salicylate	996 Glutama	glutamate
997 Phthala	phthalate		

Format of Database Species Entries

Each reaction in THERMO.DBS, TYPE6.DBS, GASES.DBS, and REDOX.DBS is specified by a two or three line entry. The explanation of each line is as follows:

FIRST line

Column(s)	Meaning	Format
1 - 7	Species reaction product ID number. If you are adding a new reaction, you create this number.	I7

	For AQUEOUS and GAS species, the 7-digit ID is formed from the 3-digit component ID # of the major cation suffixed by the 3-digit component ID# of the major anion suffixed by a single digit to ensure that the resulting 7-digit number is unique within the entire database.	
	For SOLID species, the 3-digit component ID # of the major cation is prefixed with a 2-digit code that represents the class to which the solid belongs. The 2-digit class codes are listed below. The resulting 5-digit number is suffixed with 2-digits to ensure that the final 7-digit number is unique within the entire database.	
	2-digit Codes for Classes of Solids Code Class / Code Class 00 Elemental / 51 Nitrate 10 Sulfide / 52 Borate 11 Cyanide / 60 Sulfate 12 Selenide / 61 Selenite, Selenate 14 Antimonide / 70 Phosphate 20 Oxide and Hydroxide / 72 Arsenate 30 Multiple Oxide / 43 Vanadate 40 Bromide / 80 Orthosilicate 41 Chloride / 82 Chain Silicate 42 Fluoride / 84 Framework Silicate 43 Iodide / 86 Sheet Silicate 50 Carbonate	
	For REDOX couples, the 3-digit component ID # of one member of the redox pair is prefixed by the other and the resulting 6-digit number is suffixed by a single digit to ensure that the final 7-digit ID number is unique within the entire database.	
8	blank	
9 - 20	Species reaction product name. With only 12 spaces, it may be necessary to abbreviate. Subscripts aren't possible but do use parentheses where appropriate. If the species is charged, always hang the charge on the end of the name prefixed with the appropriate algebraic sign. For SOLIDS, mineral names are preferred to chemical formula names.	A12
21 - 30	Enthalpy change, i.e., delta H for the reaction (kcal/mole). BLT-EC uses this value to adjust the equilibrium constant for temperatures other than 25 degrees C.	F10.4
31 - 40	Log K. Common logarithm of the equilibrium constant for this reaction.	F10.4

	For aqueous species, this is the thermodynamic stability or formation constant, i.e., for the reaction $wA + xB <- - - - -> yC + zD$ For BLT-EC, this reaction would be written $wA + zB - yC <- - - - -> zD$ in the thermodynamic database where A, B, and C are BLT-EC components and D is an AQUEOUS species reaction product.	
	For SOLIDS, K is the reciprocal (log K is the negative) of the solubility product. This is because BLT-EC treats precipitation reactions as if written with reactants on the left and precipitates on the right which is reversed compared with the solubility product rule. A representative BLT-EC precipitation reaction is $Ag^+ + Cl^- <- - - - -> AgCl\ (s)$ $K = \{AGCl\}/ \{Ag^+\}\ \{Cl^-\}$ where brackets { } again denote activity. The activity of solid AgCl is 1.0 because it is a pure phase sot hat we may write $K = 1/ \{Ag^+\}\ \{Cl^-\}$	
	Now, the solubility product rule applies to the silver chloride reaction gives $K_{sp} = \{Ag^+\}\ \{Cl^-\}$ Therefore, the K needed in BLT-EC is related to the K_{sp} $K = 1/K_{sp}$ $\log K = -\log K_{sp}$ In summary, the log K value for a SOLID in the database is the negative of log K_{sp}.	

	For REDOX Couples, the value entered for log K is computed form the Nernst equation $E = E^{\circ} - 2.303\ RT/nF \log Q$ where E is the potential , E° is the standard reduction potential at 25 degrees C, R is the molar gas constant, T is the absolute temperature, F is the Faraday constant, n is the number of electrons in the half-reaction, and Q is that function of concentrations (activities) of products and reactants that occurs in the equilibrium constant which is sought. For potentials measured in volts at 25 degrees C $E = E^{\circ} - (1/n)\ (0.05916) \log Q.$ Just as log K's for AQUEOUS species are referenced to an ionic strength of zero, the log K's for REDOX couples are referenced to a potential of zero. So, with rearrangement and taking E = 0, the above equation becomes $\text{Log } Q = 16.903\ nE^{\circ}$ For the Fe^{3+}/Fe^{2+} couple (species ID # 2812800), $Fe^{3+} + e^{-} \text{ - - - - - -> } Fe^{2+}$ for which the standard reduction potential is 0.771 and n = 1, the above expression gives $\log Q = 13.032.$ This is the value entered for log K in that reaction.	

