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Yucca Mountain Site Characterization Project

Total System Performance Assessment Code

TOSPAC

Volume 2: User's Guide

John H. Gauthier, Michael L. Wilson, Ralph R. Peters,
Alan L. Dudley, Lee H. Skinner

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Abstract

TOSPAC is a computer program designed to simulate the flow of water and the transport of soluble contaminants through fractured, partially saturated rock formations. The capabilities, limitations, and use of TOSPAC are described. Several example problems and a general reference section are included to aid the user in performing calculations.

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Chapter 1

INTRODUCTION

1.1 Overview

TOSPAC is a computer program that calculates partially saturated groundwater flow with the transport of water-soluble contaminants. TOSPAC Version 1 is restricted to calculations involving one-dimensional, vertical columns of one or more media.

TOSPAC was developed to help answer questions surrounding the burial of toxic wastes in arid regions. Burial of wastes in arid regions is attractive because of generally low population densities and little groundwater flow, in the unsaturated zone, to disturb the waste. TOSPAC helps to quantify groundwater flow and the spread of contamination, offering an idea of what could happen in the distant future. Figure 1.1 illustrates the problem TOSPAC was designed to investigate.

For groundwater flow, TOSPAC can provide saturations, velocities, and travel times for water in the rock matrix or the fractures in the unsaturated zone. TOSPAC can determine how hydrologic conditions vary when the rate of infiltration changes.

For contaminant transport, TOSPAC can compute how much of a contaminant is dissolved in the water and how it is distributed. TOSPAC can determine how fast the solute is moving and the shape of the concentration front. And TOSPAC can be used to investigate how much of the contaminant remains in the inventory of a repository, how much is adsorbed onto the soil or rock matrix, and how much reaches the water table.

Effective use of TOSPAC requires knowledge in a number of diverse disciplines, including real-world groundwater flow and transport, the mathematical models of groundwater flow and transport, real-world data required for the models, and the numerical solution of differential equations. Equally important is a realization of the limitations intrinsic to a computer model of complex physical phenomena. This User's Guide not only describes the mechanics of executing TOSPAC on a computer, but also examines these other topics.

Figure 1.1: The question TOSPAC was designed to examine.

1.2 User's Guide Organization

This User's Guide is a companion document to *TOSPAC Volume 1: Physical and Mathematical Basics* (Dudley *et al*, 1988). *Volume 1* provides a description of the physical models assumed during the development of TOSPAC, the mathematical models used in TOSPAC, the numerical techniques, and various example problems illustrating the application of these models and techniques.

Volume 1 was written for the person wanting to understand the ideas behind TOSPAC and the implications and limitations resulting from those ideas. This User's Guide, *Volume 2*, was written for the person wanting to understand the mechanics of TOSPAC and wanting to achieve meaningful results.

This User's Guide combines a primer, several example problems, and a reference manual. Chapter 1 is an introduction containing a general description of TOSPAC, the reasons for its development, its capabilities and limitations, and a summary of its applications. Chapter 2 is a primer describing a simple terminal session where TOSPAC is used to calculate groundwater contamination from a uranium mill-tailings pile. Chapter 3 contains descriptions of two example problems: first, a simulation of a laboratory imbibition experiment, and second, a simulation of groundwater contamination from a conceptual high-level radioactive waste repository (a problem taken from *Volume 1*). Chapter 4 is the general reference, containing a description of the structure of TOSPAC and a description of the TOSPAC modules, how they interact, their input requirements, and their output. The Appendices contain a discussion of batch-mode execution of TOSPAC and various information required by the agency funding this work.

The user is advised to read Chapter 1 and work through Chapters 2 and 3. Chapter 4 and the Appendices can be used as needed. For information about specific input data, Section 4.2 contains descriptions of the data required by the TOSPAC calculational modules, and Section 4.6 contains descriptions of the data required by the TOSPAC computer-graphics module.

1.3 Background

TOSPAC was developed at Sandia National Laboratories (SNL) for the Yucca Mountain Site Characterization Project (YMP) of the U. S. Department of Energy. TOSPAC is an acronym for the "Total System Performance Assessment Code." Initially, it was intended to model, as simply as reasonable, all the systems of a geologic waste repository for high-level radioactive waste. In its present form, TOSPAC models the unsaturated groundwater flow, the contaminant source term, and the groundwater transport systems.

One of the example problems in Chapter 3 deals with a simulation of a potential radioactive-waste repository at Yucca Mountain, Nevada. Any references to Yucca Mountain in this document are for illustrative purposes only. The calculations in this User's Guide will have no bearing on the evaluation of the suitability of Yucca Mountain as the site of a potential repository.

TOSPAC was not intended to break new ground, either in modeling or in numerical techniques. Rather, TOSPAC was designed to combine known models and techniques into a package usable by an engineer or hydrologist. The original design criteria for TOSPAC were as follows.

- Easy to learn and use: easy to enter data, easy to execute on a computer, producing results that are easy to understand;
- Fast: most problems could be solved in a single sitting at the computer terminal;
- Correct: the results had to be accurate enough to increase the user's knowledge of a repository system (based on accepted -- although not necessarily true -- physical models) without being misleading;
- Portable: written in standard FORTRAN 77 without machine-precision sensitivities so that it could be executed on most computer systems and could be readily modified should the need arise.

The design philosophy changed during the development of TOSPAC. The differential equations governing unsaturated groundwater flow through stratified, fractured rock contain nonlinear terms for hydraulic conductivity and water-storage capacity and the equations are very difficult to solve. Likewise, transport issues (such as radionuclide decay, hydrodynamic dispersion, and matrix diffusion) added complexity to TOSPAC. These issues had to be addressed in order for TOSPAC calculations to be valid. Thus, TOSPAC is not as easy to use as was first envisioned. For many problems, however, TOSPAC can provide useful results while minimizing busywork by the user.

1.4 Technical Overview

As shown in Figure 1.2, TOSPAC consists of six parts, or modules. The first module is the SHELL that controls the other five modules. Of the other five modules, one creates and modifies input data files (the INDATA module), another creates computer graphics of TOSPAC results (the OUTPLOT module), and three modules solve differential equations. The modules that perform the actual calculations and the differential equations they solve are as follows:

- STEADY: the steady-state-flow solver that solves Darcy's Law;
- DYNAMICS: the transient-flow solver that solves Richards' Equation; and
- TRANS: the transport solver that solves a general advection-dispersion equation.

The calculational modules of TOSPAC configure the differential equations as boundary-value problems in space, and initial-value problems in time. All three modules use the finite-difference method with an Eulerian mesh.

Figure 1.2: Overview of the TOSPAC module structure.

The hydrology modules (STEADY and DYNAMICS) solve for pressure head, with hydraulic conductivity and water-storage capacity (capacitance) specified as functions of pressure head. The media through which flow and transport occur are described by a composite-porosity model (Peters and Klavetter, 1988). Matrix and fracture hydrologic properties are specified separately (with saturation and hydraulic-conductivity characteristic curves for each), then combined under the assumption that the pressure head in the matrix equals the pressure head in the fractures.

The transport module (TRANS) uses the results from STEADY as the hydrologic background for transport. TRANS solves for contaminant concentration, using two coupled transport equations: one for transport through the matrix pores and one for transport through the fractures. There is a coupling-strength parameter that can be used to make the interaction between matrix and fractures stronger or weaker. For very strong coupling, the matrix and fracture concentrations are nearly equal but, for weak coupling, they can be significantly different, with contaminants moving faster through the fractures than through the matrix.

Volume 1 contains a detailed description of the mathematics used in TOSPAC. More information about the structure of TOSPAC can be found in Chapter 4 of this User's Guide.

1.5 Capabilities

TOSPAC was developed to assist in the performance assessment of a conceptual repository for high-level radioactive waste. Other computer models for unsaturated groundwater flow and transport existed, but most lacked certain essential features. For instance, most were developed for problems involving soil rather than fractured rock. Also, many did not allow for the decay of radionuclide contaminants.

TOSPAC was designed with specific capabilities to handle problems inherent to water flow and contaminant transport in fractured, unsaturated, stratified rocks. These capabilities are summarized in Figure 1.3.

TOSPAC was required to handle site-scale problems (i.e., problems with lengths measured in kilometers, contaminants measured in metric tons, geologic strata with billions of individual fractures, etc.). Site-scale problems are viewed macroscopically; microscopic features are described by bulk properties. The capability for site-scale modeling influenced much of TOSPAC's design. Rather than model fractures individually (something not possible in one dimension, anyway), TOSPAC uses a composite-porosity model. Hydrodynamic dispersion is characterized by a macroscopic approximation of an inherently microscopic process.

TOSPAC was required to solve problems in the unsaturated zone (the region above the water table). A location for a potential repository for high-level waste is in the unsaturated zone at Yucca Mountain. It is postulated that the unsaturated zone could be a significant barrier to radionuclide transport. But calculations are complicated because, according to experimental data (Klavetter and Peters, 1987), hydraulic conductivity and storage capacity are strongly nonlinear variables in predicting unsaturated-zone flow.

Many geological formations are stratified, with each stratum having its own fracture and matrix properties. Thus, TOSPAC was required to define properties for and compute results for both the rock matrix and the fractures in multiple media.

TOSPAC

- SITE SCALE
- UNSATURATED ZONE
- FRACTURED MEDIA
- STRATIFIED MEDIA
- STEADY STATE or TRANSIENT FLOW
- GWTT by
 - PARTICLE TRACKING
 - TRACER TRANSPORT
- MULTIPLE CONTAMINANTS
- DECAYING CONTAMINANTS
- SOURCE AT BOUNDARY or INTERIOR
- CHANGEABLE BOUNDARY CONDITIONS
- SOURCE TERMS
 - SOLUBILITY-DOMINATED
 - CONGRUENT LEACH
 - PARAMETERIZED (SAND91-0155)
 - FILE

Figure 1.3: TOSPAC capabilities.

Initially, TOSPAC was designed to solve only transient-flow problems (with the DYNAMICS module). Given an arbitrary initial condition, DYNAMICS was to calculate internal relaxations to the system as well as the influence of perturbations in pressure head or flux at the boundaries. (Steady-state flow could be calculated by letting a transient problem run until there is no longer any change.) DYNAMICS was also designed to handle changeable boundary conditions (e.g., the capability to model pluvial cycles, a fluctuating water table, etc.). However, because transient-flow problems are computationally expensive, an explicit steady-state solver, STEADY, was added to TOSPAC.

Regulations for waste-repository licensing require groundwater-travel-time (GWTT) estimates, and TOSPAC was designed to allow two different methods for making these calculations: particle-tracking method and a nonsorbing-tracer-transport method.

The nature of high-level radioactive waste dictated that TOSPAC be able to handle contaminants that decay. Further, TOSPAC was required to handle multiple contaminants, including contaminants that decay in chains of other contaminants. The TRANS module of TOSPAC implements Bateman's equations to compute radioactive decay. It can keep track of as many as 50 contaminants.

Because of the uncertainty involved in defining a source term (i.e., the influx of contaminants) several methods of modeling this term were incorporated into TOSPAC. Contaminants can be introduced at a boundary or at an internal source. Release of contaminants from an internal source can be defined by solubility-dominated or congruent-leach source terms, or by data from an external input file. Release of contaminants at the boundary (both into and out of the problem range) made it necessary for the TRANS module of TOSPAC to have changeable boundary conditions, similar to those in the DYNAMICS module.

Fractured rock can influence contaminant transport, primarily through a process known as matrix diffusion. TOSPAC was designed with coupled fracture and matrix transport; i.e., the capability to calculate contaminant concentrations in the matrix and the fractures and movement of contaminants between them.

Adsorption of contaminants onto rock surfaces could significantly retard the transport of contaminants. Thus, TOSPAC was designed to account for the adsorption and precipitation of contaminants.

Finally, to handle different methods of interpreting contaminant release (dictated by regulation), TOSPAC was designed to keep track of both the amount of each contaminant that crosses problem boundaries, and the amount that is outside problem boundaries at a given time.

1.6 Limitations and Assumptions

TOSPAC does not simulate everything. In the interest of efficiency, but also because some basic physics in hydrology and contaminant transport is not well understood, TOSPAC incorporates simplifying assumptions. TOSPAC's limitations and assumptions are summarized in Figure 1.4

Figure 1.4: TOSPAC limitations.

The composite-porosity model used by TOSPAC is based on the assumption that the pressure heads in the matrix and the fractures are equal. This condition is not valid for all transient flow conditions; however it could be valid for many problems. *Volume 1* discusses of the conditions under which this model is acceptable.

Only one-dimensional problems can be solved by TOSPAC. Because groundwater flow takes place in three spatial dimensions, the restriction to one dimension can be a severe limitation. Analyses involving flow in anisotropic materials and flow in tilting strata with differing conductivities are

especially presumptuous in one dimension. However, many problems can be reduced to one dimension, and calculations in one dimension have important advantages. First, one-dimensional calculations are computationally much simpler and less expensive. Second, checking the accuracy of a one-dimensional calculation is relatively easy (a point that should not be underestimated). Calculations of steady-state flow can be checked by comparing calculated flux against imposed flux. Calculations of transient flow can be checked by comparing the calculated time for water storage to change when flux is changed with a simple approximation. Similarly, one-dimensional contaminant transport can be checked against analytic approximations of various terms in the basic equations: advection, dispersion, decay, etc.

Only vertical flow is simulated by this version of TOSPAC. Arbitrary flow-tube versions of the hydrology modules of TOSPAC have been programmed; however, they have not been adequately tested and are not included in this release. Also, the hydrology modules of TOSPAC (STEADY and DYNAMICS) only calculate flow in the unsaturated zone. TRANS can handle saturated-zone transport, but only as a separate problem with user-supplied water velocities.

TOSPAC does not incorporate temperature effects. TOSPAC does not handle two-phase flow (e.g., no vapor-liquid problems, no oil-water problems). And TOSPAC cannot simulate hysteresis effects in the saturation and hydraulic-conductivity characteristic curves of the matrix or the fractures.

Contaminant transport is only simulated with steady-state flow fields; i.e., for unsaturated-zone calculations, only the STEADY module of TOSPAC can be used with the TRANS module. TOSPAC only accounts for transport of water-soluble materials (i.e., no colloidal transport). And, although TOSPAC models adsorption, it uses only a simple distribution-coefficient approximation.

Despite the limitations and simplifying assumptions built into TOSPAC, problems that fully utilize all of TOSPAC's capabilities require a large amount of input data from specialized disciplines. TOSPAC results can only be as good as the input data, and in certain cases small variations in the input data can cause large variations in the results (an effect called sensitivity to the input data).

1.7 Applications

The STEADY and DYNAMICS modules of TOSPAC preceded the TRANS module. To date, TOSPAC has primarily been used as a test bed for evaluating ideas about water flow in tuff, and as an aid in evaluating the importance of various scenarios involving water flow that could have an impact on the performance of a potential repository. For instance, TOSPAC was used to determine whether there is a difference between calculating groundwater travel times by using an "average fastest particle" as opposed to a nonsorbing tracer (answer: a significant difference exists if there is fracture flow and appreciable matrix/fracture coupling).

Several analyses using TOSPAC for the YMP are summarized in a compendium by Peters (1988), and include the following:

- An analysis of the feasibility of conducting a proposed field experiment involving flow in tuff, to determine if the experiment could be performed in a reasonable amount of time.
- An analysis of the penetration depth of high-pressure drilling fluid into tuff, using several different hydrologic properties for the tuff.
- An estimate of the travel times of water particles influenced by thermal effects of a repository.

This analysis was an attempt to use hydrologic effects to define the repository disturbed zone.

- An analysis of flooding down a generalized fault zone.
- An investigation of the time required for saturation levels in the unsaturated zone to relax after a significant fluctuation in the water-table height.

In an analysis similar to the example problem discussed in Section 3.1, TOSPAC was used to model the imbibition of water into a drill core of nonwelded tuff. TOSPAC results were compared with experimental results to determine the sufficiency of the computer model and the input data. The results are reported in an American Geophysical Union monograph paper (Peters *et al.*, 1987).

TOSPAC has been used in the analysis of time scales involved in flow through partially saturated, fractured tuff. One analysis is reported in a University of Arizona conference paper (Peters, 1986). A similar analysis, examining the influence of percolation rate on water travel times in deep, partially saturated strata, is reported by Peters *et al.* (1986).

TOSPAC has been involved in two computer-program benchmarking efforts. The first effort was known as Code Verification 2A, or COVE 2A (Gauthier *et al.*, 1990), and it involved several computer programs that were being used by the YMP. The second effort was an international project known as the Hydrologic Code Intercomparison Project, or HYDROCOIN (Prindle, 1987). TOSPAC was used to help define both the COVE 2A problem set and the HYDROCOIN problems for the unsaturated zone.

More recently, several analyses using TOSPAC related directly to the performance assessment of a potential repository for high-level radioactive waste. TOSPAC was one of the flow and transport models included in a demonstration of performance-assessment capabilities known as PACE 90 (Barnard and Dockery, 1991). TOSPAC was used to estimate the amount of water that could be applied during surface construction activities without detrimental effects on a potential repository (Fewell *et al.*, 1992). And finally, a version of TOSPAC has been incorporated in the Total-System Analyzer (TSA; Wilson *et al.*, 1991, and Wilson, 1992). The TSA uses the Monte Carlo method to take into account the uncertainty in present and possible future conditions experienced by a waste repository. TOSPAC, within the TSA, will be part of a series of total-system performance analyses planned for the potential high-level-radioactive-waste repository at Yucca Mountain.

Chapter 2

PRIMER

This chapter introduces TOSPAC through a simple example problem. The beginning user can immediately start this problem (or one of his or her own) without studying the rest of this User's Guide. This chapter contains a number of cross references to Chapter 4, a general reference. Chapter 3, the example problems, should give the user a head start on some typical real-life problems.

In this chapter we assume that the user is working on a Digital Equipment Corporation VAX computer with the VAX/VMS operating system (DEC, 1988), although if you are using a different computer, do not worry. The differences are obvious and generally insignificant. For instance, in order to run TOSPAC on a VAX, you type *RUN TOSPAC*, while on a Data General you type *EXE TOSPAC*, and on an IBM PC you type *TOSPAC*.

In this chapter, characters displayed by the computer or TOSPAC will be in a **TYPEWRITER** font, while characters you have typed will be *ITALICIZED*.

This chapter is organized by the steps you typically take when running TOSPAC. These steps are summarized in Figure 2.1.

2.1 Step One: Define the Problem

For this primer, a simple problem is constructed, as illustrated in Figure 2.2. A uranium mill-tailings pile is located on the ground surface in an arid region. The mill-tailings pile covers 1 km² and sits on unfractured sandstone. The water table is at a depth of 100 m; i.e., the bottom of the mill-tailings pile is 100 m above the water table. Because the environment is arid, the rate of water infiltration is only 5 mm/yr. Flow is vertical. The mill tailings contain several contaminants, but for this example we only consider ²³⁸U. How long does it take the ²³⁸U to reach the water table?

Figure 2.1: Steps involved in a TOSPAC calculation.

2.2 Step Two: Run TOSPAC

Turn on your terminal and log onto your computer.

TOSPAC should be installed on your computer's disk storage in an area where you have access—maybe your own area. If you do not know, ask someone. If it is in your own area, after the system prompt (which is the '\$' for DEC VAX) type...

```
$ RUN TOSPAC
```

If TOSPAC is not installed in your area, you will have to give a path name to reach it.

Figure 2.2: Overview of the simplified mill-tailings problem.

2.3 Step Three: Run INDATA

TOSPAC will display a menu on the screen, as follows...

TOSPAC VERSION 1.10 MAIN MENU

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

ENTER CHOICE:

Choice 0 simply halts execution of TOSPAC. We will do this later. The other choices correspond to TOSPAC modules. A complete discussion of this upper level of TOSPAC is contained in Section 4.1.

We want to get right to work, so type the number 1 to select the TOSPAC module that creates an

input-data file -- INDATA. You can also create an input-data file using your computer's text editor (Section 4.7.1).

TOSPAC now informs you that you are in module INDATA and asks if you want to enter hydrology data or transport data...

TOSPAC MODULE INDATA

INDATA MAIN MENU

- 0. STOP
- 1. CREATE STEADY INPUT-DATA FILE
- 2. CREATE DYNAMICS INPUT-DATA FILE
- 3. CREATE TRANS INPUT-DATA FILE
- 4. MODIFY STEADY INPUT-DATA FILE
- 5. MODIFY DYNAMICS INPUT-DATA FILE
- 6. MODIFY TRANS INPUT-DATA FILE

ENTER CHOICE:

INDATA can create or modify both hydrology input files and transport input files. If you want to create a steady-state input-data file (and you do) then enter a 1.

Throughout TOSPAC, entering only a <CR> always selects the default answer. The default to a *yes/no* question is always *NO*. The default answer to a *do-something/do-nothing* question is always *do-nothing*. The default to a *menu choice* is always *STOP* (although for a menu you have to enter <CR> three times before the stop is activated; this repetition protects against mistakes). And if there is a *list* of possible responses (set off with parentheses), the default answer is the *first item* of the list.

Now TOSPAC wants to know the name of the data file it will be creating...

ENTER STEADY INPUT-DATA FILE (DEFAULT=STEADY.DAT):

TOSPAC asks for a file name so that it can refer to this data file later and so that you can have a copy of it in your area after this run is finished. If you enter the name of an existing file here, you will get an error message and the prompt will reappear.

Because you do not have an input file to modify, and you really do not have an idea of a good input file name, just select the default by entering a <CR>. And TOSPAC responds with...

CREATING STEADY.DAT...

2.4 Step Four: Enter Hydrology Data

Now we are ready to begin the only difficult part of TOSPAC-- the input data. Actually, entering the data is not so difficult, but *knowing* the data is difficult. Modeling unsaturated flow and contaminant transport requires a large number of parameters that are not readily available. To ease the process of entering the input data, TOSPAC has been equipped with default values wherever possible. This simplified example uses many of these defaults. A complete discussion of the input data that are required is given in Section 4.2.

Return your attention to the terminal. INDATA begins to request information...

TITLE BLOCK

We will want a problem title. The title will appear on your results so that you can distinguish them several years from now. So think up something that catches the significance of this calculation--and that only uses a single line (80 characters)...

DEFAULT TITLE: NONE

ENTER PROBLEM TITLE: *Simplified Mill-Tailings Problem*

INDATA now allows various information to be placed after the title...

DEFAULT NOTE: NONE

ENTER NOTES (ENTER A PERIOD (.) IN THE 1ST COLUMN TO STOP NOTES
OR ENTER "DEFAULT" IF YOU WANT THE DEFAULT)...

We do not really have any notes to place here. But if we did, you could type in whatever you wanted (Section 4.2.5). For now, skip it. Enter a period in the first column of an otherwise blank line and TOSPAC will proceed. (Note that entering a <CR> will not select the default answer for the notes prompt--it will enter a blank line into the notes section. To every rule there is an exception....)

Continuing, TOSPAC asks for various constants (Section 4.2.6). One reason TOSPAC needs information about constants is because it is unit independent. It is up to you to be consistent with your units! TOSPAC default values are all in *Système International* or *SI* units. Most physical constants (e.g., gravity) are implicit in the equations that TOSPAC solves. Viscosity of the fluid is implicit in the characteristic curves of the flow media.

CONSTANTS BLOCK

ENTER DENSITY OF WATER (DEFAULT=1000. kg/m**3):

If you want the default--and we do--just enter a <CR>. The density of water is used to calculate the weight of water in the problem.

A further note about units: you can enter units after a value, but TOSPAC only treats the units as a special type of comment. Units *must* be separated from the data value by a single space or a single tab. Remember, TOSPAC does *not* understand the units! Be consistent with the units of the data values. Do *not* mix units.

INDATA continues prompting...

ENTER COMPRESSIBILITY OF WATER (DEFAULT=4.3E-6 /m):

Again we want the default, so enter a <CR>. Section 4.2.6 contains a discussion of this constant.

ENTER CROSS-SECTIONAL AREA OF THE COLUMN (DEFAULT=1. m**2): 1.E+6 m**2

The cross-sectional area is a constant because TOSPAC presently calculates only one-dimensional vertical flow. In hydrologic calculations the cross-sectional area is only used to calculate change of water mass. The default is a unit area, but let's make it the size of the mill-tailings pile: 1 km², or in SI units, 1,000,000 m².

ENTER TIMESTEP-CONTROL FACTOR (DEFAULT=0.1):

The timestep-control factor is a number that multiplies the timestep calculated by TOSPAC so that you can have some control over it. Steady-state calculations do not involve time and this value is ignored by STEADY.

ENTER IMPLICITNESS FACTOR (DEFAULT=0.5):

Implicitness (usually denoted by Ω) is the term used to specify when, within a given timestep, the equation variables are to be calculated. This value is also ignored by STEADY.

An important capability of TOSPAC is calculating groundwater travel times (GWTTs). One method that TOSPAC uses for this calculation is to track a water particle as it moves through the problem domain. (Sections 3.1, 3.2, 4.2.6, and 4.6.3.4 contain further discussions of GWTT calculations.) To access this calculation, you specify the starting and ending locations of the particle.

ENTER GWTT START POSITION (DEFAULT=TOP):

ENTER GWTT END POSITION (DEFAULT=BOTTOM):

The default entries tell TOSPAC to calculate GWTT from the top of the column to the bottom. If you do not want this calculation (which is very efficient in STEADY, but rather time consuming in DYNAMICS), you should enter the word *NONE*.

The last prompt in the constants block concerns restarting a DYNAMICS calculation (Section 4.4). It is not used by STEADY, and it is offered here without discussion.

ENTER TIME SNAPSHOT FOR RESTART (DEFAULT=0):

TOSPAC now begins a definition of the stratigraphy (Section 4.2.7).

Comments will be fewer now; the discussion will concentrate on what INDATA prompts in TYPEWRITER TYPE, and what you respond in *ITALICIZED TYPE*. Notice that no visible response means that the default has been selected by entering only a <CR>. We have constructed this example problem so that the defaults are used as often as possible.

GEOLOGIC-UNIT BLOCK

ENTER # OF GEOLOGIC UNITS (DEFAULT=1):

UNIT # 1

UNIT # 1 DEFAULT NAME: NONE

ENTER UNIT # 1 NAME: *Sandstone*

TOSPAC asks for names for geologic units, materials, and contaminants. As with the problem title, you can enter an arbitrary character string up to 80 characters in length.

ENTER LOWER ELEVATION (DEFAULT=0. m):

ENTER UPPER ELEVATION (DEFAULT=100. m):

ENTER MATRIX-MATERIAL INDEX (DEFAULT=1):

TOSPAC is asking for the position of the matrix material in the list of material properties (Section 4.2.8). You will enter material-property data in a minute.

ENTER FRACTURE-MATERIAL INDEX (DEFAULT=1):

ENTER FRACTURE POROSITY (DEFAULT=0.):

There are two different ways to indicate no fractures. If the fracture-material index is the same as the matrix-material index, then the fractures and the matrix have the same hydrologic properties, and the results would be the same as if there were no fractures. If the fracture porosity is zero, the fracture hydrologic properties do not contribute to the calculation. For efficiency, it is better to set the fracture porosity to zero; for understanding, it is better to do both. The default values for the fracture-material index and the fracture porosity specify no fractures.

ENTER BULK ROCK COMPRESSIBILITY (DEFAULT=0. /m):

ENTER FRACTURE COMPRESSIBILITY (DEFAULT=0. /m):

The default values imply that the bulk rock (i.e., the combination of matrix and fractures) and the fractures do not compress. TOSPAC only uses compressibilities in the water-storage term of the transient-flow equation, not in a steady-state solution.

MATERIAL-PROPERTY BLOCK

ENTER # OF MATERIALS (DEFAULT=1):

MATERIAL # 1

MATERIAL # 1 DEFAULT NAME: NONE

ENTER MATERIAL # 1 NAME: *Sandstone (van Genuchten, 1980)*

ENTER POROSITY (DEFAULT=1.): *0.25*

CHARACTERISTIC-CURVE FLAGS ARE...

1. VAN GENUCHTEN
2. VAN GENUCHTEN TABLE LOOKUP
3. SATURATION DATA-TABLE
4. DATA-TABLE
5. COMBINATION

ENTER CHARACTERISTIC-CURVE FLAG (DEFAULT=1):

The characteristic curves are the functions of saturation versus pressure head and hydraulic conductivity versus pressure head that describe how the material behaves in a partially saturated state. The characteristic-curve flag lets INDATA know how these curves will be specified and what data to expect. The default is the van Genuchten specification (van Genuchten, 1980). The methods of specifying characteristic curves are discussed in Section 4.2.8. After you select the default, TOSPAC prompts for the five parameters that are used by the van Genuchten model to define the characteristic curves:

```

ENTER TOTAL SATURATION (DEFAULT=1.):
ENTER RESIDUAL SATURATION (DEFAULT=0.0395): 0.612
ENTER ALPHA (DEFAULT=1.2851 /m): 0.79 /m
ENTER BETA (DEFAULT=4.23): 10.4
ENTER SATURATED HYDRAULIC CONDUCTIVITY (DEFAULT=4.4E-6 m/s): 1.25E-5 m/s

```

The default material specification is a typical sand taken from Freeze and Cherry (1979). We do not want a column of sand, we want sandstone, so we have entered the various values for a sandstone specified by van Genuchten (1980).

We have also entered the units. Remember, they are only a note to the user; TOSPAC cannot understand them!

TOSPAC requires a calculational mesh to solve Darcy's Law (or Richards' Equation in DYNAMICS, or the advection-dispersion equation in TRANS). The next block of input data concerns the construction of this mesh:

```

MESH BLOCK
AUTOMATIC MESH GENERATOR (N OR Y):

```

Again, the default answer for a yes/no question is always no, so entering a <CR> tells TOSPAC not to run the automatic mesh generator. (Don't try to use the automatic mesh generator before you read Section 4.2.9.)

So we have to construct the calculational mesh by hand. Actually, it is not so difficult...

```

ENTER TOTAL # OF CELLS (DEFAULT=200): 500
ENTER # OF SUBMESHES (DEFAULT=1):

SUBMESH # 1
ENTER LOWER ELEVATION (DEFAULT=0. m):
ENTER UPPER ELEVATION (DEFAULT=100. m):
ENTER # OF CELLS FOR THIS SUBMESH (DEFAULT=500):

```

We have just created a uniform mesh of 500 cells, which corresponds to 501 mesh points. (We tried to run this problem with the default 200 cells but, for accuracy, we needed more cells near the bottom boundary.)

Now TOSPAC wants to know the boundary conditions:

```

BOUNDARY-CONDITION BLOCK
ENTER # OF TIME SNAPSHOTS (DEFAULT=1):

```

Despite the fact that we are creating an input-data file for STEADY, TOSPAC still requests time information. The input-data files for hydrology calculations are organized so that they can be read by either STEADY or DYNAMICS. STEADY only reads one "time snapshot" (if more are present, they are ignored) and it ignores the time.

In another concession to input-data-file standardization, TOSPAC asks for additional time-related information. TOSPAC allows conversion of time units into more manageable numbers...


```

TIME CONVERSION MENU
0. NO CONVERSION
1. NO CONVERSION (SECONDS ASSUMED)
2. CONVERT HOURS TO SECONDS
3. CONVERT DAYS TO SECONDS
4. CONVERT YEARS TO SECONDS
5. NO CONVERSION (YEARS ASSUMED)
6. CONVERT SECONDS TO YEARS
7. CONVERT HOURS TO YEARS
8. CONVERT DAYS TO YEARS

```

```

ENTER CHOICE (DEFAULT=1):

```

We entered a choice of 1, meaning that our time units are in seconds everywhere. Actually, STEADY ignores this entry, but it is important to DYNAMICS (Section 4.2.10) and TRANS (Step Five below, and Section 4.2.17).

Finally, TOSPAC begins to ask for the actual boundary conditions (for each time snapshot)...

```

SNAPSHOT # 1
ENTER TIME (DEFAULT=0. s):
  BOUNDARY-CONDITION FLAGS ARE 2 DIGITS (LOWER/UPPER)...
  0. USE PREVIOUS BOUNDARY CONDITION
  1. PRESSURE-HEAD BOUNDARY
  2. FLUX BOUNDARY
  3. POND-DRAIN BOUNDARY (UPPER ONLY)
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=12):
ENTER LOWER-BOUNDARY PRESSURE HEAD (DEFAULT=0. m):
ENTER UPPER-BOUNDARY FLUX (DEFAULT=0. m/s): -1.585E-10 m/s
ENTER MAX POND HEIGHT (DEFAULT=0. m):

```

The boundary-condition flag, as shown, allows us to specify the pressure-head or flux conditions at either the upper or lower boundary. Actually, for a steady-state calculation, only boundary-condition flag 12 (a pressure-head lower-boundary condition and a flux upper-boundary condition) is allowed (Section 4.2.10). Notice that the default is to specify zero meters of pressure head (i.e., the water table) at the lower boundary with zero flux (i.e., no flow) going into the upper boundary. For a steady-state problem this default produces a hydrostatic condition. The maximum pond height is used by DYNAMICS and ignored by STEADY.

We do not want a hydrostatic condition: we want 5 mm/yr or 1.585×10^{-10} m/s. The flux is entered as a negative number to indicate that the flow is downward.

For a steady-state problem there is one more data block...

```

FILE BLOCK
STEADY SOLUTION FILE DEFAULT NAME: STEADY.PSI
ENTER STEADY SOLUTION FILE NAME:
PLOT-DATA FILE DEFAULT NAME: STEADY.PLT
ENTER PLOT-DATA FILE NAME:
OUTPUT-LISTING FILE DEFAULT NAME: STEADY.LIS
ENTER OUTPUT-LISTING FILE NAME:

```

ENTER OUTPUT-LISTING CONTROL (DEFAULT=1):

The file block tells TOSPAC the output files you want created (Section 4.7). The *STEADY solution file* contains the steady-state pressure-head solution in a form that can be used by the DYNAMICS module as an initial condition. The *plot-data file* contains information needed by both the OUTPLOT module in order to construct plots, and the TRANS module in order to define the mesh and the hydrologic background of a problem. The *output-listing file* contains problem results in a format that you can read. Note that the extensions PSI, PLT, and LIS stand for pressure head (ψ —not pounds per square inch), plot, and listing, respectively.

The output-listing control allows you to specify the number of mesh-point values you want written out; control number 1 means you want all the values (Section 4.2.11).

If you do not want a file created, enter the word *NONE* (in upper or lower case). The default is to create all the files. If a file name is entered, a file with that name will be created.

TOSPAC now states that it is finished creating a STEADY input-data file...

STEADY INPUT-DATA FILE STEADY.DAT CREATED.

DO YOU WANT TO HAVE STEADY.DAT CHECKED FOR ERRORS (N OR Y): *y*

And after a moment...

READING INPUT-DATA FILE STEADY.DAT.

STEADY.DAT CONTAINS NO OBVIOUS ERRORS.

If there had been errors in STEADY.DAT, they would have been listed. TOSPAC allows you to modify input-data files (Section 4.2.3). You can also modify this file with your text editor.

TOSPAC now asks a few more operational questions...

DO YOU WANT TO VIEW STEADY.DAT (N OR Y):

DO YOU WANT TO MODIFY STEADY.DAT (N OR Y):

And we are returned to the TOSPAC main menu...

TOSPAC VERSION 1.10 MAIN MENU

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

ENTER CHOICE:

Figure 2.3 shows the form and contents of the steady-state input-data file, STEADY.DAT, although we do not need to know what this file looks like to run the problem.

```

*****
*** TOSPAC HYDRO INPUT-DATA FILE ***
*****

***** TITLE BLOCK *****
Simplified Mill-Tailings Problem

***** CONSTANTS BLOCK *****
1000. kg/m**3      DENSITY OF WATER
4.3E-6 /m          COMPRESSIBILITY OF WATER
1.E+6 m**2         CROSS-SECTIONAL AREA OF COLUMN
0.1                TIMESTEP FACTOR
0.6                IMPLICITNESS FACTOR
TOP                GWTT START POSITION
BOTTOM             GWTT END POSITION
0                  TIME SNAPSHOT FOR RESTART

***** GEOLOGIC-UNIT BLOCK *****
1                  # GEOLOGIC UNITS
UNIT # 1 ...NAME:
Sandstone
0. m               MIN ELEVATION
100. m             MAX ELEVATION
1                  MATRIX MATERIAL INDEX
1                  FRACTURE MATERIAL INDEX
0.                 FRACTURE POROSITY
0. /m              BULK-ROCK COMPRESSIBILITY
0. /m              FRACTURE COMPRESSIBILITY

***** MATERIAL-PROPERTY BLOCK *****
1                  # MATERIALS
MATERIAL # 1 ...NAME:
Sandstone (van Genuchten, 1980)
0.25               MATERIAL EFFECTIVE POROSITY
1                  CHARACTERISTIC CURVE FIT
1.                 TOTAL SATURATION
0.612              RESIDUAL SATURATION
0.79 /m            ALPHA COEFFICIENT
10.4               BETA COEFFICIENT
1.28E-5 m/s        SATURATED HYDRAULIC CONDUCTIVITY

***** MESH BLOCK *****
500                TOTAL # CELLS
1                  # SUBMESHES
SUBMESH # 1:
0. m               LOWER ELEVATION
100. m             UPPER ELEVATION
500                # CELLS

***** BOUNDARY-CONDITION BLOCK *****
1                  # TIME SNAPSHOTS
1                  TIME CONVERSION NUMBER
SNAPSHOT # 1
0. sec             PROBLEM TIME
12                BOUNDARY-CONDITION FLAG
0. m               LOWER-BOUNDARY PRESSURE HEAD
-1.586E-10 m/s     UPPER-BOUNDARY FLUX
0. m               MAX POND HEIGHT

***** FILE BLOCK *****
STEADY.PSI         STEADY SOLUTION FILE
STEADY.PLT         PLOT-DATA FILE
STEADY.LIS         OUTPUT-LISTING FILE
1                  OUTPUT-LISTING CONTROL

```

Figure 2.3: STEADY input-data file for the simplified mill-tailings problem.

2.5 Step Five: Enter Transport Data

We still need a transport input-data file in order to make this example complete. Type 1 in response to the TOSPAC main menu to get the INDATA main menu back...

TOSPAC MODULE INDATA

INDATA MAIN MENU

- 0. STOP
- 1. CREATE STEADY INPUT-DATA FILE
- 2. CREATE DYNAMICS INPUT-DATA FILE
- 3. CREATE TRANS INPUT-DATA FILE
- 4. MODIFY STEADY INPUT-DATA FILE
- 5. MODIFY DYNAMICS INPUT-DATA FILE
- 6. MODIFY TRANS INPUT-DATA FILE

ENTER CHOICE: 3

INDATA queries for a transport input-data file name...

ENTER TRANS INPUT-DATA FILE (DEFAULT=TRANS.DAT):
CREATING TRANS.DAT...

TITLE BLOCK

DEFAULT TITLE: NONE

ENTER PROBLEM TITLE: *Simplified Mill-Tailings Problem*

DEFAULT NOTE: NONE

ENTER NOTES (ENTER A PERIOD (.) IN THE 1ST COLUMN TO STOP NOTES
OR ENTER "DEFAULT" IF YOU WANT THE DEFAULT)...

We still have no notes to add, so enter a period.

SOURCE BLOCK

SOURCE FLAGS ARE...

- 0. SOURCE SET BY BOUNDARY CONDITION
- 1. INTERIOR, CONGRUENT-LEACH SOURCE
- 2. INTERIOR, SOLUBILITY-LIMIT SOURCE
- 3. INTERIOR, FILE-DEFINED SOURCE
- 4. INTERIOR, SAND91-0155 SOURCE

ENTER SOURCE FLAG (DEFAULT=0):

The source, or source term, consists of the location, the amount, and the method of release of the contaminant. TOSPAC allows you to locate the source at the boundary (as a boundary condition), or somewhere within the mesh. You just told TOSPAC that you want the contaminant at the boundary. (Section 4.2.13 contains details.)

ENTER AREA OF REPOSITORY (DEFAULT=1. m**2): *1.E+6 m**2*

TOSPAC wants to know the area of the repository it is dealing with so that it can compute release amounts for the total amount of contaminant. (Remember, TOSPAC is a one-dimensional model, so when we talk about total release, it is as if every flow path under the contaminant is the same as the one given by the steady-state solver.) We have entered a square kilometer as the area of repository. If the number looks familiar, we also entered it in the STEADY input-data file as the cross-sectional area of the column.

The TRANS module of TOSPAC can solve transport problems in either the unsaturated or the saturated zone, but not both at the same time. (STEADY and DYNAMICS can only solve problems in the unsaturated zone.) TOSPAC asks the domain for this problem...

UNSATURATED- OR SATURATED-ZONE PROBLEM (U OR S):

We have an unsaturated-zone problem, so just select the default.

TOSPAC continues by asking for more information about geologic units (Section 4.2.14). This information must be for the same geologic units given in the hydrology input-data file...

GEOLOGIC-UNIT BLOCK

ENTER # OF GEOLOGIC UNITS (DEFAULT=1):

UNIT # 1

UNIT # 1 DEFAULT NAME: NONE

ENTER UNIT # 1 NAME: *Sandstone*

ENTER BULK DENSITY (DEFAULT=2000. kg/m**3): *1800. kg/m**3*

ENTER FRACTURE SURFACE AREA PER UNIT VOLUME (DEFAULT=0. /m):

ENTER FRACTURE SPACING (DEFAULT=0. m):

ENTER LONGITUDINAL MATRIX DISPERSIVITY (DEFAULT=0. m): *10. m*

ENTER LONGITUDINAL FRACTURE DISPERSIVITY (DEFAULT=0. m):

ENTER MATRIX-VELOCITY CORRELATION LENGTH (DEFAULT=0. m): *30. m*

ENTER FRACTURE-VELOCITY CORRELATION LENGTH (DEFAULT=0. m):

ENTER MATRIX TORTUOSITY (DEFAULT=1.): *5.*

ENTER FRACTURE TORTUOSITY (DEFAULT=1.):

ENTER MATRIX/FRACTURE COUPLING FACTOR (DEFAULT=1.):

TOSPAC now asks for contaminant properties (Section 4.2.16)...