	For GASES, the log K entered is log K^p where the partial pressure of the gas is in atmospheres. The values currently in the database files are for a partial pressure of one atmosphere. If you want to compute equilibria at pressures other than one atm, you will need to adjust the log K^p accordingly. ECIN makes this adjustment for you by asking for the desired partial pressure, obtaining the constant for the atm from the database, and entering the corrected log K in your input file. An example of a gas reaction and the partial pressure adjustment is species 3301403 $CO_3^{-2} + 2H^{+1} - H_2O <- - - - -> CO_2\,(g)$ The log K_p at one atm is 18.16. The log of the partial pressure of CO_2 (g) in the atmosphere is aboiut -3.5. Therefore, the corrected log K_p is $\log K_p = \log K_p - \log 10^{-3.5}$ $= 18.16 - (-3.5)$ $= 21.66$ BLT-EC requires that the partial pressures of all gases be fixed for a given problem.	
41 - 48	Maximum reported log K. This entry is made only for SOLID species and is not actually used in BLT-EC's equilibria calculations. It is intended to provide a means of judging the reliability of the log K given in columns 31 - 40.	F8.3
49 - 56	Minimum reported log K. This entry is made for SOLID species only and is not actually used IN BLT-EC's equilibria calculations. It is intended to provide a means of judging the reliability of the log K given in columns 31 - 40.	F8.3
57 - 61	Charge of species reaction product.	F5.2
62 - 66	Debye-Huckel a parameter for species reaction product.	F5.2
67 - 71	Debye-Huckel b parameter for species reaction product.	F5.2
72 - 80	Gram formula weight of species reaction product. No entry for REDOX couples.	F9.4
<u>SECOND line</u>		
Column(s)	Meaning	Format

1 - 5	Carbonate alkalinity factor. This entry is made only for AQUEOUS species that have carbonate (ID # 140) as a component. In cases where the user has chosen to specify the inorganic carbon as alkalinity (this is an option when executing BLT-EC), the carbonate alkalinity factor is used to determine total dissolved inorganic carbon concentration from a measure of alkalinity. To compute the carbonate alkalinity factor for a new species, use the formula: alkalinity factor = 2 x STOIC (CO_3^{2-}) - STOIC (H^+) Where STOIC(x) is the stoichiometry of component x in the reaction.	F5.2
6	blank	
7	Number of components (as reactants or products in this reaction. Maximum = 9.	I1
8 - 10	blank	
11 - 17	Stoichiometry of the first component. Negative if the component is a reaction product, that is if it occurs in the left-hand side of the chemical equation with a negative coefficient.	F7.3
18	blank	
19 - 21	ID number of the first component.	
22 - ?	Additional stoichiometry/component ID # pairs with separating spaces so that the total number of pairs is equal to the number of components as specified in column 7. These are entered in the same manner as the first pair in columns 8 - 21. That is, 3 blank columns followed by seven columns for the stoichiometry in F7.3 format, one blank column and finally, three columns for the component ID # in I3 format. The remainder of the second line will hold 4 additional pairs through column 77. If the total number of components is greater than 5, continue on a third line with the 3 columns 78 - 80 of the second line counted as the 3 blank columns for the sixth pair. Use columns 1 - 7 of the third line for the stoichiometry of the sixth pair. Column 8 should be blank and columns 9 - 10 should contain the component ID #. Continue with the 3X, F7.3, 1X, I3 format for up to three additional pairs on the third line.	

Examples of Entries in the Thermodynamic Database Files

The following are excerpts from the thermodynamic database files. Each excerpt is followed by an explanation

of all entries. The explanation is presented with the component names just as they appear in BLT-EC.

AQUEOUS Species

```
3300020  OH-          13.345        -13.998                    -1.   3.5  0.0   17.0074
      2        1.000  2      -1.000 330
1501401  CACO3 AQ    4.0300        3.1500                     0.   0.0  0.0   100.0890
 2.00  2        1.000  150    1.000  140
2113300  CR+3         -20.1400       9.62        3.00 0.00 0.00  51.9960
 0.00  3        1.0000 211    2.000  330  -2.000 2
```

EXPLANATION:

First reaction - -

Species ID number:	3300020	Minimum Log K:	not used
Species name:	OH	Species charge:	-1
Delta H:	13.345 Kcal/mole	Debye-Huckel a:	3.5
Log K:	-13.998	Debye-Huckel b:	0 or unknown
Maximum Log K:	not used	Gram Formula Wt.:	17.0074

Alkalinity factor: none Number of components: 2
Chemical Equation (from stoichiometry/components):

$$H_2O \; - \; H^{+1} \; <- - - - > OH$$

or, in terms of (stoichiometry component ID #'s:

$$1(002) \; - \; 1(300) \; <- - - - - > \; 3300020$$

Second reaction - -

Species ID number:	1501401	Minimum Log K:	not used
Species name:	CaCo3 (aq)	Species charge:	0
Delta H:	4.03 kcal/mole	Debye-Huckel a:	0 or unknown
Log K:	3.15	Debye Huckel b:	0 or unknown
Maximum Log K:	not used	Gram Formul Wt.:	100.089

Alkalinity factor: 2.0 Number of components: 2
Chemical Equation (from stoichiometry/components):

$$Ca \; + \; CO_3^{-2} <- - - - > \; CaCO_3$$

or, in terms of (stoichiometry) component ID#'s:

$$1(150) \; + \; 1(140) \; <- - - - > 1501401$$

Third reaction:

Species ID number:	2113300	Minimum Log K:	not used
Species name:	Cr+3	Species charge:	+3
Delta H:	-20.140 kcal/mole	Debye-Huckel a:	0 or unknown
Log K:	9.62	Debye Huckel b:	0 or unknown
Maximum Log K:	not used	Gram Formul Wt.:	51.996

Alkalinity factor: none Number of components: 3
Chemical Equation (from stoichiometry/components):

$$Cr(OH)_2^{+} + 2H^{+1} - 2H_20 \text{ <- - - -> } Cr^{+3}$$

or in terms of (stoichiometry component ID #'s:

$$1(211 + 2(330) - 2(002) \text{ <- - - - -> } 2113300$$

SOLID (Mineral) species

6010000 BARITE -6.280 9.976 .000 9.773 233.4016
2 1.000 100 1.000 732

EXPLANATION:

Species ID number:	6010000	Minimum Log K:	9.773
Species name:	Barite	Spceies charge:	0
Delta H:	-6.280 kcal/mole	Debye-Huckel a:	unkown
Log K:	9.976	Debye-Huckel b:	unknown
Maximum Log K:	unknown	Gram Formula Wt.:	233.4016

Alkalinity factor: none Number of components: 2
Chemical Equation (from stoichiometry/components):

$$Ba^{+2} + SO_4^{-2} \text{ <- - - - - -> } BaSO_4 \text{ (Barite)}$$

Or, in terms of (stoichiometry) component ID #'s:

$$1(100) + 1(732) \text{ <- - - - - -> } 6010000$$

REDOX Couple

2812800 Fe+3/Fe+2 -10.0 13.032
3 1.000 281 -1.000 280 1.000 1

EXPLANATION:

Species ID number:	2812800	Minimum Log K:	not used
Species name:	Fe+3/Fe+2	Spceies charge:	not used
Delta H:	-10.0 kcal/mole	Debye-Huckel a:	not used
Log K:	13.032	Debye-Huckel b:	not used
Maximum Log K:	not used	Gram Formula Wt.:	not used

Alkalinity factor: none Number of components: 3
Chemical Equation (from stoichiometry/components):

$$FE^{+3} - Fe^{+2} + E^{-1} \text{ <- - - - -> Activity ratio of } Fe^{+3}/Fe^{+2}$$

Or, in terms of (stoichiometry) component ID #'s:

1(281) + 1(280) + 1(001) <- - - -> 2812800

GAS species

3301403 CO2 (GAS) -0.53 18.16
3 1.000 140 2.000 330 -1.000 2

EXPLANATION:

Species ID number:	3301403	Minimum Log K:	not used
Species name:	CO2 (g)	Spceies charge:	0
Delta H:	-0.53	Debye-Huckel a:	unknown
Log K:	18.16	Debye-Huckel b:	unknown
Maximum Log K:	not used	Gram Formula Wt.:	41.010

Alkalinity factor: none Number of components: 3

Chemical Equation (from stoichiometry/components):

$$CO_3^{-2} + 2H^{+1} - H_2O \quad <- - - - > CO_2\,(g)$$

Or, in terms of (stoichiometry) component ID #'s:

1(140) + 2(330) - 1(002) <- - - -> 3301403

APPENDIX F
CHEMISTRY MODULE ERROR DIAGNOSTICS

If an error occurs during the execution of the chemistry module, the chemistry output file will contain an error code of the form BLT-EC Vx.xx-yy where x.xx is the BLT-EC version number and yy refers to an error message code. All error message codes are written to the chemistry output file along with a suggested REMEDY and sometimes an ALTERNATIVE remedy. The complete set of error message codes and their corresponding remedies are listed below along with additional explanation and remedial suggestions if appropriate.