CONTAMINANT-PROPERTY BLOCK

ENTER # OF CHAINS (DEFAULT=1):

ENTER # OF SPECIES FOR CHAIN # 1 (DEFAULT=1):

ENTER # OF GEOLOGIC UNITS (DEFAULT=1):

CONTAMINANT # 1 CHAIN # 1 SPECIES # 1

CONTAMINANT # 1 DEFAULT NAME: NONE

ENTER CONTAMINANT # 1 NAME: *U-238*

ENTER INITIAL INVENTORY (DEFAULT=0. mol):

ENTER HALF-LIFE (DEFAULT=INFINITY): *1.41E+17 s*

ENTER ACTIVITY (DEFAULT=0. Ci/mol): *8.00E-5 Ci/mol*

ENTER RELEASE LIMIT (DEFAULT=0. Ci):

ENTER SOLUBILITY (DEFAULT=0. mol/m**3): *2.1E-4 mol/m**3*

```

ENTER DIFFUSION COEFF (DEFAULT=0. m**2/s): 1.E-9 m**2/s
ENTER MATRIX DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m**3/kg): 5.3E-3 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m):

```

In the above sequence of prompts, the activity and the release limit pertain to Environmental Protection Agency (EPA) regulations and are only used by TOSPAC to compute the EPA ratio. We will not worry about them here.

Also, notice that TOSPAC asks for the number of geologic units again. This entry allows TOSPAC to cross check the input-data file, and allows modification of the contaminant-property block independent of the geologic-unit block.

Now the boundary conditions must be given (notice the similarity between the transport boundary-condition block, Section 4.2.17, and the hydrology boundary-condition block, Section 4.2.10)...

BOUNDARY-CONDITION BLOCK

```

ENTER # OF TIME SNAPSHOTS (DEFAULT=1): 33

```

The number of time snapshots corresponds to the number of data segments we want in the output files. At any or all of these snapshot times we could change the boundary conditions. (Section 4.2.10). We want quite a few time snapshots for this problem so that our plots will be informative and provide smooth time histories.

As mentioned previously, TOSPAC input data can be in any units as long as the data are consistent. Unfortunately, this freedom is cumbersome when having to enter very long times in seconds. Just for the boundary-condition block, TOSPAC allows conversion of time units into more manageable numbers...

TIME CONVERSION MENU

- 0. NO CONVERSION
- 1. NO CONVERSION (SECONDS ASSUMED)
- 2. CONVERT HOURS TO SECONDS
- 3. CONVERT DAYS TO SECONDS
- 4. CONVERT YEARS TO SECONDS
- 5. NO CONVERSION (YEARS ASSUMED)
- 6. CONVERT SECONDS TO YEARS
- 7. CONVERT HOURS TO YEARS
- 8. CONVERT DAYS TO YEARS

```

ENTER CHOICE (DEFAULT=1): 4

```

We entered choice 4, meaning that our time units are really seconds, but we are going to enter snapshot times in years. If we want to enter time in seconds, then we could have entered a choice of 1, or the default <CR>. But entering the time in years is much easier. Also, the time axes on any plots we request will now be shown in years. Notice that if we had consistently used other time units throughout the input-data file (e.g., weeks or millennia), we should enter 0 as our choice. A choice of 0 tells TOSPAC that the time snapshots should not be converted to different units and the OUTPLOT module of TOSPAC should not assume seconds or years in labeling the plots.

As a consistency check, TOSPAC asks again for the number of contaminants...

ENTER # OF CONTAMINANTS (DEFAULT=1):

TOSPAC now begins prompting for time and boundary-condition information at every snapshot...

SNAPSHOT # 1

ENTER TIME (DEFAULT=0. yr):

The first default is 0 yr because TOSPAC wants to start every problem at time 0. We could have entered 1993 or -10,000 or any real number as the problem start time.

BOUNDARY-CONDITION FLAGS ARE 2 DIGITS (LOWER/UPPER)...

0. USE PREVIOUS BOUNDARY CONDITION

1. CONCENTRATION BOUNDARY

2. CONCENTRATION-FLUX BOUNDARY

3. ZERO-CONCENTRATION-GRADIENT BOUNDARY

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=12): 31

In the source block above, we told TOSPAC that we were going to put the contaminant source at the boundary, and boundary-condition flag 31 means a concentration is to be specified at the upper boundary, but the lower boundary is to be defined by setting the spatial derivative of the concentration to zero (allowing whatever amount of contaminant that reaches the lower boundary to exit the mesh; Section 4.2.17)...

ENTER CONTAMINANT # 1

UPPER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3): 1.E-6 mol/m**3

ENTER CONTAMINANT # 1

UPPER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):

We specified that a matrix concentration of 10^{-6} mol/m³ of ²³⁸U be imposed at the upper boundary. No prompts are issued for the lower boundary because TOSPAC already knows that we want to set the spatial derivative to zero. There are no fractures, thus the fracture data are superfluous. These boundary conditions are in effect until the next time snapshot is specified.

And we continue...

SNAPSHOT # 2

ENTER TIME (DEFAULT=0. yr): 5000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

Some brief notes: first, the snapshot time default is two times whatever the previous time was (in this case, a not-so-useful 0 yr); second, a boundary-condition flag of 00 means to use the previous lower and upper boundary conditions.

SNAPSHOT # 3

ENTER TIME (DEFAULT=10000. yr):

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 4

ENTER TIME (DEFAULT=20000. yr):

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 5
ENTER TIME (DEFAULT=40000. yr): 30000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 6
ENTER TIME (DEFAULT=60000. yr): 40000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 7
ENTER TIME (DEFAULT=80000. yr): 50000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 8
ENTER TIME (DEFAULT=100000. yr): 60000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 9
ENTER TIME (DEFAULT=120000. yr): 70000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 10
ENTER TIME (DEFAULT=140000. yr): 80000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 11
ENTER TIME (DEFAULT=160000. yr): 90000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 12
ENTER TIME (DEFAULT=180000. yr): 100000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 13
ENTER TIME (DEFAULT=200000. yr): 110000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 14
ENTER TIME (DEFAULT=220000. yr): 120000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 15
ENTER TIME (DEFAULT=240000. yr): 130000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 16
ENTER TIME (DEFAULT=260000. yr): 140000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

Around this time we estimate that the mill-tailings pile has run out of ^{238}U . Therefore, at the next time snapshot we are going to shut off the source by changing the boundary condition. . .

SNAPSHOT # 17

ENTER TIME (DEFAULT=280000 yr): 150000 yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 32

Boundary-condition flag 32 means that the lower boundary is still to be specified by zero concentration gradient, but now the upper boundary is to be specified by a concentration flux...

ENTER CONTAMINANT # 1

UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):

ENTER CONTAMINANT # 1

UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):

We specified that nothing is to enter the upper boundary after 150,000 yr.

SNAPSHOT # 18

ENTER TIME (DEFAULT=300000. yr): 155000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 19

ENTER TIME (DEFAULT=310000. yr): 160000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 20

ENTER TIME (DEFAULT=320000. yr): 170000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 21

ENTER TIME (DEFAULT=340000. yr): 180000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 22

ENTER TIME (DEFAULT=360000. yr): 190000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 23

ENTER TIME (DEFAULT=380000. yr): 200000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 24

ENTER TIME (DEFAULT=400000. yr): 210000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 25

ENTER TIME (DEFAULT=420000. yr): 220000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 26

ENTER TIME (DEFAULT=440000. yr): 230000. yr

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):

SNAPSHOT # 27

```
ENTER TIME (DEFAULT=460000. yr): 240000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):
```

```
SNAPSHOT # 28
ENTER TIME (DEFAULT=480000. yr): 250000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):
```

```
SNAPSHOT # 29
ENTER TIME (DEFAULT=500000. yr): 260000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):
```

```
SNAPSHOT # 30
ENTER TIME (DEFAULT=520000. yr): 270000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):
```

```
SNAPSHOT # 31
ENTER TIME (DEFAULT=540000. yr): 280000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):
```

```
SNAPSHOT # 32
ENTER TIME (DEFAULT=560000. yr): 290000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00):
```

```
SNAPSHOT # 33
ENTER TIME (DEFAULT=580000. yr): 300000. yr
```

The TRANS module must know the initial concentrations to be assigned to the mesh points at the start of the problem (Section 4.2.18). TOSPAC prompts for this information as follows...

```
INITIAL-CONDITION BLOCK
  INITIAL-CONDITION FLAGS ARE...
  0. ZERO CONCENTRATION, ALL CONTAMINANTS, ALL MESH POINTS
  1. CONSTANT CONCENTRATIONS
  2. FILE-DEFINED CONCENTRATIONS
ENTER INITIAL-CONDITION FLAG (DEFAULT=0):
```

Because we want zero concentration everywhere and this value is the default, we enter <CR>.

Lastly, we need to enter the file information required by TRANS (Section 4.2.11)...

```
FILE BLOCK
STEADY PLOT-DATA FILE DEFAULT NAME: STEADY.PLT
ENTER STEADY PLOT-DATA FILE NAME:
TRANS PLOT-DATA FILE DEFAULT NAME: TRANS.PLT
ENTER TRANS PLOT-DATA FILE NAME:
OUTPUT-LISTING FILE DEFAULT NAME: TRANS.LIS
ENTER OUTPUT-LISTING FILE NAME:
ENTER OUTPUT-LISTING CONTROL (DEFAULT=1):
```

The STEADY plot-data file is required to set up the hydrologic background needed for a transport calculation. The TRANS plot-data and output-listing files will contain the TRANS output.

The INDATA module of TOSPAC is now finished creating a TRANS input-data file and says so...

```
TRANS INPUT-DATA FILE TRANS.DAT CREATED.  
DO YOU WANT TO HAVE TRANS.DAT CHECKED FOR ERRORS (N OR Y): Y
```

And after a moment...

```
READING INPUT-DATA FILE TRANS.DAT.  
TRANS.DAT CONTAINS NO OBVIOUS ERRORS.
```

A copy of TRANS.DAT is presented in Figure 2.4. Notice how it follows our input session; the major difference is that the data are placed before the comments on each line so that TOSPAC can read them more easily.

After INDATA checks your TRANS input-data file, it asks if you would like to view or modify this file...

```
DO YOU WANT TO VIEW TRANS.DAT (N OR Y):  
DO YOU WANT TO MODIFY TRANS.DAT (N OR Y):
```

and then returns you to the TOSPAC SHELL (i.e., the main menu)...

```
TOSPAC VERSION 1.10 MAIN MENU
```

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

```
ENTER CHOICE:
```

In order to complete this example, we need to determine the steady-state hydrology by executing the STEADY module; then we must determine the transport of our contaminant by executing the TRANS module. After these two calculations we can make some computer-generated plots of the results by executing the OUTPLOT module.

But now is a good time to take a break. Enter choice 0, and log off.

```

*****
*** TOSPA TRANS INPUT-DATA FILE ***
*****

***** TITLE BLOCK *****
Simplified Mill-Tailings Problem

***** SOURCE BLOCK *****
0 SOURCE-TERM FLAG
1.E+6 m**2 AREA OF REPOSITORY

***** GEOLOGIC-UNIT BLOCK *****
1 # GEOLOGIC UNITS
UNIT # 1... NAME:
Sandstone
1800. kg/m**3 BULK DENSITY
0. /m FRACTURE SURFACE AREA PER UNIT VOLUME
0. m FRACTURE SPACING
10. m LONGITUDINAL MATRIX DISPERSIVITY
0. m LONGITUDINAL FRACTURE DISPERSIVITY
30. m MATRIX VELOCITY CORRELATION LENGTH
0. m FRACTURE VELOCITY CORRELATION LENGTH
5. MATRIX TORTUOSITY
1. FRACTURE TORTUOSITY
1. MATRIX/FRACTURE COUPLING FACTOR

***** CONTAMINANT-PROPERTY BLOCK *****
1 # CHAINS
1 # SPECIES FOR CHAIN # 1
1 # GEOLOGIC UNITS (CONSISTENCY CHECK)
CONTAMINANT # 1 CHAIN # 1 SPECIES # 1... NAME:
U-238
0. mol INITIAL INVENTORY
1.41E+17 s HALF-LIFE
8.00E-6 Ci/mol ACTIVITY
0. Ci RELEASE LIMIT
2.1E-4 mol/m**3 SOLUBILITY
1.E-9 m**2/s DIFFUSION COEFFICIENT
5.3E-3 m**3/kg MATRIX DISTRIBUTION COEFFICIENT FOR UNIT 1
0. m FRACTURE DISTRIBUTION COEFFICIENT FOR UNIT 1

***** BOUNDARY-CONDITION BLOCK *****
33 # TIME SNAPSHOTS
4 TIME CONVERSION NUMBER
1 # CONTAMINANTS (CONSISTENCY CHECK)
SNAPSHOT # 1
0. yr PROBLEM TIME
31 BOUNDARY-CONDITION FLAG
1.E-6 mol/m**3 CONTAMINANT # 1 UPPER-BOUNDARY MATRIX CONC
0. mol/m**3 CONTAMINANT # 1 UPPER-BOUNDARY FRACTURE CONC
SNAPSHOT # 2
5000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 3
10000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 4
20000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 5
30000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 6
40000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 7
50000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 8
60000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 9
70000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 10
80000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 11
90000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG
SNAPSHOT # 12
100000. yr PROBLEM TIME
00 BOUNDARY-CONDITION FLAG

```

Figure 2.4: TRANS input-data file for the simplified mill-tailings problem.

```

SNAPSHOT # 13
110000. yr
00
SNAPSHOT # 14
120000. yr
00
SNAPSHOT # 15
130000. yr
00
SNAPSHOT # 16
140000. yr
00
SNAPSHOT # 17
150000. yr
32
0. mol/m**2/s
0. mol/m**2/s
SNAPSHOT # 18
155000. yr
00
SNAPSHOT # 19
160000. yr
00
SNAPSHOT # 20
170000. yr
00
SNAPSHOT # 21
180000. yr
00
SNAPSHOT # 22
190000. yr
00
SNAPSHOT # 23
200000. yr
00
SNAPSHOT # 24
210000. yr
00
SNAPSHOT # 25
220000. yr
00
SNAPSHOT # 26
230000. yr
00
SNAPSHOT # 27
240000. yr
00
SNAPSHOT # 28
250000. yr
00
SNAPSHOT # 29
260000. yr
00
SNAPSHOT # 30
270000. yr
00
SNAPSHOT # 31
280000. yr
00
SNAPSHOT # 32
290000. yr
00
SNAPSHOT # 33
300000. yr

***** INITIAL-CONDITION BLOCK *****
0
INITIAL-CONDITION FLAG

***** FILE BLOCK *****
STEADY.PLT STEADY PLOT-DATA FILE
TRANS.PLT TRANS PLOT-DATA FILE
TRANS.LIS OUTPUT-LISTING FILE
1 OUTPUT-LISTING CONTROL

```

Figure 2.4- Concluded.

2.6 Step Six: Run STEADY

Log back onto your computer system. Again type the following, or the equivalent for your system, on your computer terminal...

```
$ RUN TOSPAC
```

TOSPAC responds with the main menu...

```
TOSPAC VERSION 1.10 MAIN MENU
0. STOP
1. INDATA
2. STEADY
3. DYNAMICS
4. TRANS
5. OUTPLOT
```

```
ENTER CHOICE:
```

Now, if you remember, we already produced two input-data files, so we can proceed to the calculations. For the menu choice, enter 2...

```
ENTER CHOICE: 2
```

We descend into the STEADY module (Section 4.3)...

```
TOSPAC MODULE STEADY
ENTER STEADY INPUT-DATA FILE (DEFAULT=STEADY.DAT):
```

The STEADY input-data file we created in Step Four was called STEADY.DAT, the default, and now we just enter a <CR>.

STEADY begins to work, writing status messages to your terminal screen...

```
READING INPUT-DATA FILE STEADY.DAT.
CREATING STEADY SOLUTION FILE STEADY.PSI.
CREATING STEADY PLOT-DATA FILE STEADY.PLT.
CREATING STEADY OUTPUT-LISTING FILE STEADY.LIS.
INITIALIZING VARIABLES...
```

```
BEGINNING STEADY-STATE FLOW CALCULATION...
```

```
ITERATION =    1 WORKING ON UNIT #  1
ITERATION =   10 WORKING ON UNIT #  1
ITERATION =   20 WORKING ON UNIT #  1
ITERATION =   30 WORKING ON UNIT #  1
ITERATION =   40 WORKING ON UNIT #  1
```

```
STEADY STATE REACHED AT ITERATION NUMBER 40.
```

```
MAX FLUX DEVIATION= 0.29778    % AT MESH POINT= 10 ELEVATION=      1.8000
NORMAL STEADY TERMINATION.
```

The STEADY module works on a calculation in a piecemeal fashion, one geologic unit at a time, starting from the bottom. Our problem has only a single geologic unit, so STEADY only works on one geologic unit.

Unsaturated-zone hydrology calculations are often difficult because they can use highly nonlinear characteristic curves and the solution is not always smooth at the interfaces between geologic units. Sections 4.3 and 4.4, as well as *Volume 1*, contain more information about flow calculations. But this steady-state-flow calculation was relatively easy.

Immediately preceding the message that STEADY terminated normally, TOSPAC has displayed a measure of how accurate the calculation was. The message tells how much the calculated flux deviates from the imposed flux and where in the mesh this deviation occurs. All mesh points having flux deviations greater than 10% are listed; if no mesh point has a flux deviation greater than 10%, then only the mesh point with the maximum deviation is listed. (Section 4.3 contains a discussion of the possible messages given here.) The maximum flux deviation in this case is less than 1%, a satisfactory result.

So that you can take a look at some numbers, Figure 2.5 presents a portion of the output-listing file, STEADY.LIS, created by STEADY. Section 4.7.3 contains a description of this file.

And we are returned to the TOSPAC main menu...

```
TOSPAC VERSION 1.10 MAIN MENU
```

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

```
ENTER CHOICE:
```

2.7 Step Seven: Run TRANS

Now we will execute TRANS (Section 4.5). In response to the main menu, enter choice 4...

```
ENTER CHOICE: 4
```

```
TOSPAC MODULE TRANS
```

```
ENTER TRANS INPUT-DATA FILE (DEFAULT=TRANS.DAT):
```

We used the default file name when we created the TRANS input-data file, so just enter a <CR> to select the default name again.

And the TRANS module begins running...

```
READING INPUT-DATA FILE TRANS.DAT.
```

```
CREATING TRANS PLOT-DATA FILE TRANS.PLT.
```

```

STEADY STATE REACHED AT ITERATION NUMBER 40.
MAX FLUX DEVIATION= 0.29778 % AT MESH POINT= 10 ELEVATION= 1.8000

FINAL CONDITIONS OF MESH
AVERAGE COLUMN SATURATION = 0.623478
TOTAL VOID VOLUME = 2.500000E+07
TOTAL WATER VOLUME = 1.558696E+07
TOTAL AIR VOLUME = 9.413044E+06
TOTAL WATER MASS = 1.558696E+10

BOUNDARY CONDITIONS: FLAG = 12
FLUX = -1.58500E-10
BOTTOM PRESSURE HEAD = 0.00000E+00

J UNIT MAT FRK Z PRES HEAD %QDEVIATION FLUX FLXMAT FLXFRK HK
501 1 1 1 100.0 -1.952 0.0000E+00 -1.5850E-10 -1.5850E-10 0.0000E+00 1.5850E-10
500 1 1 1 99.80 -1.952 1.1491E-02 -1.5848E-10 -1.5848E-10 0.0000E+00 1.5846E-10
499 1 1 1 99.60 -1.952 2.2989E-02 -1.5846E-10 -1.5846E-10 0.0000E+00 1.5846E-10
498 1 1 1 99.40 -1.952 2.2989E-02 -1.5846E-10 -1.5846E-10 0.0000E+00 1.5846E-10
497 1 1 1 99.20 -1.952 2.2989E-02 -1.5846E-10 -1.5846E-10 0.0000E+00 1.5846E-10
o
o
o
5 1 1 1 0.8000 -0.8000 4.5435E-04 -1.5850E-10 -1.5850E-10 0.0000E+00 1.2124E-05
4 1 1 1 0.6000 -0.6000 5.4034E-04 -1.5850E-10 -1.5850E-10 0.0000E+00 1.2475E-05
3 1 1 1 0.4000 -0.4000 1.0025E-03 -1.5850E-10 -1.5850E-10 0.0000E+00 1.2499E-05
2 1 1 1 0.2000 -0.2000 7.1233E-04 -1.5850E-10 -1.5850E-10 0.0000E+00 1.2500E-05
1 1 1 1 0.0000E+00 0.0000E+00 0.0000E+00 -1.5850E-10 -1.5850E-10 0.0000E+00 1.2500E-05

J UNIT MAT FRK SAT DSAT SATMAT SATFRK VEL VELMAT VELFRK
501 1 1 1 0.6185 3.1171E-02 0.6185 0.6185 -9.6872E-08 -9.6872E-08 0.0000E+00
500 1 1 1 0.6185 3.1167E-02 0.6185 0.0000E+00 -9.6863E-08 -9.6863E-08 0.0000E+00
499 1 1 1 0.6185 3.1167E-02 0.6185 0.0000E+00 -9.6854E-08 -9.6854E-08 0.0000E+00
498 1 1 1 0.6185 3.1167E-02 0.6185 0.0000E+00 -9.6854E-08 -9.6854E-08 0.0000E+00
497 1 1 1 0.6185 3.1167E-02 0.6185 0.0000E+00 -9.6854E-08 -9.6854E-08 0.0000E+00
o
o
o
5 1 1 1 0.9971 3.7959E-02 0.9971 0.0000E+00 -1.6706E-09 -1.6706E-09 0.0000E+00
4 1 1 1 0.9999 2.5793E-03 0.9999 0.0000E+00 -1.6374E-09 -1.6374E-09 0.0000E+00
3 1 1 1 1.000 5.7094E-05 1.000 0.0000E+00 -1.6342E-09 -1.6342E-09 0.0000E+00
2 1 1 1 1.000 8.4511E-08 1.000 0.0000E+00 -1.6340E-09 -1.6340E-09 0.0000E+00
1 1 1 1 1.000 0.0000E+00 1.000 1.000 -1.6340E-09 -1.6340E-09 0.0000E+00

***** GROUNDWATER TRAVEL TIME *****
START POSITION = 100.00
END POSITION = 0.00000E+00
AVERAGE FASTEST PARTICLE = 0.17938257E+10 SEC
COMPOSITE = 0.17938257E+10 SEC
MATRIX = 0.17938257E+10 SEC (100.00% OF RANGE)
FRACTURES = NO FLOW
CALCULATIONAL CUTOFF USED TO DETERMINE SIGNIFICANT FLOW = 0.10000E-01

```

Figure 2.5: Part of the STEADY output-listing file for the simplified mill-tailings problem.