Chemistry Module Error Codes and Messages

BLT-EC V1.00-01

The number of COMPONENTS specified exceeds the maximum allowed, NXDIM.

REMEDY: Eliminate unnecessary components (those that are chemically non-reactive in this system, the reduced members of redox couples when the pe is very high or vice versa, etc,).

ALTERNATIVE: Re-compile BLTEC3.FOR with a larger value for parameter NXDIM in the file EQCHEM..INC.

Too many components are specified in the chemistry input file. Eliminate those that would probably remain as free species at equilibrium anyway. If eliminating such components adversely affects the ionic strength , fix it at the appropriate value. The effect of Na^+, Cl^-, NO_3^-, and K^+ on the final equilibrium composition can frequently be adequately modeled by merely fixing the ionic strength.

BLT-EC V1.00-02

The number of species read from the database exceeds the maximum allowed, NYDIM.

REMEDY: Eliminate unnecessary components (those that are chemically non-reactive in this system, the reduced members of redox couples when the pe is very high or vice versa, etc.). This will result in fewer species.

ALTERNATIVE: Re-compile BLTEC3.FOR with a larger value for parameter NYDIM in the file EQCHEM.INC.

Same comment as for BLT-EC V1.00-01

BLT-EC V1.00-03

A species included in the input file as TYPE 3, 4, 5, or 6 was not in the thermodynamic database.

REMEDY: Check to make sure that the ID numbers of TYPE 3, 4, 5, and 6 entries in the input file are valid.

If the input file ID numbers are all legitimate database species, check to be sure you have not inadvertently changed the database.

BLT-EC V1.00-04

The number of adsorption parameters entered is insufficient for the adsorption model specified.

REMEDY: Check the input file to be sure that the solid sorbent concentration, specific surface area, and capacitance parameters are entered as appropriate for the model specified. ECIN inserts the appropriate parameters for each model.

Use ECIN to set-up input files for adsorption runs; do not try to insert adsorption parameters by using an editor. Also, do not attempt to change the adsorption model of an input file in ECIN; that characteristic of a file cannot be changed in ECIN.

BLT-EC V1.00-05

The input file is interpreted to have a species TYPE greater than six.

REMEDY: This usually results from having used an editor to modify the input file outside ECIN. Check for misplaced blank lines or the wrong number of entries specified for TYPE 3, 4, 5, or 6 in the input file.

There is no legitimate type number greater than six. If things are out of place in thechemistry input file, BLT-EC may misinterpret an input field.

BLT-EC V1.00-06

A component ID listed in the input file is not a valid BLT-EC component ID number.

REMEDY: This error may be a typo resulting form using an editor to modify the input file. If it is not a typo but rather is an attempt to use a new component previously unknown to BLT-EC, be aware that you must edit the component database file COMP.DBS and insert the new component therein.

New components cannot be defined by specifying them in ECIN. The component database COMP.DBS file must be edited to define a new component.

BLT-EC V1.00-07 RESERVED - NOT CURRENTLY USED

BLT-EC V1.00-08

As requested via an input option, execution is halted due to charge imbalance.

REMEDY: Obtain more accurate or complete analyses of total dissolved concentrations or reset the input option via ECIN to continue in spite of charge imbalance.

BLT-EC V1.00-09 06

Computations have resulted in a singular matrix.

REMEDY: Check initial activity guesses. Poor guesses may lead to divergence rather than convergence. If this is a fixed pH or fixed pe run, use of the sweep option starting at a pH or pe where you can make good guesses to compute equilibria at a difficult pH or pe by specifying a small increment with each sweep.

This error is generated by the routine that estimates the change in component activities with each successive iteration. It indicates that the problem is not converging and results either from poor initial activity guesses or from an improperly posed chemical problem. Re-think the chemical problem in terms of a laboratory system and make sure it is formulated properly for BLT-EC. If it seems to be a reasonable chemical problem, try making better initial activity guesses.

BLT-EC V1.00-10 07

Computations have resulted in an estimate of zero for the activity of some component.

REMEDY: Check initial activity guesses. Poor guesses may lead to divergence rather than convergence. For fixed pH or fixed pe runs, use the sweep option starting at a pH or pe where you can make good guesses to compute equilibria at a difficult pH or pe by specifying a small increment with each sweep.

ALTERNATIVE: Eliminate the component whose activity has become zero.

Same comment as BLT-EC V1.00-09

A phase rule violation has occurred.

REMEDY: Explained in detail in Appendix C.

Phase rule violations are more likely when a FINITE solid with non-zero concentration is specified in the input file. This is because the solid specified may not be the most insoluble at equilibrium If it is not, BLT-EC will dissolve it in favor of the more insoluble form. Should the replacing mineral precipitate before the initial one has dissolved, a phase rule violation may occur. The remedy is to either remove the FINITE solid from the input file or set its concentration to zero. In either case, the total dissolved concentrations of its constituent components must be supplemented.

Also, phase rule violations are more likely when all over saturated solids of the database are allowed to precipitate. If this option is used and a phase rule violation occurs, execute the model a second time with no solids allowed. The saturation indices of database solids will be printed out and can be used as a guide for deciding which solids to specifically allow.

A general observation regarding this type of phase rule violation is illustrated by imagining a model run with several metal components. In such a run, imagine that after converging several times and precipitating a solid each time, a solid of metal "M" precipitates. Iterations continue and several more solids precipitate, none involving metal "M." Finally, a second solid of metal "M" precipitates and execution ends with a phase rule violation. It is usually the case that the correct remedy is to run the model again with that solid of metal "M" that precipitated first explicitly EXCLUDED. That this is the correct remedy can be verified by examining the listing of saturation indices in PART 6 of the output file. If no phase rule violation occurs and the index calculated for the EXCLUDED solid is less than zero, the problem has been correctly resolved. It may be that the first phase rule violation will be eliminated, but a new one involving a different solid (which has taken the place of the one you excluded and is now the first precipitate of metal "M") now occurs. Try applying the same procedure again, excluding the new offending solid as well as that which was formerly excluded. It may be necessary to repeat the procedure several times before the most insoluble solid is finally the first to precipitate.

BLT-EC V1.00-12 04

The number of degrees of freedom is zero. This problem is over-constrained.

REMEDY: Specify additional components or reduce the number of fixed species. Remember that each solid that precipitates introduces an additional fixed constraint on the system.

There are too many fixed species for computations to continue. If, for example, Ca^{+}, CO_3^{2}, and H^{+} are the only components (other than H_2O) and if the pH is fixed and a $CO_2(g)$ phase with fixed partial pressure is imposed, and if solids are allowed to precipitate, this error will occur when a solid containing calcium precipitates. In that case, there will be four components and four fixed species and no variables remaining in the problem. Add inert components to allow computations to continue or restrict certain solids from precipitation.

The number of iterations has reached the maximum allowed as specified in the input file.

REMEDY: Use ECIN to re-set this to a larger value or else make better initial activity guesses to produce convergence in fewer iterations.

Most well-formulated problems take fewer than 100 iterations unless there are many solid phases.

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10. SUPPLEMENTARY NOTES

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11. ABSTRACT *(200 words or less)*

The BLT-EC computer code has been developed, implemented, and tested. BLT-EC is a two-dimensional finite element computer code capable of simulating the time-dependent release and reactive transport of aqueous phase species in a subsurface soil system. BLT-EC contains models to simulate the processes (container degradation, waste-form performance, transport, chemical reactions, and radioactive production and decay) most relevant to estimating the release and transport of contaminants from a subsurface disposal system. Water flow is provided 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, and solubility. Chemical reactions accounted for include complexation, sorption, dissolution-precipitation, oxidation-reduction, and ion exchange. Radioactive production and decay in the waste form is simulated. Transport considers the processes of advection, dispersion, diffusion, chemical reaction, radioactive production and decay, and sources (waste form releases). To improve the usefulness of BLT-EC, a pre-processor, ECIN, which assists in the creation of chemistry input files, and a post-processor, BLTPLOT, which provides a visual display of the data have been developed. BLT-EC also includes an extensive database of thermodynamic data that is also accessible to ECIN. This document reviews the models implemented in BLT-EC and serves as a guide to creating input files and applying BLT-EC.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*

low-level radioactive waste, ground disposal, radioactive waste disposal, radionuclide migration, chemical reactions, containers, decay, finite element method, leaching, radioactivity transport, waste management, thermodynamic properties, waste forms, underground disposal

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