2.7. STEP SEVEN: RUN TRANS

35

CREATING TRANS OUTPUT-LISTING FILE TRANS.LIS.
READING STEADY PLOT-DATA FILE STEADY.PLT.

INITIALIZING VARIABLES...

BEGINNING TRANSPORT CALCULATION...

SNAPSHOT 1... TIME(YR) = 0.00000E+00

ITERATION =	1	STEP(DY) =	57.870	TIME(DY) =	57.870
ITERATION =	10	STEP(DY) =	63.332	TIME(YR) =	1.5994
ITERATION =	20	STEP(DY) =	152.75	TIME(YR) =	4.6812
ITERATION =	30	STEP(DY) =	318.42	TIME(YR) =	11.307

o
o
o

ITERATION =	393	STEP(YR) =	10000.	TIME(YR) =	2.80000E+05
SNAPSHOT 31...		TIME(YR) =	2.80000E+05		
ITERATION =	394	STEP(YR) =	10000.	TIME(YR) =	2.90000E+05
SNAPSHOT 32...		TIME(YR) =	2.90000E+05		
ITERATION =	395	STEP(YR) =	10000.	TIME(YR) =	3.00000E+05
SNAPSHOT 33...		TIME(YR) =	3.00000E+05		

NORMAL TRANS TERMINATION.

That is it. To understand better what TRANS is doing and telling you, see Section 4.5. To see a portion of the numbers generated by TRANS, see Figure 2.6. A description of the TRANS output-listing file is given in Section 4.7.10.

After TRANS is executed, TOSPAC returns to the main menu...

TOSPAC VERSION 1.10 MAIN MENU

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

ENTER CHOICE:

HYDROLOGIC QUANTITIES:

MESH CELL	UNIT #	ELEV	MATRIX MOISTURE	FRACTURE MOISTURE	MATRIX VELOCITY	FRACTURE VELOCITY	ADVECTIVE COUPLING
500	1	99.90	0.1546	0.0000E+00	-1.0250E-09	0.0000E+00	0.0000E+00
499	1	99.70	0.1546	0.0000E+00	-1.0248E-09	0.0000E+00	0.0000E+00
498	1	99.50	0.1546	0.0000E+00	-1.0248E-09	0.0000E+00	0.0000E+00
497	1	99.30	0.1546	0.0000E+00	-1.0248E-09	0.0000E+00	0.0000E+00
5	1	0.9000	0.2461	0.0000E+00	-6.4394E-10	0.0000E+00	0.0000E+00
4	1	0.7000	0.2496	0.0000E+00	-6.3498E-10	0.0000E+00	0.0000E+00
3	1	0.5000	0.2500	0.0000E+00	-6.3404E-10	0.0000E+00	0.0000E+00
2	1	0.3000	0.2500	0.0000E+00	-6.3399E-10	0.0000E+00	0.0000E+00
1	1	0.1000	0.2500	0.0000E+00	-6.3400E-10	0.0000E+00	0.0000E+00

TRANSPORT COEFFICIENTS FOR SPECIES 1 OF DECAY CHAIN 1: U-238

MESH CELL	UNIT #	ELEV	MATRIX RETARD	FRACTURE RETARD	MATRIX DISPERSN	FRACTURE DISPERSN	DISPERSIVE COUPLING
500	1	99.90	62.69	1.000	2.3411E-10	1.0000E-09	0.0000E+00
499	1	99.70	62.69	1.000	3.0196E-10	1.0000E-09	0.0000E+00
498	1	99.50	62.69	1.000	3.6938E-10	1.0000E-09	0.0000E+00
497	1	99.30	62.69	1.000	4.3634E-10	1.0000E-09	0.0000E+00
5	1	0.9000	39.76	1.000	6.4026E-09	1.0000E-09	0.0000E+00
4	1	0.7000	39.22	1.000	6.3179E-09	1.0000E-09	0.0000E+00
3	1	0.5000	39.16	1.000	6.3105E-09	1.0000E-09	0.0000E+00
2	1	0.3000	39.16	1.000	6.3116E-09	1.0000E-09	0.0000E+00
1	1	0.1000	39.16	1.000	6.3131E-09	1.0000E-09	0.0000E+00

TIME STEP 395 TIME 9.46728E+12 DELTA TIME 3.15576E+11
 FINAL TIME: SNAPSHOT 33

U-238

MESH CELL	UNIT #	ELEV	MATRIX CONC	FRACTURE CONC
500	1	99.90	2.3845E-12	0.0000E+00
499	1	99.70	3.9996E-12	0.0000E+00
498	1	99.50	6.2461E-12	0.0000E+00
497	1	99.30	9.2226E-12	0.0000E+00
5	1	0.9000	6.1280E-07	0.0000E+00
4	1	0.7000	6.1291E-07	0.0000E+00
3	1	0.5000	6.1299E-07	0.0000E+00
2	1	0.3000	6.1302E-07	0.0000E+00
1	1	0.1000	6.1302E-07	0.0000E+00

MASS CONSERVATION TIME STEP 395 TIME 9.46728E+12

CHAIN #	SPECIES # NAME	MATRIX MASS	FRACTURE MASS	ADSORBED MASS	PRECIP MASS	SOURCE MASS	T BDRY MASS	B BDRY MASS	MASS IN MESH + MASS RELEASED	MASS INJECTED INTO MESH	PERCENT DIFF
1	1 U-238	3.88E+00	0.00E+00	2.35E+02	0.00E+00	0.00E+00	7.53E+02	-5.14E+02	7.52E+02	7.53E+02	-8.97E-02

MASS RELEASE

CHAIN #	SPECIES # NAME	TOP TOTAL	TOP CUMULATIVE	BOTTOM TOTAL	BOTTOM CUMULATIVE
1	1 U-238	-7.53E+02	-7.53E+02	5.14E+02	5.14E+02

Figure 2.6: Part of the TRANS output-listing file for the simplified mill-tailings problem.

2.8 Step Eight: Run OUTPLOT

We are in the home stretch.

Waiting to be used, but currently invisible to us, are the results STEADY and TRANS have created. These results consist of large arrays of numbers corresponding to pressure heads, concentrations, releases, etc., at each mesh point or each boundary or each time snapshot. We showed you a part of them in Figures 2.5 and 2.6. Now we need to somehow digest this information.

TOSPAC contains a module, OUTPLOT, to produce computer plots of the results. OUTPLOT is described in detail in Section 4.6. To create these plots, enter 5 as your choice from the TOSPAC main menu...

ENTER CHOICE: 5

And TOSPAC responds...

TOSPAC MODULE OUTPLOT

ENTER OUTPLOT PLOT-DEFINITION FILE (DEFAULT=OUTPLOT.PDF):

A brief description of how OUTPLOT works is necessary here. Basically, OUTPLOT reads a file that tells it what plots are desired (the *plot-definition file*) and a data file (the *plot-data file*), then it produces a file of computer-graphics commands that can only be interpreted by a computer-graphics device (the *graphics-driver file*). If the plot-definition file does not exist, the OUTPLOT module enters into a procedure that prompts for plot-definition data. As you answer the prompts, OUTPLOT creates a plot-definition file. When you finish defining the plots you want, OUTPLOT produces the actual plots on the graphics-driver file. (At some installations, OUTPLOT may produce the plots directly on the user's terminal screen.) The main purpose of the plot-definition file is to avoid repeating the prompting procedure every time a new set of plots is required. With time, you can tailor a plot-definition file that produces most of the plots that you find useful, and you will be able to create the plots by simply telling TOSPAC the file name.

But we do not have a plot-definition file yet. Choose the default plot-definition file name by entering a <CR>. TOSPAC responds with the following message...

OUTPLOT.PDF DOES NOT EXIST...

CREATING OUTPLOT.PDF.

Then TOSPAC presents the top-level menu for OUTPLOT...

OUTPLOT MAIN MENU

0. STOP

1. DEFINE STEADY PLOTS

2. DEFINE DYNAMICS PLOTS

3. DEFINE TRANS PLOTS

4. CONSTRUCT GRAPHICS-DRIVER FILE

ENTER CHOICE:

If the plot-definition file already exists, the same menu is presented. If any new plots are defined, they

are appended to the the plot-definition file. No provision is made to modify or delete plot definitions. These tasks must be performed using your computer's text editor.

We want to plot results from both STEADY and TRANS. First, we will define plots for STEADY. Enter choice 1...

ENTER CHOICE: 1

First, TOSPAC asks for the STEADY plot-data file...

ENTER STEADY PLOT-DATA FILE (DEFAULT=NONE):

TOSPAC allows you to name plot-data files in the plot-definition file. The advantage is that an audit trail is kept. The disadvantage is that the plot-definition file will only work with the specified plot-data file. Select the default.

And TOSPAC presents the menu for the various steady-state plots that are available...

OUTPLOT (STEADY RESULTS) MENU

- 0. STOP
- 1. PLOT MESH/STRATIGRAPHY
- 2. PLOT CHARACTERISTIC CURVES
- 3. PLOT COMPOSITE CONDUCTIVITY AND CAPACITANCE CURVES
- 4. PLOT PRESSURE HEAD VS ELEVATION
- 5. PLOT SATURATION VS ELEVATION
- 6. PLOT FLUX VS ELEVATION
- 7. PLOT VELOCITY VS ELEVATION
- 8. PLOT CONDUCTIVITY VS ELEVATION
- 9. PLOT CAPACITANCE VS ELEVATION
- 10. PLOT TRAVEL TIMES

ENTER CHOICE:

A description of each type of steady-state plot is contained in Section 4.6.3. Steady-state plots are often more useful if you include several different steady-state calculations on the same plot (Section 4.6.2). We will produce a mesh/stratigraphy plot to check our input data, and we will make a water-velocity plot in order to demonstrate the process for producing a more typical plot.

First, the mesh/stratigraphy plot. Enter choice 1...

ENTER CHOICE: 1

And the TOSPAC OUTPLOT module responds...

DEFINING MESH/STRATIGRAPHY PLOT...

ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):

TOSPAC is asking you to specify an axis type. The default axis type is the one listed first; in this case, linear. For a mesh/stratigraphy plot, it is usually best to use a linear axis.

Now OUTPLOT seeks information about the units of the axis. . .

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

OUTPLOT assumes *SI* units. If we wanted English units instead, we could change the axis labels. If we had used *SI* units, but wanted elevation in centimeters, we could change the axis labels and we could enter a scale factor to scale the data. But *SI* units are what we want.

Next, TOSPAC asks about the axis limits. The default is to show the mesh/stratigraphy for the whole column, but you could specify some other limits, if you wanted a "blow-up" of a particular region, for example.

SET AXIS LIMITS. . .

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

Notice that the OUTPLOT module handles defaults differently than the INDATA module. OUTPLOT does not tell you what the default value is: if you enter a <CR>, the word DEFAULT is written in the plot-definition file. OUTPLOT does not calculate the actual default values until it creates the graphics-driver file. OUTPLOT was designed this way so that one plot-definition file could be used to create plots with several different plot-data files (for several TOSPAC calculations). On the debit side, the user does not know beforehand what the default value is.

TOSPAC now queries for two more parameters. . .

ENTER # OF MESH POINTS IN BOX:

ENTER STEP SIZE FOR MESH-POINT-NUMBER LABEL:

These parameters allow you to adjust the mesh-column drawing but, for now, enter <CR> to select the default.

And after a time. . .

PLOT DEFINITION COMPLETED.

That is easy enough, but where is your plot? OUTPLOT has only written the mesh/stratigraphy request onto the plot-definition file. We are going to define all the plots first. Then we are going to use these plot definitions to create a file that will drive a computer-graphics device. When it is finally drawn on a computer-graphics device, the mesh/stratigraphy plot you have just defined should look like the one presented in Figure 2.7.

A moment later, on your terminal the STEADY results menu will reappear. . .

Figure 2.7: Mesh/stratigraphy plot for the simplified mill-tailings problem.

OUTPLOT (STEADY RESULTS) MENU

- 0. STOP
- 1. PLOT MESH/STRATIGRAPHY
- 2. PLOT CHARACTERISTIC CURVES
- 3. PLOT COMPOSITE CONDUCTIVITY AND CAPACITANCE CURVES
- 4. PLOT PRESSURE HEAD VS ELEVATION
- 5. PLOT SATURATION VS ELEVATION
- 6. PLOT FLUX VS ELEVATION
- 7. PLOT VELOCITY VS ELEVATION
- 8. PLOT CONDUCTIVITY VS ELEVATION
- 9. PLOT CAPACITANCE VS ELEVATION
- 10. PLOT TRAVEL TIMES

ENTER CHOICE:

Now let's make the water-velocity plot, choice 7...

ENTER CHOICE: 7

And TOSPAC responds...

DEFINING VELOCITY-VS-ELEVATION PLOT...

In TOSPAC, "velocity" is the average linear velocity of a parcel of water. Actually, there is more than one type of plot for the average linear velocity, so TOSPAC responds with the velocity plot menu...

OUTPLOT (STEADY RESULTS) VELOCITY MENU

- 0. STOP
- 1. PLOT COMPOSITE-WATER VELOCITY
- 2. PLOT MATRIX-WATER VELOCITY
- 3. PLOT FRACTURE-WATER VELOCITY
- 4. PLOT ALL

ENTER CHOICE:

Our example problem has no fractures, thus the velocity plots for the fractures will not be useful. Also, without fractures, composite water velocity is the same as matrix water velocity. Try the following...

ENTER CHOICE: 2

And TOSPAC begins several queries to define the axes...

ENTER ORIENTATION (PORTRAIT OR LANDSCAPE):

ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

```
ENTER VELOCITY-AXIS TYPE (LIN, LOG, NEGLOG):  NEGLOG
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER VELOCITY-AXIS MINIMUM:
ENTER VELOCITY-AXIS MAXIMUM:
```

The default orientation is portrait. Portrait orientation places the plot with the longer sides of the page vertical; landscape turns the longer sides horizontal. We have defined a portrait orientation with a linear elevation axis and a logarithmic velocity axis with negative velocities. The default units (*SI*) are to be used.

The OUTPLOT module of TOSPAC has self-scaling capability and the default value is what TOSPAC considers to be the best. But you may not always like it, so you are given a chance to change it. For this example, defaults have been chosen for all the axis limits.

And finally...

```
DO YOU WANT A LEGEND (N OR Y OR SAME):
```

We do not need a legend for only one curve: enter *<CR>* to select the default (which, again, in the case of a yes/no question is no).

And after a time, TOSPAC indicates that the plot is defined...

PLOT DEFINITION COMPLETED.

The plot of the average linear velocity of water in the matrix versus elevation for the example problem is presented in Figure 2.8.

A moment later, on your terminal the STEADY results menu will reappear...

```
OUTPLOT (STEADY RESULTS) MENU
0. STOP
1. PLOT MESH/STRATIGRAPHY
2. PLOT CHARACTERISTIC CURVES
3. PLOT COMPOSITE CONDUCTIVITY AND CAPACITANCE CURVES
4. PLOT PRESSURE HEAD VS ELEVATION
5. PLOT SATURATION VS ELEVATION
6. PLOT FLUX VS ELEVATION
7. PLOT VELOCITY VS ELEVATION
8. PLOT CONDUCTIVITY VS ELEVATION
9. PLOT CAPACITANCE VS ELEVATION
10. PLOT TRAVEL TIMES
```

```
ENTER CHOICE:
```

Enter choice 0 here and the OUTPLOT main menu will appear...

Figure 2.8: Water velocity for the simplified mill-tailings problem.

OUTPLOT MAIN MENU

- 0. STOP
- 1. DEFINE STEADY PLOTS
- 2. DEFINE DYNAMICS PLOTS
- 3. DEFINE TRANS PLOTS
- 4. CONSTRUCT GRAPHICS-DRIVER FILE

ENTER CHOICE: 3

At this time we enter choice 3 to see what OUTPLOT can do with the transport results. First, as with the STEADY plots, TOSPAC asks for a plot-data file...

ENTER TRANS PLOT-DATA FILE (DEFAULT=NONE):

Select the default and this plot-definition file can be used with any TRANS plot-data file.

Now TOSPAC presents the menu for the various TRANS-related plots...

OUTPLOT (TRANS RESULTS) MENU

- 0. STOP
- 1. PLOT MOISTURE CONTENT VS ELEVATION
- 2. PLOT VELOCITY VS ELEVATION
- 3. PLOT DISPERSION COEFF VS ELEVATION
- 4. PLOT RETARDATION VS ELEVATION
- 5. PLOT COUPLING CONSTANT VS ELEVATION
- 6. PLOT CONCENTRATION VS ELEVATION
- 7. PLOT CONC VS ELEVATION VS TIME (3-D)
- 8. PLOT CONCENTRATION VS TIME
- 9. PLOT RELEASE VS TIME

ENTER CHOICE:

Section 4.6.5 contains a discussion of the plotting options for transport results.

Plots of release versus time are informative; enter choice 9, and TOSPAC responds...

DEFINING RELEASE-VS-TIME PLOT...

Because there are several different release plots, TOSPAC displays another menu...

OUTPLOT (TRANS RESULTS) RELEASE MENU

- 0. STOP
- 1. PLOT BOTH ACTUAL AND CUMULATIVE AMOUNTS TOGETHER
- 2. PLOT ACTUAL AMOUNT PRESENT
- 3. PLOT CUMULATIVE RELEASE
- 4. PLOT RATE OF RELEASE

ENTER CHOICE: 1

The actual amount present is the amount of contaminant that has crossed a problem boundary, adjusted for radioactive decay as time passes while it is outside of the problem boundary. The

cumulative release is a running total of contaminant that has crossed the boundary. If the contaminant does not decay, the actual amount equals the cumulative amount. The rate of release is the time derivative of the release.

TOSPAC now queries about the type of plot...

ENTER RELEASE TYPE (MASS, RADIOACTIVITY, OR EPA RATIO):

The default is MASS, which we have again selected. Also select the default for the next prompt...

ENTER RELEASE BOUNDARY (BOTTOM, TOP, OR BOTH):

Now TOSPAC prompts for information about the axes...

ENTER RELEASE-AXIS TYPE (LIN, LOG, NEGLOG): LOG
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER RELEASE-AXIS MINIMUM:
ENTER RELEASE-AXIS MAXIMUM:

ENTER TIME-AXIS TYPE (LIN, LOG, NEGLOG):
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER TIME-AXIS MINIMUM:
ENTER TIME-AXIS MAXIMUM:

We have specified a logarithmic release axis and a linear time axis. We will stay with the default units and axes limits.

TOSPAC now asks for the contaminants we would like as the subject of the plot...

ENTER CONTAMINANT:

An acceptable response is the number representing the position in the input-data file of the contaminant, or the name of the contaminant. A separate plot will be made for each contaminant listed. We only have one contaminant in the input-data file; we could have entered the number 1, the name U-238, or the default.

And again we are allowed to specify a legend...

DO YOU WANT A LEGEND (N OR Y OR SAME): Y

We do want a legend, this time, in order to discriminate between the curves for actual amount and cumulative amount.

ENTER LEGEND LOCATION:

And TOSPAC signals that the release-versus-time plot is defined...

PLOT DEFINITION COMPLETED.

The plot produced by the TOSPAC OUTPLOT module for this problem is presented in Figure 2.9. Because of the long half-life for ^{238}U , the curve for the actual amount overlays the curve for the cumulative release.

The transport plot menu returns to your terminal screen...

```
OUTPLOT (TRANS RESULTS) MENU
0. STOP
1. PLOT MOISTURE CONTENT VS ELEVATION
2. PLOT VELOCITY VS ELEVATION
3. PLOT DISPERSION COEFF VS ELEVATION
4. PLOT RETARDATION VS ELEVATION
5. PLOT COUPLING CONSTANT VS ELEVATION
6. PLOT CONCENTRATION VS ELEVATION
7. PLOT CONC VS ELEVATION VS TIME (3-D)
8. PLOT CONCENTRATION VS TIME
9. PLOT RELEASE VS TIME
```

ENTER CHOICE:

Three-dimensional plots are nice: select choice 7, and TOSPAC responds...

DEFINING CONC-VS-ELEVATION-VS-TIME PLOT...

```
OUTPLOT (TRANS RESULTS) CONCENTRATION MENU
0. STOP
1. PLOT CONC IN THE MATRIX
2. PLOT CONC IN THE FRACTURES
3. PLOT CONC IN THE MATRIX AND FRACTURES
```

ENTER CHOICE: 1

OUTPLOT can either plot matrix concentration or fracture concentration; in most cases, where there is a fairly strong matrix/fracture coupling, the plots will look identical. For our problem the point is moot because we did not include any fractures.

```
ENTER VIEW RADIUS (DEFAULT=125.):
ENTER VIEW POLAR ANGLE (DEFAULT=75.):
ENTER VIEW AZIMUTHAL ANGLE (DEFAULT=340.):
```

Three-dimensional plots are drawn in perspective. You need to tell TOSPAC in spherical coordinates where to place your eye with respect to the plot (Section 4.6.5). You can look at it from above, behind, below, or wherever. But for now, take the defaults.

And take the defaults for the axis units, axis scaling, and axis limits...

```
CONCENTRATION AXIS...
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER CONCENTRATION-AXIS MINIMUM:
ENTER CONCENTRATION AXIS MAXIMUM:
```

Simplified Mill-Tailings Problem
Release for U-238; Bottom Boundary

Figure 2.9: ^{238}U release at the water table for the simplified mill-tailings problem.

```
ELEVATION AXIS...  
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):  
SET AXIS LIMITS...  
ENTER ELEVATION-AXIS MINIMUM:  
ENTER ELEVATION-AXIS MAXIMUM:
```

```
TIME AXIS...  
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):  
SET AXIS LIMITS...  
ENTER TIME-AXIS MINIMUM:  
ENTER TIME-AXIS MAXIMUM:
```

Note that log scales are not allowed on three-dimensional plots.

TOSPAC now prompts for the numbers of the contaminants (from the order in the input-data file) that you want plotted...

```
ENTER CONTAMINANT:
```

And finally, TOSPAC lets you define (within limits!) the coarseness of the fabric of the three-dimensional surface...

```
ENTER # OF ELEVATION LINES:  
ENTER # OF TIME LINES:
```

You can enter whatever positive integers you want, but TOSPAC will not put in more elevation lines or time lines than the data contain.

Now TOSPAC finishes the plot definition...

```
PLOT DEFINITION COMPLETED.
```

The three-dimensional plot produced by OUTPLOT for this problem is presented in Figure 2.10. Notice how the concentration is a constant (10^{-6} mol/m³) at the top of the mesh—it forms a triangular table top—for the first 150,000 yr, then it is shut off. The concentration falls to zero as the contaminant mixes with the water at the water table.

OUTPLOT now returns you to the transport plot menu...

Simplified Mill-Tailings Problem
U-238 Concentration in the Matrix Water

Figure 2.10: ^{238}U concentration over time and elevation for the simplified mill-tailings problem.

OUTPLOT (TRANS RESULTS) MENU

- 0. STOP
- 1. PLOT MOISTURE CONTENT VS ELEVATION
- 2. PLOT VELOCITY VS ELEVATION
- 3. PLOT DISPERSION COEFF VS ELEVATION
- 4. PLOT RETARDATION VS ELEVATION
- 5. PLOT COUPLING CONSTANT VS ELEVATION
- 6. PLOT CONCENTRATION VS ELEVATION
- 7. PLOT CONC VS ELEVATION VS TIME (3-D)
- 8. PLOT CONCENTRATION VS TIME
- 9. PLOT RELEASE VS TIME

ENTER CHOICE:

We would like one more plot, a plot of concentration versus elevation with multiple time lines. This plot has the same information as the three-dimensional plot we just made, but using it, one can more easily discern concentration values.

Entering choice 6, we get...

DEFINING CONC-VS-ELEVATION PLOT...

Again, several different types of plots showing concentration versus elevation are available through a menu...

OUTPLOT (TRANS RESULTS) CONCENTRATION MENU

- 0. STOP
- 1. PLOT CONC IN THE MATRIX
- 2. PLOT CONC IN THE FRACTURES
- 3. PLOT CONC IN BOTH MATRIX AND FRACTURES TOGETHER

ENTER CHOICE: 1

Next, TOSPAC asks for several drawing parameters...

ENTER ORIENTATION (PORTRAIT OR LANDSCAPE):

ENTER CONCENTRATION-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER CONCENTRATION-AXIS MAXIMUM:

ENTER CONCENTRATION-AXIS MAXIMUM:

ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

Just select the defaults. TOSPAC now asks for the contaminant that is the subject of the plot...

ENTER CONTAMINANT:

And the times at which you want a curve of concentration versus elevation...

ENTER TIME-SPAPSHOTS TO BE PLOTTED:

The time-snapshot numbers correspond to the order number of the snapshots in the input-data file. We want quite a few time lines on our plot, but not all of them, so enter the following...

ENTER TIME-SNAPSHOT TO BE PLOTTED: 1 2 4 7 12 17 18 20 23 28 33

All these numbers must be entered before you enter a <CR>.

TOSPAC now asks about a legend as follows...

DO YOU WANT A LEGEND (N OR Y OR SAME): Y

SPECIFY LABELS...

ENTER LABEL FOR SNAPSHOT # 1:
 ENTER LABEL FOR SNAPSHOT # 2:
 ENTER LABEL FOR SNAPSHOT # 4:
 ENTER LABEL FOR SNAPSHOT # 7:
 ENTER LABEL FOR SNAPSHOT # 12:
 ENTER LABEL FOR SNAPSHOT # 17:
 ENTER LABEL FOR SNAPSHOT # 18:
 ENTER LABEL FOR SNAPSHOT # 20:
 ENTER LABEL FOR SNAPSHOT # 23:
 ENTER LABEL FOR SNAPSHOT # 28:
 ENTER LABEL FOR SNAPSHOT # 33:

The default labels (the labels we selected) are the times entered in the boundary-condition block of the TRANS input-data file.

Now TOSPAC allows us to locate the legend on the plot...

ENTER LEGEND LOCATION: RIGHT, BOTTOM

We told TOSPAC to locate the legend in the lower right corner of the plot.

And TOSPAC announces...

PLOT DEFINITION COMPLETED.

The plot we just produced is presented in Figure 2.11. It is interesting to compare this plot with the three-dimensional plot shown in Figure 2.10.

TOSPAC now returns us to the transport plot menu...

Simplified Mill-Tailings Problem U-238 Concentration in the Matrix Water

Figure 2.11: ^{238}U concentration for the simplified mill-tailings problem.

OUTPLOT (TRANS RESULTS) MENU

- 0. STOP
- 1. PLOT MOISTURE CONTENT VS ELEVATION
- 2. PLOT VELOCITY VS ELEVATION
- 3. PLOT DISPERSION COEFF VS ELEVATION
- 4. PLOT RETARDATION VS ELEVATION
- 5. PLOT COUPLING CONSTANT VS ELEVATION
- 6. PLOT CONCENTRATION VS ELEVATION
- 7. PLOT CONC VS ELEVATION VS TIME (3-D)
- 8. PLOT CONCENTRATION VS TIME
- 9. PLOT RELEASE VS TIME

ENTER CHOICE:

Enter choice 0 here and the OUTPLOT main menu will appear.

OUTPLOT MAIN MENU

- 0. STOP
- 1. DEFINE STEADY PLOTS
- 2. DEFINE DYNAMICS PLOTS
- 3. DEFINE TRANS PLOTS
- 4. CONSTRUCT GRAPHICS-DRIVER FILE

ENTER CHOICE:

We now have all the plots we want defined in OUTPLOT.PDF, the plot-definition file. You do not need to know what OUTPLOT.PDF looks like for this example, but if you are interested, it is presented in Figure 2.12.

But we do not as yet have any plots. To produce the plots, we must first produce a graphics-driver file. The graphics-driver file contains the actual commands that tell a computer-graphics device how to draw the plots. A graphics-driver file is created when you enter choice 4. (Some installations will not produce a graphics-driver file, but will produce these plots on the user's terminal screen.) So enter choice 4...

ENTER CHOICE: 4

TOSPAC asks for a name for the output graphics file...

ENTER OUTPLOT GRAPHICS-DRIVER FILE (DEFAULT=OUTPLOT.DRV):

Select the default. The DRV extension refers to the fact that this file is a graphics-device driver. You cannot read this file; only a computer-graphics device can.

TOSPAC now reads the plot-definition file. The plot-data file names were not entered when we defined the plots, so TOSPAC asks for them now. First, TOSPAC asks for the STEADY plot-data file...

STEADY PLOT SECTION

ENTER STEADY PLOT-DATA FILE (DEFAULT=STEADY.PLT):

```

*****
***  TOSAPC OUTPLOT PLOT-DEFINITION FILE  ***
*****

***** STEADY PLOT SECTION *****

***** MESH PLOT BLOCK *****
XAXIS LIN          ELEVATION AXIS TYPE
XLIMITS DEFAULT,DEFAULT  ELEVATION AXIS LIMITS
BOX DEFAULT        MESH POINTS PER BOX
NUMBER DEFAULT     MESH POINTS PER LABEL

***** VELOCITY PLOT BLOCK *****
XAXIS LIN          ELEVATION AXIS TYPE
XLIMITS DEFAULT,DEFAULT  ELEVATION AXIS LIMITS
YAXIS NEGLOG       VELOCITY AXIS TYPE
YLIMITS DEFAULT,DEFAULT  VELOCITY AXIS LIMITS
LEGEND NONE        LEGEND LOCATION
PLOTTYPE MATRIX    VELOCITY TYPE
MODE MULTI         PLOT MODE
ORIENT PORTRAIT    PLOT ORIENTATION

***** TRANS PLOT SECTION *****

***** RELEASE PLOT BLOCK *****
YAXIS LOG          RELEASE AXIS TYPE
YLIMITS DEFAULT,DEFAULT  RELEASE AXIS LIMITS
XAXIS LIN          TIME AXIS TYPE
XLIMITS DEFAULT,DEFAULT  TIME AXIS LIMITS
LEGEND DEFAULT     LEGEND LOCATION
PLOTTYPE BOTH      PLOT BOTH ACTUAL AND CUMULATIVE CURVES
RELEASE MASS        PLOT RELEASES IN TERMS OF MASS
BOUNDARY BOTTOM     PLOT RELEASES FROM BOTTOM BOUNDARY
MODE SINGLE        PLOT MODE
SPECIES ALL         PLOT CURVES FOR ALL SPECIES

***** 3-D PLOT BLOCK *****
PLOTTYPE MATRIX    PLOT MATRIX CONCENTRATION
VIEW 125.,75.,340. VIEWPOINT LOCATION
ZLIMITS DEFAULT,DEFAULT  CONCENTRATION AXIS LIMITS
YLIMITS DEFAULT,DEFAULT  ELEVATION AXIS LIMITS
XLIMITS DEFAULT,DEFAULT  TIME AXIS LIMITS
NUMX DEFAULT       NUMBER OF TIME LINES
NUMY DEFAULT       NUMBER OF ELEVATION LINES
SPECIES ALL        PLOT CURVES FOR ALL SPECIES

***** CVSE PLOT BLOCK *****
PLOTTYPE MATRIX    PLOT MATRIX CONCENTRATION
MODE MULTI         PLOT MODE
ORIENT PORTRAIT    PLOT ORIENTATION
YAXIS LIN          CONCENTRATION AXIS TYPE
YLIMITS DEFAULT,DEFAULT  CONCENTRATION AXIS LIMITS
XAXIS LIN          ELEVATION AXIS TYPE
XLIMITS DEFAULT,DEFAULT  ELEVATION AXIS LIMITS
SPECIES ALL        PLOT CURVES FOR ALL SPECIES
SNAPSHOT 1         SNAPSHOT TO PLOT
SNAPSHOT 2         SNAPSHOT TO PLOT
SNAPSHOT 4         SNAPSHOT TO PLOT
SNAPSHOT 7         SNAPSHOT TO PLOT
SNAPSHOT 12        SNAPSHOT TO PLOT
SNAPSHOT 17        SNAPSHOT TO PLOT
SNAPSHOT 18        SNAPSHOT TO PLOT
SNAPSHOT 20        SNAPSHOT TO PLOT
SNAPSHOT 23        SNAPSHOT TO PLOT
SNAPSHOT 28        SNAPSHOT TO PLOT
SNAPSHOT 33        SNAPSHOT TO PLOT
LEGEND RIGHT, BOTTOM  LEGEND LOCATION

```

Figure 2.12: OUTPLOT plot-definition file for the simplified mill-tailings problem.

Just select the default (we used the default plot-data file name back in Step Four). Then surprise! TOSPAC asks the same thing again...

ENTER STEADY PLOT-DATA FILE (DEFAULT=NONE):

The OUTPLOT module can plot the results from several STEADY runs on a single plot, so it allows you to enter the names of several plot-data files. We only have one plot-data file, and we have already entered its name, so now we want to enter *NONE*, the default.

TOSPAC begins to create the graphics-driver file. The following messages appear on your terminal screen. At this point, for some installations of TOSPAC, the actual plots will appear on the user's terminal screen. In these cases, after a plot is drawn, it will remain on the screen until the user enters a <CR>. The next plot will then be drawn.

CREATING MESH PLOTS.

CREATING VELOCITY VS. ELEVATION PLOTS.

When TOSPAC comes to the transport plots, it asks for the TRANS plot-data file...

TRANS PLOT SECTION

ENTER TRANS PLOT-DATA FILE (DEFAULT=TRANS.PLT):

Again, just select the default (we used the default plot-data file name back in Step Five).

CREATING RELEASE PLOTS.

CREATING 3-D CONCENTRATION PLOTS.

CREATING CONCENTRATION VS. ELEVATION PLOTS.

NORMAL OUTPLOT TERMINATION. 5 PLOTS PRODUCED.

Now the OUTPLOT main menu reappears on your terminal screen for the fourth time.

OUTPLOT MAIN MENU

0. STOP

1. DEFINE STEADY PLOTS

2. DEFINE DYNAMICS PLOTS

3. DEFINE TRANS PLOTS

4. CONSTRUCT GRAPHICS-DRIVER FILE

ENTER CHOICE:

We are finished. Enter choice 0 and the TOSPAC main menu will appear.

Enter choice 0 to the TOSPAC main menu and this session terminates.

2.9 Step Nine: Finish

Send the file OUTPLOT.DRV to your computer-graphics device. OUTPLOT.DRV is formatted to be read by a specific computer-graphics device that was specified when TOSPAC was installed on your computer system. For the system that is used by the authors, the command used to plot OUTPLOT.DRV is as follows. . .

```
$ IMPRINT/IMPRESS OUTPLOT.DRV
```

After OUTPLOT.DRV has been sent to the your computer-graphics device, you can fetch the hardcopy of the plots and congratulate yourself!

Chapter 3

EXAMPLE PROBLEMS

This chapter contains a description of two example problems and a discussion of how to use TOSPAC to solve each of them. The first problem concerns transient water flow and illustrates the use of the DYNAMICS module of TOSPAC. The second problem concerns steady-state water flow with contaminant transport; this repository-scale problem is taken from *Volume 1*, and illustrates the use of the STEADY and TRANS modules.

The emphasis in this chapter is on transforming the problem for input to TOSPAC and examining the output. There is little discussion of the mechanics of the computer-terminal session involved in the calculation. Chapter 2 contains an example of a terminal session.

3.1 Simulation of a Laboratory Imbibition Experiment

The DYNAMICS module of TOSPAC can be used to simulate the following laboratory experiment. A section of dry drillhole core is supported above a pan of water so that only the bottom face contacts the water. The sample imbibes water. Periodically the sample is removed and weighed. It is of interest to simulate this process in order to determine whether the computer model and input data can be extrapolated accurately to processes of this, and perhaps larger, size. Figure 3.1 shows an illustration of the experimental setup and how the setup can be envisioned for input into TOSPAC.

To simulate the experiment, we assume one-dimensional flow upward through the sample. Then we create one "geologic unit"—the piece of core—and assign it material properties measured from a very small sample (approximately 1 cm³ in volume) taken from the same stratum. The material properties are taken from sample BB#10 on page B.33 of Klavetter and Peters (1987).

It should be noted that these saturation and hydraulic-conductivity curves come from measurements made by drying the sample: they are "drying curves." The imbibition experiment we want to simulate is a wetting process. Typically, drying and wetting curves for a material are different (an effect called hysteresis) and we can expect differences because of it.

The calculational mesh assigned to the geologic unit has 150 cells (151 mesh points) in three submeshes. The 50 cells near the bottom are 0.08 mm tall; the next 50 cells are 0.4 mm tall; the final

Figure 3.1: Experimental setup and TOSPAC setup for the laboratory imbibition experiment.

50 cells are 1.4 mm tall. More mesh points are located near the bottom of the sample because there are very strong pressure-head gradients in this region when the simulation begins, and the mesh spacing must be fine for the difference equations to behave like the differential equation. (More mesh points typically lead to much longer computer-processing times; however, DYNAMICS uses a direct, tridiagonal-matrix solver for the linear system that it defines, and it is relatively efficient).

The upper boundary condition is zero flux, i.e., no water is exiting the top of the sample. (Water vapor could escape through the top surface, but TOSPAC does not simulate vapor flow.) The lower boundary condition is zero pressure head, i.e., the “water table.” These boundary conditions remain constant throughout the simulation.

TOSPAC transient-flow problems must present results at user-defined times (problem times), called time snapshots, in order to monitor the flow dynamics. The times of the time snapshots are selected by experience. A rough guess of the imbibition time scale can be made by dividing the length of the sample by the velocity of the water. An estimate of the velocity can be made by assuming a unit head gradient (which in a saturated sample with gravity as the driving force makes the flux equal to the saturated conductivity) and dividing it by the porosity. In this case...

$$t = \frac{nl}{K_s},$$

where t is time, n is porosity, l is the length of the sample, and K_s is the saturated conductivity. This time is divided by an appropriate number of time snapshots. Other methods can be devised.

The initial condition is a dry sample. A dry sample is a paradox. Totally dry implies no water, which is typically less than the estimated residual saturation. In TOSPAC, the saturation is calculated from the pressure head using the material-property data, and thus, the saturation cannot be less than the residual saturation of the material. Also, totally dry implies no hydraulic conductivity (no flow possible). Indeed, the drier the sample is, the greater the pressure-head gradients, and the more difficult it is to solve the problem numerically. But for the material hydrologic properties used in this example problem, the imbibition rate is relatively independent of the initial saturation (a finding based on computer simulation). With this information, we will assign as an initial condition a very low pressure head, $-20,000$ m, which corresponds to a saturation of approximately 4% for this material.

The DYNAMICS input-data file for this example problem is given in Figure 3.2. This input-data file can be created using the INDATA module of TOSPAC as described in Chapter 2. In INDATA the user can either name this file or accept the default name, DYNAMICS.DAT. Notice that the input prompts given in INDATA correspond almost exactly to the data layout in the input-data file, so that with Figure 3.2, recreating this input-data file is trivial. This input-data file can also be created using the user's text editor. Section 4.7.1 describes the format of an input-data file. Also, Section 4.2 contains a description of the input-data requirements.

When the DYNAMICS input-data file given in Figure 3.2 exists, the user can execute this example problem. First, the user logs onto the computer and runs TOSPAC...

\$RUN TOSPAC

TOSPAC responds with the main menu...

TOSPAC VERSION 1.10 MAIN MENU

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

ENTER CHOICE:

The user selects choice 3 and receives the following message and prompt to name the input-data file...

TOSPAC MODULE DYNAMICS

ENTER DYNAMICS INPUT-DATA FILE (DEFAULT=DYNAMICS.DAT):

If the DYNAMICS module can find the input-data file, it checks to see if it contains a file block with the names of the initial-condition file and the output files. The input-data file in Figure 3.2 does contain a file block but, if it did not, TOSPAC would issue the following prompts...

ENTER DYNAMICS INITIAL-CONDITION FILE (DEFAULT=STEADY.PSI):

ENTER DYNAMICS OUTPUT-LISTING FILE (DEFAULT=DYNAMICS.LIS):

ENTER DYNAMICS PLOT-DATA FILE (DEFAULT=DYNAMICS.PLT):

Continuing with the example problem, TOSPAC indicates that it is reading the input-data file and creating the output files listed in the file block...

```

*****
***  TOSPAC HYDRO INPUT-DATA FILE  ***
*****

***** TITLE BLOCK *****
IMBIBITION EXPERIMENT EXAMPLE

***** CONSTANTS BLOCK *****
1000. kg/m**3      DENSITY OF WATER
4.3E-6 /m          COMPRESSIBILITY OF WATER
0.003 m**2         CROSS-SECTIONAL AREA OF COLUMN
0.1                TIMESTEP FACTOR
0.6                IMPLICITNESS FACTOR
BOTTOM            GWIT START POSITION
TOP               GWIT END POSITION
0                TIME SNAPSHOT FOR RESTART

***** GEOLOGIC-UNIT BLOCK *****
1                # GEOLOGIC UNITS
UNIT # 1 ...NAME:
BB#10
0. m              MIN ELEVATION
0.094 m           MAX ELEVATION
1                MATRIX MATERIAL INDEX
1                FRACTURE MATERIAL INDEX
0                FRACTURE POROSITY
5.8E-7 /m         BULK-ROCK COMPRESSIBILITY
0. /m             FRACTURE COMPRESSIBILITY

***** MATERIAL-PROPERTY BLOCK *****
1                # MATERIALS
MATERIAL # 1 ...NAME:
BB#10 (Klavetter & Peters, SAND86-0286)
0.11             MATERIAL EFFECTIVE POROSITY
2               CHARACTERISTIC CURVE FIT
1               TOTAL SATURATION
0.0194          RESIDUAL SATURATION
0.0227 /m       ALPHA COEFFICIENT
1.624           BETA COEFFICIENT
5.3E-12 m/s     SATURATED HYDRAULIC CONDUCTIVITY

***** MESH BLOCK *****
160             TOTAL # CELLS
3               # SUBMESHES
SUBMESH # 1:
0. m            LOWER ELEVATION
0.004 m         UPPER ELEVATION
50             # CELLS
SUBMESH # 2:
0.004 m         LOWER ELEVATION
0.024 m         UPPER ELEVATION
50             # CELLS
SUBMESH # 3:
0.024 m         LOWER ELEVATION
0.094 m         UPPER ELEVATION
50             # CELLS

***** BOUNDARY-CONDITION BLOCK *****
12             # TIME SNAPSHOTS
1             TIME CONVERSION NUMBER
SNAPSHOT # 1
0. s           PROBLEM TIME
12            BOUNDARY-CONDITION FLAG
0. m           LOWER-BOUNDARY PRESSURE HEAD
0. m/s         UPPER-BOUNDARY FLUX
0. m           MAX POND HEIGHT
SNAPSHOT # 2
60. s          PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 3
600. s         PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 4
6000. s        PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 5
86400. s       PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 6
604800. s      PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 7
2592000. s     PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 8
5184000. s     PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 9
7889400. s     PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 10
15778800. s    PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 11
23668200. s    PROBLEM TIME
00            BOUNDARY-CONDITION FLAG
SNAPSHOT # 12
31557600. s    PROBLEM TIME

***** INITIAL-CONDITION BLOCK *****
3             INITIAL-CONDITION FLAG
-2.0E+4 m     INITIAL PRESSURE HEAD

***** FILE BLOCK *****
NONE          INITIAL-CONDITION FILE
EX2DYNAMICS.PLT  PLOT-DATA FILE
EX2DYNAMICS.LIS  OUTPUT-LISTING FILE
15            OUTPUT-LISTING CONTROL

```

Figure 3.2: DYNAMICS input-data file for the imbibition-experiment simulation (in two columns).

```

READING INPUT-DATA FILE DYNAMICS.DAT.
CREATING DYNAMICS PLOT-DATA FILE EX2DYNAMICS.PLT.
CREATING DYNAMICS OUTPUT-LISTING FILE EX2DYNAMICS.LIS.

```

Then DYNAMICS begins the calculation, writing status messages to the terminal screen...

INITIALIZING VARIABLES...

BEGINNING TRANSIENT FLOW CALCULATION...

```

SNAPSHOT 1... TIME(SEC) = 0.00000E+00
  ITERATION =   1 STEP(SEC) = 3.25633E-05 TIME(SEC) = 3.25633E-05
  ITERATION =  10 STEP(SEC) = 1.25184E-03 TIME(SEC) = 3.69040E-03
  ITERATION =  20 STEP(SEC) = 7.21876E-02 TIME(SEC) = 0.21650
  ITERATION =  30 STEP(SEC) = 3.5944    TIME(SEC) = 11.875
  ITERATION =  37 STEP(SEC) = 1.5151    TIME(SEC) = 60.000
SNAPSHOT 2... TIME(SEC) = 60.000
  ITERATION =  40 STEP(SEC) = 5.1136    TIME(SEC) = 70.795
SLOW CONVERGENCE...
  REDO IT =   46 STEP(SEC) = 22.045    NEW STEP(SEC) = 15.431
  ITERATION =  50 STEP(SEC) = 15.431    TIME(SEC) = 222.86

```

```

  o
  o
  o

```

```

  ITERATION = 2282 STEP(DY) = 22.608    TIME(DY) = 182.63
SNAPSHOT 10... TIME(SEC) = 1.57788E+07
  ITERATION = 2285 STEP(DY) = 6.5310    TIME(DY) = 273.94
SNAPSHOT 11... TIME(SEC) = 2.36682E+07
  ITERATION = 2290 STEP(DY) = 11.715    TIME(YR) = 1.0000
SNAPSHOT 12... TIME(SEC) = 3.15576E+07
NORMAL DYNAMICS TERMINATION.

```

Notice that DYNAMICS has difficulty converging to a solution at iteration 46. Slow convergence (more than ten Newton subiterations) is a sign of numerical instability. Another sign is when the automatic timestep controller calculates a significantly smaller timestep (less than one-half the previous timestep). In both cases, DYNAMICS deals with the problem by reverting to the conditions at the time of the previous iteration, calculating a smaller timestep, and then taking the new timestep. This process is repeated until conditions stabilize. It does not imply that the results are inaccurate.

DYNAMICS takes 2290 timesteps (approximately eight minutes on a VAX 8700) to finish this example. Upon completion, the user is returned to the TOSPAC SHELL and the TOSPAC main menu.

Figure 3.3 presents part of the DYNAMICS output-listing file that was created for the imbibition-experiment simulation. Section 4.7.7 contains a description of the format of the DYNAMICS output-listing file. Shown in Figure 3.3 are a part of the initial conditions and the results of the time snapshots at 1 day (84,600 sec) and 1 yr (31,577,600 sec) into the simulation. The initial-conditions section begins with the average column saturation, the volume of the void space, the volume occupied by water and by air, and the mass of water in the column. The boundary conditions imposed at the initial timestep are presented next. Following is a table of calculated hydrologic variables given at

selected mesh points. (Selection of mesh points is controlled by the output-listing-control parameter in the file block of the input-data file--Section 4.2.11. In this case, output for every fifteenth mesh point is specified.) All values are given in the units used in the calculation; in this case, *SI* units. The time-snapshots sections are organized similarly to the initial-conditions section, with two exceptions. First, the results of a mass-balance calculations are included after the total-water-mass value. The mass balance compares the actual mass of water in the column with what the mass should be given the changes at the boundaries. It is a measure of the accuracy of the calculation. Second, the results of a groundwater-travel-time (GWTT) calculation are included after the hydrologic variables table. The GWTT calculation is based on tracking water particles. A particle is released at every time snapshot and is tracked between two positions specified in the constants block of the input-data-file (Section 4.2.6). The particle is tracked using two different algorithms: the average-fastest-particle method computes particle position using either the velocity of water in the matrix or in the fractures, depending on which is faster; the composite-velocity method uses the area-weighted average of the velocities in the matrix and in the fractures. The average-fastest-particle method approximates a worst-case GWTT. The composite-velocity method more closely approximates GWTT in media that allow matrix diffusion. GWTT is discussed further in Sections 3.2 and 4.6.3.4.

In Figure 3.3, the initial average column saturation is slightly more than 4%; after 1 day it is approximately 14%; after 1 yr it is virtually one. The total void space within the column is approximately 31 cm^3 (or $3.1 \times 10^{-5} \text{ m}^3$ in the units used in the calculation). Initially, the water occupies approximately 1.3 cm^3 of the void space and air occupies approximately 29.7 cm^3 . After 1 day, the water occupies approximately 4.5 cm^3 and air occupies approximately 26.5 cm^3 ; after 1 yr, the water occupies almost the entire void space. Initially, the total water mass--the amount of water actually calculated to be in the column--is 1.3 g (0.0013 kg); after 1 day it is approximately 4.5 g; after 1 yr it is approximately 31 g.

At the 1-day and 1-yr time snapshots, the amount of water crossing the top boundary is very small; the mass gain is caused by water entering through the bottom boundary. At 1 day, the difference between the mass that is in the column and the mass that should be in the column is approximately 4%; at 1 year, the difference is approximately 1%. These differences are caused by inaccuracies in calculating the boundary conditions and in solving the difference equations. The mass balance is acceptably small for such a nonlinear problem.

The table of hydrologic variables for the initial conditions shows a constant pressure head of $-20,000 \text{ m}$. There is a very small flux and velocity downward because a constant initial pressure head under the force of gravity causes water movement. At 1 day, at the top of the column, the flux has been set to a number sufficiently close to 0 for the precision of the VMS FORTRAN. At the bottom of the column, the pressure head has been set exactly to 0 and the pressure-head pulse extends past mesh point 60, only about 7.6 mm into the sample. (At other time snapshots, the flux and the water velocity can be seen to extend somewhat higher into the column than the pressure head, because they are calculated by pressure-head difference across three mesh points.) At 1 yr, flow in the column approaches zero everywhere because the imbibition has completed.

GWTT information is given in two tables; one table for the average-fastest-particle method, the other for composite-velocity method. In this example problem, without fractures, both methods return the same results. For each particle released--i.e., each time snapshot--the time of release (entry time), the current position in the column, the current time or the time the particle leaves the column (current or exit time), and the travel time (the time to go from the start position to the end position) are listed.

The table at 1 day shows that five particles have been released. The first three particles are approximately 1 cm above the lower boundary; the fourth particle is approximately 7 mm into the

INITIAL CONDITIONS OF MESH

AVERAGE COLUMN SATURATION = 4.095625E-02
 TOTAL VOID VOLUME = 3.102000E-05
 TOTAL WATER VOLUME = 1.270463E-06
 TOTAL AIR VOLUME = 2.974954E-06
 TOTAL WATER MASS = 1.270463E-03

INITIAL BOUNDARY CONDITIONS: FLAG = 12

TOP FLUX = 0.00000E+00
 BOTTOM PRESSURE HEAD = 0.00000E+00
 MAXIMUM POND HEIGHT = 0.00000E+00

J	UNIT	MAT	FRK	Z	PRES HEAD	SAT	FLUX	VEL	HYD COND	CAPACITANCE	DSAT
151	1	1	1	9.4000E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
150	1	1	1	9.2600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
135	1	1	1	7.1600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
120	1	1	1	5.0600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
105	1	1	1	2.9600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
90	1	1	1	1.9600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
75	1	1	1	1.3600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
60	1	1	1	7.6000E-03	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
45	1	1	1	3.5200E-03	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
30	1	1	1	2.3200E-03	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
15	1	1	1	1.1200E-03	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
1	1	1	1	0.0000E+00	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07

o
o
o

ITERATION = 358
 TIME = 1.00000 DY
 AVERAGE COLUMN SATURATION = 0.143663
 TOTAL VOID VOLUME = 3.102000E-05
 TOTAL WATER VOLUME = 4.456422E-06
 TOTAL AIR VOLUME = 2.666358E-05
 TOTAL MASS IN COLUMN = 4.456422E-03
 CUMULATIVE MASS IN TOP = -5.218003E-27 (1.17090E-22% OF TOTAL)
 CUMULATIVE MASS IN BOTTOM = 3.379988E-03 (75.845 % OF TOTAL)
 MASS THAT SHOULD BE IN COLUMN = 4.650451E-03
 MASS DIFFERENCE = -1.940289E-04 MASS BALANCE = -4.35392 %

BOUNDARY CONDITIONS: FLAG = 12

TOP FLUX = 0.00000E+00
 BOTTOM PRESSURE HEAD = 0.00000E+00
 MAXIMUM POND HEIGHT = 0.00000E+00

J	UNIT	MAT	FRK	Z	PRES HEAD	SAT	FLUX	VEL	HYD COND	CAPACITANCE	DSAT
151	1	1	1	9.4000E-02	-2.0000E+04	4.0956E-02	2.0131E-32	8.4899E-30	2.7278E-22	9.4373E-08	6.7298E-07
150	1	1	1	9.2600E-02	-2.0000E+04	4.0956E-02	-1.3637E-22	-5.7513E-20	2.7278E-22	9.4373E-08	6.7298E-07
135	1	1	1	7.1600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
120	1	1	1	5.0600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
105	1	1	1	2.9600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
90	1	1	1	1.9600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
75	1	1	1	1.3600E-02	-2.0000E+04	4.0956E-02	-2.7278E-22	-1.1504E-19	2.7278E-22	9.4373E-08	6.7298E-07
60	1	1	1	7.6000E-03	-22.49	0.8968	5.9650E-09	6.1853E-08	8.5166E-13	6.7344E-04	6.1141E-03
45	1	1	1	3.5200E-03	-6.206	0.9845	6.3157E-09	5.9490E-08	2.6735E-12	4.2250E-04	3.8315E-03
30	1	1	1	2.3200E-03	-3.648	0.9934	6.3326E-09	5.9104E-08	3.3028E-12	3.1541E-04	2.8579E-03
15	1	1	1	1.1200E-03	-1.569	0.9983	6.3383E-09	5.8864E-08	4.0699E-12	1.8890E-04	1.7077E-03
1	1	1	1	0.0000E+00	0.0000E+00	1.0000	6.3390E-09	5.8768E-08	5.3000E-12	1.0630E-06	0.0000E+00

PARTICLE TRAVEL TIMES: START POSITION = 0.00000E+00
 END POSITION = 9.40000E-02

PARTICLE NUMBER	ENTRY TIME	CURRENT POSITION	AVERAGE FASTEST PARTICLE		TRAVEL TIME
			CURRENT POSITION	EXIT TIME	
1	0.000000E+00 SEC	1.115521E-02	1.00000	DY	(STILL IN RANGE)
2	60.0000 SEC	1.112600E-02	1.00000	DY	(STILL IN RANGE)
3	600.000 SEC	1.025833E-02	1.00000	DY	(STILL IN RANGE)
4	1.66667 HR	7.868055E-03	1.00000	DY	(STILL IN RANGE)
5	1.00000 DY	0.000000E+00	1.00000	DY	(STILL IN RANGE)

PARTICLE NUMBER	ENTRY TIME	CURRENT POSITION	COMPOSITE VELOCITY		TRAVEL TIME
			CURRENT POSITION	EXIT TIME	
1	0.000000E+00 SEC	1.115521E-02	1.00000	DY	(STILL IN RANGE)
2	60.0000 SEC	1.112600E-02	1.00000	DY	(STILL IN RANGE)
3	600.000 SEC	1.025833E-02	1.00000	DY	(STILL IN RANGE)
4	1.66667 HR	7.868055E-03	1.00000	DY	(STILL IN RANGE)
5	1.00000 DY	0.000000E+00	1.00000	DY	(STILL IN RANGE)

Figure 3.3: Part of the DYNAMICS output-listing file for the imbibition-experiment simulation.

```

o
o
o
ITERATION = 2290          SNAPSHOT = 12
TIME = 1.00000 YR        PRV TIME STEP = 11.7153 DY
AVERAGE COLUMN SATURATION = 0.999993
TOTAL VOID VOLUME = 3.102000E-05
TOTAL WATER VOLUME = 3.101979E-05
TOTAL AIR VOLUME = 2.088229E-10
TOTAL MASS IN COLUMN = 3.101979E-02
CUMULATIVE MASS IN TOP = -1.375805E-21 ( 4.43525E-18% OF TOTAL)
CUMULATIVE MASS IN BOTTOM = 3.001143E-02 ( 96.749 % OF TOTAL)
MASS THAT SHOULD BE IN COLUMN = 3.128189E-02
MASS DIFFERENCE = -2.621031E-04 MASS BALANCE = -0.844954 %

```

J	UNIT	MAT	FRK	Z	PRES HEAD	SAT	FLUX	VEL	HYD COND	CAPACITANCE	DSAT
151	1	1	1	9.4000E-02	-9.4000E-02	1.000	0.0000E+00	0.0000E+00	5.0747E-12	3.3880E-05	2.9843E-04
150	1	1	1	9.2600E-02	-9.2600E-02	1.000	3.7263E-19	3.4546E-18	5.0767E-12	3.3585E-05	2.9575E-04
135	1	1	1	7.1600E-02	-7.1600E-02	1.000	-4.0297E-18	-3.7359E-17	5.1105E-12	2.8613E-05	2.5054E-04
120	1	1	1	5.0600E-02	-5.0600E-02	1.000	-2.8676E-17	-2.6585E-16	5.1462E-12	2.3351E-05	2.0299E-04
105	1	1	1	2.9600E-02	-2.9600E-02	1.000	-1.4347E-17	-1.3301E-16	5.1897E-12	1.7038E-05	1.4532E-04
90	1	1	1	1.9600E-02	-1.9600E-02	1.000	1.6603E-17	1.5392E-16	5.2149E-12	1.3367E-05	1.1195E-04
75	1	1	1	1.3600E-02	-1.3600E-02	1.000	3.0525E-17	2.8299E-16	5.2322E-12	1.0854E-05	8.9099E-05
60	1	1	1	7.6000E-03	-7.6001E-03	1.000	6.0019E-17	5.5843E-16	5.2526E-12	7.9022E-06	6.2266E-05
45	1	1	1	3.5200E-03	-3.5201E-03	1.000	8.4357E-17	7.8206E-16	5.2708E-12	5.2642E-06	3.8284E-05
30	1	1	1	2.3200E-03	-2.3200E-03	1.000	9.4270E-17	8.7396E-16	5.2775E-12	4.3012E-06	2.9529E-05
15	1	1	1	1.1200E-03	-1.1200E-03	1.000	1.0577E-16	9.8056E-16	5.2857E-12	3.1111E-06	1.8710E-05
1	1	1	1	0.0000E+00	0.0000E+00	1.000	1.2174E-16	1.1286E-15	5.3000E-12	1.0530E-06	0.0000E+00

PARTICLE TRAVEL TIMES: START POSITION = 0.00000E+00
END POSITION = 9.40000E-02

PARTICLE NUMBER	ENTRY TIME	AVERAGE FASTEST CURRENT POSITION	PARTICLE CURRENT OR EXIT TIME	TRAVEL TIME
1	0.000000E+00 SEC	9.225512E-02	1.00000 YR	(STILL IN RANGE)
2	60.0000 SEC	9.225389E-02	1.00000 YR	(STILL IN RANGE)
3	600.000 SEC	9.205376E-02	1.00000 YR	(STILL IN RANGE)
4	1.66667 HR	8.995978E-02	1.00000 YR	(STILL IN RANGE)
5	1.00000 DY	8.217153E-02	1.00000 YR	(STILL IN RANGE)
6	7.00000 DY	6.554964E-02	1.00000 YR	(STILL IN RANGE)
7	30.0000 DY	3.707456E-02	1.00000 YR	(STILL IN RANGE)
8	60.0000 DY	1.448047E-02	1.00000 YR	(STILL IN RANGE)
9	91.3125 DY	2.564524E-07	365.250 DY	(STILL IN RANGE)
10	182.625 DY	0.000000E+00	182.625 DY	0.000000E+00 SEC WARNING
11	273.938 DY	1.186435E-09	1.00000 YR	(STILL IN RANGE)
12	1.00000 YR	0.000000E+00	1.00000 YR	(STILL IN RANGE)

PARTICLE NUMBER	ENTRY TIME	COMPOSITE VELOCITY CURRENT POSITION	CURRENT OR EXIT TIME	TRAVEL TIME
1	0.000000E+00 SEC	9.225512E-02	1.00000 YR	(STILL IN RANGE)
2	60.0000 SEC	9.225389E-02	1.00000 YR	(STILL IN RANGE)
3	600.000 SEC	9.205376E-02	1.00000 YR	(STILL IN RANGE)
4	1.66667 HR	8.995978E-02	1.00000 YR	(STILL IN RANGE)
5	1.00000 DY	8.217153E-02	1.00000 YR	(STILL IN RANGE)
6	7.00000 DY	6.554964E-02	1.00000 YR	(STILL IN RANGE)
7	30.0000 DY	3.707456E-02	1.00000 YR	(STILL IN RANGE)
8	60.0000 DY	1.448047E-02	1.00000 YR	(STILL IN RANGE)
9	91.3125 DY	2.564524E-07	365.250 DY	(STILL IN RANGE)
10	182.625 DY	0.000000E+00	182.625 DY	0.000000E+00 SEC WARNING
11	273.938 DY	1.186435E-09	1.00000 YR	(STILL IN RANGE)
12	1.00000 YR	0.000000E+00	1.00000 YR	(STILL IN RANGE)

Figure 3.3: Concluded.

column; and the fifth particle, which has just been released, is at the lower boundary. At 1 day, none of the particles have reached the end position at the upper boundary. The note STILL IN RANGE is given in the place of a travel time.

At 1 yr, twelve particles have been released, none of which have reached the upper boundary—although the first particles are close, having traveled approximately 9.2 cm of the 9.4 cm. Indeed, it is unlikely that any particles will reach the upper boundary because of the no-flux upper boundary condition. The first and furthest particle is in the center of the inflowing pulse, and this pulse dissipated when it reached the upper boundary. One particle has, however, left the column at the start position, because after the inflowing pulse dissipated, flow reversed slightly (this flow reversal could be a numerical artifact). The exit time is given for this particle, as well as a travel time. The WARNING note indicates that the given travel time is incorrect.

To finish the example problem, several computer graphs can be produced. Computer plots are useful in giving the user a quick grasp of the overall imbibition process in this problem. Select choice 5 in response to the TOSPAC main menu...

TOSPAC VERSION 1.10 MAIN MENU

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

ENTER CHOICE: 5

And TOSPAC switches to the plotting module, OUTPLOT...

TOSPAC MODULE OUTPLOT

ENTER PLOT-DEFINITION FILE (DEFAULT=OUTPLOT.PDF): EX2OUTPLOT.PDF

EX2OUTPLOT.PDF DOES NOT EXIST...

CREATING EX2OUTPLOT.PDF.

OUTPLOT MAIN MENU

- 0. STOP
- 1. DEFINE STEADY PLOTS
- 2. DEFINE DYNAMICS PLOTS
- 3. DEFINE TRANS PLOTS
- 4. CONSTRUCT GRAPHICS-DRIVER FILE

ENTER CHOICE: 2

ENTER DYNAMICS PLOT-DATA FILE (DEFAULT=NONE): EX2DYNAMICS.PLT

OUTPLOT (DYNAMICS RESULTS) MENU

0. STOP
1. PLOT MESH/STRATIGRAPHY
2. PLOT CHARACTERISTIC CURVES
3. PLOT COMPOSITE CONDUCTIVITY AND CAPACITANCE CURVES
4. PLOT PRESSURE HEAD VS ELEVATION
5. PLOT SATURATION VS ELEVATION
6. PLOT FLUX VS ELEVATION
7. PLOT VELOCITY VS ELEVATION
8. PLOT CONDUCTIVITY VS ELEVATION
9. PLOT CAPACITANCE VS ELEVATION
10. PLOT SATURATION VS TIME
11. PLOT MASS VS TIME

ENTER CHOICE:

At this point, the user is directed to Section 4.6 for a discussion of OUTPLOT and the plot-definition file. For DYNAMICS plots, Section 4.6.4 contains a description of the questions, and the meaning of the questions, that appear when the user requests a particular plot.

Eleven plots have been created for the imbibition-experiment example, one for each of the categories listed in the OUTPLOT (DYNAMICS RESULTS) menu. The plots are shown in Figures 3.4 through 3.15, and are described below in the order they appear in the OUTPLOT (DYNAMICS RESULTS) menu.

Figure 3.4 shows the mesh/stratigraphy plot—choice 1 on the OUTPLOT (DYNAMICS RESULTS) menu. The left-hand stack of rectangles represents the mesh, with the horizontal lines indicating mesh points. Note that the bottom of each mesh-point number aligns with the appropriate mesh point. The right-hand rectangle represents the geologic unit(s) and presents the material assignments. The purpose of this plot is to make certain that the calculational mesh matches both the physical layout and the user's intended layout. Compare this graphic with the illustration in Figure 3.1 to check the mesh design.

Figure 3.5 presents the curves for saturation versus pressure head and hydraulic conductivity versus pressure head for the section of drill core used in the experiment. These curves are known as the characteristic curves for the material. The curves are specified in the material-property block of the input-data file (Figure 3.2), in this case, using the parameters for the van Genuchten formulation.

DYNAMICS uses the characteristic curves of the matrix and fractures to compute the composite hydraulic-conductivity curve and composite capacitance (or storage capacity) curve for each geologic unit. The composite curves are then used by DYNAMICS to solve Richards' Equation. Plots of the composite curves can be used to verify that the input data are correct (i.e., that the hydrologic properties are reasonable and that they are assigned to the correct geologic unit) and to interpret results.

Figure 3.6 presents the composite curve of hydraulic conductivity versus pressure head for the single geologic unit defined in the geologic unit block of the input-data file (Figure 3.2). The composite curve is calculated as the area-weighted average of the hydraulic conductivity of the matrix and the hydraulic conductivity of the fractures (Peters and Klavetter, 1988). Also shown in Figure 3.6 are the characteristic curves for the matrix and the fractures that are used in defining the composite curve. When a geologic unit is defined without fractures, the composite hydraulic-conductivity curve is the

Figure 3.4: Mesh/stratigraphy plot for the imbibition-experiment simulation.

Figure 3.5: Characteristic curves of the sample used for the imbibition-experiment simulation.

same as the hydraulic-conductivity curve of the matrix material (Figure 3.5). A more interesting composite curve is given in Figure 3.26 in Section 3.2.

Figure 3.7 presents the composite curves of capacitance versus pressure head for the "geologic unit" defined for the problem. (As with the composite hydraulic conductivity curves, this plot is also selected by choice 3 on the OUTPLOT (DYNAMICS RESULTS) menu.) The solid line on the plot is the composite curve; the dashed line is the first derivative of the saturation of the matrix material. If we had specified a fracture material, it would also be shown on the plot. A more interesting composite capacitance curve is given in Figure 3.27 in Section 3.2.

The composite capacitance coefficient is the sum of the storage capacities caused by matrix saturation (the area-weighted derivative of the saturation of the matrix material), fracture saturation (the area-weighted derivative of the saturation of the fracture material), bulk-rock compressibility, fracture compressibility, and the compressibility of water. Peters and Klavetter (1988) give a complete discussion of the capacitance coefficient. In this example problem the significant terms are the matrix storage capacity and the bulk-rock compressibility. The capacitance influences the rate at which flow changes in a problem: low capacitance allows quick changes in flow; high capacitance forces slow changes because large amounts of water are required to fill or drain the material before the new flow can be supported.

Figure 3.8 presents the profiles of pressure head versus elevation. The vertical line on the left is the initial pressure head of $-20,000$ m. The vertical line on the right is the final pressure head of approximately 0 m. Each horizontal line is the distinguishable part of a time line, or profile, showing the "shape" of the pressure head at a given time snapshot.

Examination of the plot shows that the pressure-head profile is very steep. That is, the water moves into the sample predominantly as a saturated front. (See Figure 3.6 to determine the increase in hydraulic conductivity with the increase in pressure head for this sample.) The front is widening as it progresses, and it is slowing down. Widening of the front decreases the pressure-head gradient at a point, thus slowing the water movement.

DYNAMICS solves for pressure head. Figures 3.9 through 3.15 present quantities calculated from pressure head.

Figure 3.9 shows the profiles of saturation versus elevation for the calculation. The saturation profiles do not exactly resemble the pressure-head profiles (Figure 3.8). The saturation profiles are calculated from the pressure head, but the relationship is nonlinear and the profiles are not the same shape. Indeed, the saturation change appears to lag behind the pressure-head change. The 60-day time line in Figure 3.8 shows that the middle part of the sample is in a local steady state according to pressure head; the 60-day time line in Figure 3.9 shows that the middle part of the sample is still filling with water. This observation is important when attempting to run a transient-flow calculation to a steady-state conclusion.

It may be possible to check these saturation results during the course of the experiment. Although the amount of water is small, visual observation of the front is possible. Also, if the sample were cut in half after approximately 15 days, one-half should be almost dry and one-half almost saturated. In a uniform material this prediction could be checked by weighing.

Figure 3.10 presents the profiles of matrix flux versus elevation. The plot was constructed with a linear scale; logarithmic scales are also available, as are plots of normalized data. Initially, the flux is approximately zero in the sample (actually, a slight downward flux is present, as shown in Figure 3.3,

IMBIBITION EXPERIMENT EXAMPLE
Composite Hydraulic Conductivity For BB#10

Figure 3.6: Composite hydraulic conductivity of the sample used for the imbibition-experiment simulation.

IMBIBITION EXPERIMENT EXAMPLE Composite Capacitance Coefficients For BB#10

Figure 3.7: Composite capacitance of the sample used for the imbibition-experiment simulation.

IMBIBITION EXPERIMENT EXAMPLE Pressure Head of the Water

Figure 3.8: Pressure-head results for the imbibition-experiment simulation.

IMBIBITION EXPERIMENT EXAMPLE Pore Saturation in the Matrix

Figure 3.9: Saturation profiles for the imbibition-experiment simulation.

but it is not visible at this scale). With the start of the experiment, very large upward (positive) fluxes are expected, and are shown in the figure. The flux indicated by the first time line extends off the plot; it is approximately three times larger than the flux at the second time line (Figure 3.3). The magnitude of the flux continues to drop as the front extends into the sample.

Flux is calculated from Darcy's Law:

$$q = -K(\psi)\left(\frac{\Delta\psi}{\Delta z} + 1\right),$$

where q is the flux, K is the hydraulic conductivity, ψ is the pressure head, and z is the elevation. Thus the slight widening of the pressure-head front observed in Figure 3.8 has a profound slowing effect on the movement of water.

When large changes in flux are caused by slight changes in pressure head, flux is said to be sensitive to pressure head. This sensitivity allows us to measure the stability of the calculation. Any unexplained wiggles or oscillations in the flux profiles imply a numerical instability. Such instability may or may not significantly affect the results; however, the user must examine it further. A further discussion of numerical instability is included at the end of this section.

Figure 3.11 presents the average linear velocity of water in the sample versus elevation. The plot shows the upward velocities of water into the sample. The velocities decline over time, as is observed with flux. Notice that a slight upward velocity is still indicated at 90 days. If flux were plotted in this manner, we would see almost identical curves. The order-of-magnitude difference between velocity and flux is caused by dividing the flux by the moisture content, which is the product of porosity (0.11) and saturation (approximately 1). This dependence on flux means that velocity is also sensitive to pressure head; hence, velocity can also be used as a measure of numerical stability.

The plot of matrix hydraulic conductivity versus elevation is presented in Figure 3.12. As with saturation (Figure 3.9), hydraulic conductivity distinctly lags behind pressure head. This plot serves as a diagnostic tool for interpreting complex results.

Figure 3.13 presents the plot of capacitance (storage capacity) coefficients versus elevation. Capacitance has a large influence on transient water flow, because a large storage capacity holds water and damps pressure-head fronts attempting to move through, while a small storage capacity allows fronts to move through quickly. Capacitance coefficients are lowest at very unsaturated and saturated conditions. At these extremes, capacitance is dominated by various compressibility factors. Between these extremes, capacitance is dominated by the derivative of the saturation with respect to pressure head (Peters and Klavetter, 1988). Because this problem goes from a dry condition to a saturated condition, the capacitance coefficient is a profile of the rise and fall of the storage capacity of the rock. As with the plot of hydraulic conductivity versus elevation, the capacitance plot is primarily used as a tool to understand complex behavior.

Figure 3.14 presents the average sample saturation versus time and Figure 3.15 presents the water mass versus time, both plotted on a linear scale. These plots are constructed with choices number 10 and 11 on the OUTPLOT (DYNAMICS RESULTS) menu. The average sample saturation is calculated by summing over the entire mesh as follows: the average saturation between every two neighboring mesh points multiplied by the ratio of the distance between the neighboring points over the entire distance (elevation) covered by the mesh. The shape of this curve follows the shape of the water-mass curve. The water mass is calculated by summing the volume of water in each mesh cell

IMBIBITION EXPERIMENT EXAMPLE Water Flux in the Matrix

Figure 3.10: Flux profiles for the imbibition-experiment simulation.

IMBIBITION EXPERIMENT EXAMPLE Water Velocity in the Matrix

Figure 3.11: Average linear velocity of water for the imbibition-experiment simulation.

IMBIBITION EXPERIMENT EXAMPLE Hydraulic Conductivity in the Matrix

Figure 3.12: Hydraulic-conductivity profiles for the imbibition-experiment simulation.

IMBIBITION EXPERIMENT EXAMPLE Composite Water Capacitance

Figure 3.13: Capacitance-coefficient profiles for the imbibition-experiment simulation.

(determined by taking the average of the moisture contents at the mesh points, then multiplying by the distance across the cell), and multiplying by the density of water (an input parameter).

The information in Figure 3.15 is the information being sought in the experiment; hence, this plot allows correspondence between the simulated experiment and the experimental data. Discrepancies between experimental and simulated results are possible, and indeed, should be expected. For example, TOSPAC does not handle hysteresis effects in the definition of the material hydrologic properties; therefore, because these hydrologic properties were measured by draining the sample, they may not be satisfactory for modeling an imbibition experiment.

By changing certain hydrologic material properties, it is often possible to match experimental results. In this manner, errors in the input data can be estimated and potentially more accurate characteristic curves can be constructed (Peters *et al.*, 1987).

Consider the following three hydrologic parameters:

- 1) The van Genuchten α parameter. This parameter is based on the air-entry pressure head: a large α implies that the material contains large pores and that it begins to desaturate at high pressure heads. Setting α to a larger value causes the average-sample-saturation change and the mass change to occur over a longer time scale. The curves appear to retain the same shape, but the time axis is expanded. Changing α can effectively mimic hysteresis effects: increasing α makes a draining curve more like a wetting curve; decreasing α makes a wetting curve more like a draining curve.
- 2) The saturated hydraulic conductivity (K_s). The product of this parameter with the relative conductivity (K_{rel}) determines the unsaturated hydraulic conductivity. Reducing K_s reduces the unsaturated hydraulic conductivity, and effectively shifts the hydraulic-conductivity characteristic curve so that a higher pressure head is required to achieve the same conductivity. Thus, reducing K_s produces changes similar to increasing the van Genuchten α parameter; the time scale of the mass-change curve increases.
- 3) The van Genuchten β parameter. This parameter is based on the uniformity of pore sizes and is a measure of the steepness of the characteristic curve (the more uniform the pore sizes, the steeper the characteristic curve and the larger the value of β). Changing β produces competing effects. Increasing β causes changes in saturation and hydraulic conductivity to occur at higher pressure heads, and therefore, should lengthen the time scale of the mass change. However, increasing β causes the problem to become more nonlinear. The pressure-head gradients increase causing the mass-change time scale to shorten. In the end, changing β primarily causes changes in the shape of the saturation- and mass-change curves. Increasing β causes the curves to become more linear, i.e., straighten out (on a linear scale). Decreasing β cause the curves to become more logarithmically shaped (on a linear scale).

The OUTPLOT module also allows plots of average sample saturation and water mass on a logarithmic scale. Mass and saturation plots on a logarithmic scale are most useful with events that change rapidly at early times, but then extend over very long time scales. With this experiment, results are more understandable on a linear scale. Peters *et al.* (1987) documents a similar experiment that was more understandable with a logarithmic plot.

The OUTPLOT plot-definition file used to define the plots discussed in this section is presented in Figure 3.16.

Figure 3.14: Average sample saturation for the imbibition experiment.

Figure 3.15: Sample mass change for the imbibition experiment.

```

*****
***  TOSPA OUTPLOT PLOT-DEFINITION FILE  ***
*****

***** DYNAMICS PLOT SECTION *****

***** PLOT FILE BLOCK *****
EX2DYNAMICS.PLT          DYNAMICS PLOT-DATA FILENAME

***** MESH PLOT BLOCK *****
XAXIS LIN                ELEVATION AXIS TYPE
XLIMITS DEFAULT,DEFAULT  ELEVATION AXIS LIMITS
BOX DEFAULT              MESH POINTS PER BOX
NUMBER DEFAULT           MESH POINTS PER LABEL

***** CHARACTERISTIC-CURVE PLOT BLOCK *****
XAXIS NEGLOG             PRESSURE-HEAD AXIS TYPE
XLIMITS DEFAULT,DEFAULT  PRESSURE-HEAD AXIS LIMITS
ZAXIS LIN                SATURATION AXIS TYPE
ZLIMITS DEFAULT,DEFAULT  SATURATION AXIS LIMITS
YAXIS LOG                CONDUCTIVITY AXIS TYPE
YLIMITS DEFAULT,DEFAULT  CONDUCTIVITY AXIS LIMITS
MATERIAL ALL             PLOT CURVES FOR MATERIAL

***** COMPOSITE-CONDUCTIVITY PLOT BLOCK *****
UNIT ALL                 PLOT CURVES FOR GEOLOGIC UNIT
YAXIS LOG                CONDUCTIVITY AXIS TYPE
YLIMITS DEFAULT,DEFAULT  CONDUCTIVITY AXIS LIMITS
XAXIS NEGLOG             PRESSURE-HEAD AXIS TYPE
XLIMITS DEFAULT,DEFAULT  PRESSURE-HEAD AXIS LIMITS
LEGEND RIGHT,TOP         LEGEND LOCATION

***** COMPOSITE-CAPACITANCE PLOT BLOCK *****
UNIT ALL                 PLOT CURVES FOR GEOLOGIC UNIT
YAXIS LOG                CAPACITANCE AXIS TYPE
YLIMITS DEFAULT,DEFAULT  CAPACITANCE AXIS LIMITS
XAXIS NEGLOG             PRESSURE-HEAD AXIS TYPE
XLIMITS DEFAULT,DEFAULT  PRESSURE-HEAD AXIS LIMITS
LEGEND RIGHT,TOP         LEGEND LOCATION

***** PRESSURE-HEAD PLOT BLOCK *****
XAXIS LIN                ELEVATION AXIS TYPE
XLIMITS DEFAULT,DEFAULT  ELEVATION AXIS LIMITS
YAXIS LIN                PRESSURE-HEAD AXIS TYPE
YLIMITS DEFAULT,DEFAULT  PRESSURE-HEAD AXIS LIMITS
SNAPSHOT 1               SNAPSHOT TO PLOT
LABEL initial
SNAPSHOT 2               SNAPSHOT TO PLOT
LABEL 60 sec
SNAPSHOT 3               SNAPSHOT TO PLOT
LABEL 600 sec
SNAPSHOT 4               SNAPSHOT TO PLOT
LABEL 6000 sec
SNAPSHOT 5               SNAPSHOT TO PLOT
LABEL 1 day
SNAPSHOT 6               SNAPSHOT TO PLOT
LABEL 7 days
SNAPSHOT 7               SNAPSHOT TO PLOT
LABEL 30 days
SNAPSHOT 8               SNAPSHOT TO PLOT
LABEL 60 days
SNAPSHOT 9               SNAPSHOT TO PLOT
LABEL 0.25 yr
LEGEND RIGHT,TOP         LEGEND LOCATION
MODE MULTI               PLOT MODE
ORIENT PORTRAIT          PLOT ORIENTATION

***** SATURATION PLOT BLOCK *****
XAXIS LIN                ELEVATION AXIS TYPE
XLIMITS DEFAULT,DEFAULT  ELEVATION AXIS LIMITS
YAXIS LIN                SATURATION AXIS TYPE
YLIMITS DEFAULT,DEFAULT  SATURATION AXIS LIMITS
SNAPSHOT 1               SNAPSHOT TO PLOT
LABEL initial
SNAPSHOT 2               SNAPSHOT TO PLOT
LABEL 60 sec
SNAPSHOT 3               SNAPSHOT TO PLOT
LABEL 600 sec
SNAPSHOT 4               SNAPSHOT TO PLOT
LABEL 6000 sec
SNAPSHOT 5               SNAPSHOT TO PLOT
LABEL 1 day

```

Figure 3.16: OUTPLOT plot-definition file for the imbibition-experiment simulation.

SNAPSHOT 6	SNAPSHOT TO PLOT
LABEL 7 days	
SNAPSHOT 7	SNAPSHOT TO PLOT
LABEL 30 days	
SNAPSHOT 8	SNAPSHOT TO PLOT
LABEL 60 days	
SNAPSHOT 9	SNAPSHOT TO PLOT
LABEL 0.25 yr	
LEGEND RIGHT, TOP	LEGEND LOCATION
PLOTTYPE MATRIX	SATURATION TYPE
MODE MULTI	PLOT MODE
ORIENT PORTRAIT	PLOT ORIENTATION
***** FLUX PLOT BLOCK *****	
XAXIS LIN	ELEVATION AXIS TYPE
XLIMITS DEFAULT, DEFAULT	ELEVATION AXIS LIMITS
YAXIS LIN	FLUX AXIS TYPE
YLIMITS -1.E-8, 8.E-8	FLUX AXIS LIMITS
SNAPSHOT 1	SNAPSHOT TO PLOT
LABEL initial	
SNAPSHOT 2	SNAPSHOT TO PLOT
LABEL 60 sec	
SNAPSHOT 3	SNAPSHOT TO PLOT
LABEL 600 sec	
SNAPSHOT 4	SNAPSHOT TO PLOT
LABEL 6000 sec	
SNAPSHOT 5	SNAPSHOT TO PLOT
LABEL 1 day	
SNAPSHOT 6	SNAPSHOT TO PLOT
LABEL 7 days	
SNAPSHOT 7	SNAPSHOT TO PLOT
LABEL 30 days	
SNAPSHOT 8	SNAPSHOT TO PLOT
LABEL 60 days	
SNAPSHOT 9	SNAPSHOT TO PLOT
LABEL 0.25 yr	
LEGEND RIGHT, TOP	LEGEND LOCATION
PLOTTYPE MATRIX	FLUX TYPE
MODE MULTI	PLOT MODE
ORIENT PORTRAIT	PLOT ORIENTATION
***** VELOCITY PLOT BLOCK *****	
XAXIS LIN	ELEVATION AXIS TYPE
XLIMITS DEFAULT, DEFAULT	ELEVATION AXIS LIMITS
YAXIS LOG	VELOCITY AXIS TYPE
YLIMITS DEFAULT, DEFAULT	VELOCITY AXIS LIMITS
SNAPSHOT 1	SNAPSHOT TO PLOT
LABEL initial	
SNAPSHOT 2	SNAPSHOT TO PLOT
LABEL 60 sec	
SNAPSHOT 3	SNAPSHOT TO PLOT
LABEL 600 sec	
SNAPSHOT 4	SNAPSHOT TO PLOT
LABEL 6000 sec	
SNAPSHOT 5	SNAPSHOT TO PLOT
LABEL 1 day	
SNAPSHOT 6	SNAPSHOT TO PLOT
LABEL 7 days	
SNAPSHOT 7	SNAPSHOT TO PLOT
LABEL 30 days	
SNAPSHOT 8	SNAPSHOT TO PLOT
LABEL 60 days	
SNAPSHOT 9	SNAPSHOT TO PLOT
LABEL 0.25 yr	
LEGEND RIGHT, TOP	LEGEND LOCATION
PLOTTYPE MATRIX	VELOCITY TYPE
MODE MULTI	PLOT MODE
ORIENT PORTRAIT	PLOT ORIENTATION
***** CONDUCTIVITY PLOT BLOCK *****	
XAXIS LIN	ELEVATION AXIS TYPE
XLIMITS DEFAULT, DEFAULT	ELEVATION AXIS LIMITS
YAXIS LOG	CONDUCTIVITY AXIS TYPE
YLIMITS DEFAULT, DEFAULT	CONDUCTIVITY AXIS LIMITS
SNAPSHOT 1	SNAPSHOT TO PLOT
LABEL initial	
SNAPSHOT 2	SNAPSHOT TO PLOT
LABEL 60 sec	
SNAPSHOT 3	SNAPSHOT TO PLOT
LABEL 600 sec	
SNAPSHOT 4	SNAPSHOT TO PLOT
LABEL 6000 sec	

Figure 3.16: Continued.

SNAPSHOT 5	SNAPSHOT TO PLOT
LABEL 1 day	
SNAPSHOT 6	SNAPSHOT TO PLOT
LABEL 7 days	
SNAPSHOT 7	SNAPSHOT TO PLOT
LABEL 30 days	
SNAPSHOT 8	SNAPSHOT TO PLOT
LABEL 60 days	
SNAPSHOT 9	SNAPSHOT TO PLOT
LABEL 0.25 yr	
LEGEND RIGHT, TOP	LEGEND LOCATION
PLOTTYPE MATRIX	CONDUCTIVITY TYPE
MODE MULTI	PLOT MODE
ORIENT PORTRAIT	PLOT ORIENTATION
***** CAPACITANCE PLOT BLOCK *****	
XAXIS LIN	ELEVATION AXIS TYPE
XLIMITS DEFAULT, DEFAULT	ELEVATION AXIS LIMITS
YAXIS LOG	CAPACITANCE AXIS TYPE
YLIMITS 1.E-8, 1.E-1	CAPACITANCE AXIS LIMITS
SNAPSHOT 1	SNAPSHOT TO PLOT
LABEL initial	
SNAPSHOT 2	SNAPSHOT TO PLOT
LABEL 60 sec	
SNAPSHOT 3	SNAPSHOT TO PLOT
LABEL 600 sec	
SNAPSHOT 4	SNAPSHOT TO PLOT
LABEL 6000 sec	
SNAPSHOT 5	SNAPSHOT TO PLOT
LABEL 1 day	
SNAPSHOT 6	SNAPSHOT TO PLOT
LABEL 7 days	
SNAPSHOT 7	SNAPSHOT TO PLOT
LABEL 30 days	
SNAPSHOT 8	SNAPSHOT TO PLOT
LABEL 60 days	
SNAPSHOT 9	SNAPSHOT TO PLOT
LABEL 0.25 yr	
LEGEND RIGHT, TOP	LEGEND LOCATION
MODE MULTI	PLOT MODE
ORIENT PORTRAIT	PLOT ORIENTATION
***** AVERAGE-SATURATION PLOT BLOCK *****	
YAXIS LIN	SATURATION AXIS TYPE
YLIMITS DEFAULT, DEFAULT	SATURATION AXIS LIMITS
XAXIS LIN	TIME AXIS TYPE
XLIMITS 0., 100.	TIME AXIS LIMITS
XUNITS days	UNITS FOR TIME
XFACTOR 1.16E-5	CONVERSION FACTOR, SECONDS TO DAYS
***** WATER-MASS PLOT BLOCK *****	
YAXIS LIN	MASS AXIS TYPE
YLIMITS DEFAULT, DEFAULT	MASS AXIS LIMITS
XAXIS LIN	TIME AXIS TYPE
XLIMITS 0., 100.	TIME AXIS LIMITS
XUNITS days	UNITS FOR TIME
XFACTOR 1.16E-5	CONVERSION FACTOR, SECONDS TO DAYS

Figure 3.16: Concluded.

Transient-flow calculations offer many possibilities for error and numerical instability. The calculation is routinely rerun with different, and usually more accurate, parameters to determine if there is any change in the results. Adjusting the following parameters can influence the accuracy and stability of a calculation.

- 1) The timestep factor: decreasing this factor decreases the length of the timesteps and should lead to a more accurate solution (Section 4.2.6). However, this action causes longer run times.
- 2) The mesh: decreasing the mesh-point spacing (increasing the number of mesh points) allows the difference equations to approximate the differential equations more closely, and should lead to a more accurate solution (Section 4.2.9). This action also causes longer run times.
- 3) The implicitness factor: should be set between 0.5 and 1, with 0.5 the most accurate and 1 the most stable (Section 4.2.6). Larger implicitness factors can potentially cause inaccuracy, but typically reduce run times. Notice that in Figure 3.2 the implicitness factor is set to 0.6. When this calculation was made with an implicitness factor of 0.5, it was unstable.

Sections 4.2.6 and 4.2.9 contain more information about numerical stability.

The authors were confident of the accuracy of the results of this example problem and therefore attempted a less accurate solution method to determine whether the results would deteriorate significantly. Setting the implicitness factor to 1 and the timestep factor to 0.5 allows a faster solution—approximately three times as fast—and gives good agreement with the original calculation. Figure 3.17 shows the plot of pressure head versus elevation for the degraded calculation; compare this figure to the original results shown in Figure 3.8.

SECOND IMBIBITION CALCULATION Pressure Head of the Water

Figure 3.17: Pressure-head results for the imbibition-experiment simulation (with the implicitness factor set to 1 and the timestep factor set to 0.5).

3.2 Simulation of a Potential Waste Repository in Stratified Tuff

This section contains a description of one of the example problems discussed in *TOSPAC Volume 1: Physical and Mathematical Bases* (Dudley *et al.*, 1988). Although this problem involves a calculation representative of Yucca Mountain, it is only used as an example and is not meant to offer any conclusions as to the suitability of the site as a location for a high-level-radioactive-waste repository. This calculation is not acceptable for repository licensing activities.

This example problem demonstrates the capabilities of the STEADY module of TOSPAC to solve a highly nonlinear flow problem, and the TRANS module of TOSPAC to solve a complicated transport problem with multiple radioactive contaminants on this hydrologic background.

Briefly, the problem investigates placing a potential high-level-radioactive-waste repository in a partially saturated mountain with strata of fractured, welded and nonwelded tuffs. Figure 3.18 shows the physical layout of the mountain with the potential repository. Figure 3.19 shows how the problem is simplified for input into TOSPAC.

For this problem we assume that flow is in steady state downward through a one-dimensional, vertical column (a requirement of TOSPAC), at a constant percolation rate of 4 mm/yr. The flow media

Figure 3.18: Cross-section of Yucca Mountain showing the geologic stratigraphy and the location of the potential repository.

Figure 3.19: Simplification of the geometry and geology of Yucca Mountain for a TOSPAc calculation.

consist of five geologic units defined in a stratigraphy similar to that reported for drillhole USW G-4 at Yucca Mountain (Ortiz *et al.*, 1985):

- 1) Calico Hills unit, designated CHuz, predominantly composed of zeolitized, nonwelded ash-fall tuffs, extending from 0 m (the water table and lower boundary of the problem) to 129.5 m above the water table;
- 2) Topopah Spring unit, lower half, designated TSw2-3, composed of welded ash-flow tuffs with less than 10% by volume of vugs, extending from 129.5 to 335.2 m above the water table;
- 3) Topopah Spring unit, upper half, designated TSw1, composed of welded ash-flow tuffs with greater than 10% by volume of vugs, extending from 335.2 to 465.3 m above the water table;
- 4) Paintbrush unit, designated PTn, composed of nonwelded ash-fall tuffs, extending from 465.3 to 503.4 m above the water table;
- 5) Tiva Canyon unit, designated TCw, composed of welded ash-flow tuffs, extending from 503.4 to 530.4 m above the water table (nominally the ground surface; the upper boundary of the problem).

All five geologic units are fractured; the welded units are highly fractured. Material hydrologic properties, fracture porosities, and bulk-rock compressibilities can be found in Klavetter and Peters (1986) and in *Volume 1*. For this calculation, material properties are assumed to be uniform throughout each geologic unit.

Construction of a calculational mesh for this problem requires an understanding of the numerics, experience, and often a certain amount of trial and error. Mesh points must be placed close enough together so that little information is lost in going from the differential equations to the difference equations used in STEADY and TRANS. For example, a material should not go from full saturation to residual saturation between adjacent mesh points (although this situation may be unavoidable at a material interface).

This example problem uses 2303 mesh points. The mesh block in Figure 3.20 contains the definition of the mesh, and Figure 3.24 contains an illustration of the mesh. This number is more than necessary for an accurate steady-state solution, but in *Volume 1* the STEADY results were also to be used as the initial condition for DYNAMICS calculations. Hence, the mesh is structured as if for a transient problem. Equation 2.3-21 in Section 2.3 of *Volume 1* can be used to determine mesh-point spacing for a DYNAMICS problem in terms of the radii of curvature of the leading and trailing edges of a flux pulse. The equation is reproduced in Section 4.2.9 of this User's Guide. (Section 4.2.9 also contains bounding equations for STEADY and TRANS meshes.) In geologic unit TSw2-3, a flux pulse from 4 to 8 mm/yr has a radius of curvature of approximately 0.3 m at the leading edge; thus, the mesh points are spaced at 0.25 m throughout most of TSw2-3.

With this information, the mesh was constructed using the trial-and-error method, as follows. First, a mesh was constructed with uniformly spaced mesh points, and a steady-state solution was calculated. Then, the regions of the mesh were identified where the solution was unacceptable. The authors typically define "unacceptable" as a region where the calculated flux differs from the imposed flux by more than 10%. In general, mesh points must be finely spaced at the interfaces between geologic units and at asymptotic approaches to the characteristic solution. A new mesh was then constructed by placing mesh points closer together, by adding more mesh points, in the unacceptable regions. (Surprisingly, you may find that increasing the number of mesh points may occasionally make

the solution worse; increase or decrease the number of mesh points again and it should improve.) The solution was recalculated and this procedure was repeated as many times as necessary to achieve an acceptable solution.

Looking ahead, note that in the 4 mm/yr steady-state solution the pressure head is a constant in most of TSw2-3 (Figure 3.28). For a constant pressure head in a steady-state problem, the mesh points can be spaced very far apart. However, because steady-state problems are relatively easy to compute (in terms of computer time), reducing the mesh to two or three mesh points in the upper part of TSw2-3 would be more trouble than it is worth—first, because the solution would have to be known in advance, and second, because the upcoming transport calculation needs more mesh points (Section 4.2.9).

The boundary condition for the hydrology problem is a constant influx of 4 mm/yr (-1.27×10^{-9} m/s) at the top of the column, and a pressure head of 0 m (the water table) at the bottom of the column. The maximum pond at the top of the column is specified as 0 m, but this parameter does not play a part in the problem. This influx was chosen because it results in flow predominantly through the fractures of the welded tuffs.

Figure 3.20 shows the STEADY input-data file for the waste-repository problem. Notice that fractures are included in the definition of the geologic units and the fracture properties are given in entries 2, 4, 6, 8, and 10 in the material-property block. The fractures are defined as having the same hydrologic properties as sand. Because the fracture porosity is given in the geologic unit block, it is listed as 1 in the material-property block (Section 4.2.8).

Figure 3.21 shows the transport input-data file for this example problem. For the transport calculation, the source region is internal to the calculational mesh, at an elevation between 230 and 235 meters above the water table in unit TSw2-3. The potential repository is planned to cover an area of 1260 acres (5.1×10^6 m²) and to have 21,000 waste canisters implanted, containing 70,000 metric tons of heavy metal (MTHM). The canisters will cover approximately 0.15% of the area of the potential repository.

For this example problem, a source of seven species contained in five chains is defined:

Chain 1: ^{238}U .

Chain 2: ^{240}Pu , ^{236}U , ^{232}Th .

Chain 3: ^{14}C .

Chain 4: ^{99}Tc .

Chain 5: ^{129}I .

The source term used is a congruent-leach model. Congruent leach means that all the contaminants in the source are released at a rate proportional to the leach rate of the major contaminant, in this case, ^{238}U . The rationale behind using a congruent-leach model is that the contaminants are all embedded within the major contaminant, and thus can only be exposed to leaching as the major contaminant dissolves. The TRANS input-data file has a flag that allows choosing the congruent-leach source term, a solubility-limit source term, or a source term read from a file (Section 4.2.13). When a congruent-leach source term is chosen, the major contaminant is the first one specified in the contaminant-property block of the TRANS input-data file (Section 4.2.16). Properties of contaminants and transport-related properties of geologic units can be found in documents by the DOE (1986), Travis *et al.* (1985), and Daniels *et al.* (1982), as well as in *Volume 1*.

```

*****
*** TOSPAC HYDRO INPUT-DATA FILE ***
*****

***** TITLE BLOCK *****
YUCCA MOUNTAIN EXAMPLE PROBLEM

This example problem is based on the stratigraphy of drill hole USW-G4.
It assumes a steady-state percolation rate of 4 mm/yr.

***** CONSTANTS BLOCK *****
1000. kg/m**3      density of water
4.3E-6 /m          compressibility of water
5.1E+6 m**2        cross-sectional area of column
0.1                timestep factor
0.5                implicitness factor

***** GEOLOGIC-UNIT BLOCK *****
5                  # geologic units
unit # 1 ...name:
CHnz
0. m              min elevation
129.5 m           max elevation
1                 matrix material index
2                 fracture material index
4.6E-5            fracture porosity
2.6E-7 /m         bulk-rock compressibility
2.8E-8 /m         fracture compressibility
unit # 2 ...name:
TSw2-3
129.5 m           min elevation
335.2 m           max elevation
3                 matrix material index
4                 fracture material index
1.8E-5            fracture porosity
5.8E-7 /m         bulk-rock compressibility
12.E-8 /m         fracture compressibility
unit # 3 ...name:
TSw1
335.2 m           min elevation
465.3 m           max elevation
5                 matrix material index
6                 fracture material index
4.1E-5            fracture porosity
12.E-7 /m         bulk-rock compressibility
5.6E-8 /m         fracture compressibility
unit # 4 ...name:
PTn
465.3 m           min elevation
503.4 m           max elevation
7                 matrix material index
8                 fracture material index
2.7E-5            fracture porosity
82.E-7 /m         bulk-rock compressibility
19.E-8 /m         fracture compressibility
unit # 5 ...name:
TCw
503.4 m           min elevation
530.4 m           max elevation
9                 matrix material index
10                fracture material index
14.E-5            fracture porosity
6.2E-7 /m         bulk-rock compressibility
132.E-8 /m        fracture compressibility

***** MATERIAL-PROPERTY BLOCK *****
10                # materials
material # 1 ...name:
CHnz/G4-11 (Klavetter & Peters, SAND84-2642)
0.28              material effective porosity
1                 characteristic curve fit
1                 total saturation
0.11              residual saturation
0.00308 /m        alpha coefficient
1.602             beta coefficient
2.0E-11 m/s        saturated hydraulic conductivity
material # 2 ...name:
CHnz/G4-4F (Klavetter & Peters, SAND84-2942)
1                 material effective porosity

```

Figure 3.20: STEADY input-data file for the waste-repository simulation.


```

1          characteristic curve fit
1          total saturation
0.0395     residual saturation
1.2851 /m  alpha coefficient
4.23       beta coefficient
2.0E-5 m/s saturated hydraulic conductivity
material # 3 . . .name:
TSw2/G4-6 (Klavetter & Peters, SAND84-2642)
0.11       material effective porosity
1          characteristic curve fit
1          total saturation
0.080      residual saturation
0.00567 /m alpha coefficient
1.798      beta coefficient
1.9E-11 m/s saturated hydraulic conductivity
material # 4 . . .name:
TSw2/G4-2F (Klavetter & Peters, SAND84-2642)
1          material effective porosity
1          characteristic curve fit
1          total saturation
0.0395     residual saturation
1.2851 /m  alpha coefficient
4.23       beta coefficient
1.7E-5 m/s saturated hydraulic conductivity
material # 5 . . .name:
TSw1/G4-6 (Klavetter & Peters, SAND84-2642)
0.11       material effective porosity
1          characteristic curve fit
1          total saturation
0.080      residual saturation
0.00567 /m alpha coefficient
1.798      beta coefficient
1.9E-11 m/s saturated hydraulic conductivity
material # 6 . . .name:
TSw1/G4-2F (Klavetter & Peters, SAND84-2642)
1          material effective porosity
1          characteristic curve fit
1          total saturation
0.0395     residual saturation
1.2851 /m  alpha coefficient
4.23       beta coefficient
2.2E-5 m/s saturated hydraulic conductivity
material # 7 . . .name:
PTn/GU3-7 (Klavetter & Peters, SAND84-2642)
0.40       material effective porosity
1          characteristic curve fit
1          total saturation
0.1        residual saturation
0.015 /m  alpha coefficient
6.872     beta coefficient
3.9E-7 m/s saturated hydraulic conductivity
material # 8 . . .name:
PTn/G4-3F (Klavetter & Peters, SAND84-2642)
1          material effective porosity
1          characteristic curve fit
1          total saturation
0.0395     residual saturation
1.2851 /m  alpha coefficient
4.23       beta coefficient
6.1E-5 m/s saturated hydraulic conductivity
material # 9 . . .name:
TCw/G4-1 (Klavetter & Peters, SAND84-2642)
0.08       material effective porosity
1          characteristic curve fit
1          total saturation
0.002      residual saturation
0.00821 /m alpha coefficient
1.558      beta coefficient
9.7E-12 m/s saturated hydraulic conductivity
material # 10 . . .name:
TCw/G4-2F (Klavetter & Peters, SAND84-2642)
1          material effective porosity
1          characteristic curve fit
1          total saturation
0.0395     residual saturation
1.2851 /m  alpha coefficient
4.23       beta coefficient
3.8E-5 m/s saturated hydraulic conductivity

```

Figure 3.20: Continued.

```

***** MESH BLOCK *****
2302          total # cells
11           # submeshes
submesh # 1:
0. m         lower elevation
2. m         upper elevation
20           # cells
submesh # 2:
2. m         lower elevation
130. m       upper elevation
512          # cells
submesh # 3:
130. m       lower elevation
142. m       upper elevation
120          # cells
submesh # 4:
142. m       lower elevation
335. m       upper elevation
772          # cells
submesh # 5:
335. m       lower elevation
336. m       upper elevation
10           # cells
submesh # 6:
336. m       lower elevation
465. m       upper elevation
516          # cells
submesh # 7:
465. m       lower elevation
466. m       upper elevation
10           # cells
submesh # 8:
466. m       lower elevation
503. m       upper elevation
74           # cells
submesh # 9:
503. m       lower elevation
507. m       upper elevation
160          # cells
submesh # 10:
507. m       lower elevation
530. m       upper elevation
92           # cells
submesh # 11:
530. m       lower elevation
530.4 m      upper elevation
16           # cells

***** BOUNDARY-CONDITION BLOCK *****
1           # time snapshots
1           time conversion number
snapshot # 1
0. s        problem time
12          boundary-condition flag
0. m        lower-boundary pressure head
-1.27E-10 m/s upper-boundary flux
0. m        max pond height

***** FILE BLOCK *****
none        STEADY solution file
ex3steady.plt plot-data file
ex3steady.lis output-listing file
200        output-listing control

```

Figure 3.20: Concluded.

```

*****
***  TOSPAG TRANS INPUT-DATA FILE  ***
*****

***** TITLE BLOCK *****
YUCCA MOUNTAIN EXAMPLE PROBLEM

This example problem contains seven radionuclides in five decay chains:
(U-238) (Pu-240, U-236, Th-232) (C-14) (Tc-99) (I-129). It assumes
a 70,000 MTHM inventory uniformly distributed on 1260 acres, with waste
on 0.15 canister-failure time of 3,000 years.

***** SOURCE BLOCK *****
1          source-term flag
230. m     elevation of source lower boundary
235. m     elevation of source upper boundary
5.1E+6 m**2 area of repository
0.0015     fraction of repository area covered by contaminant

***** GEDLOGIC-UNIT BLOCK *****
5          # geologic units
unit # 1... name:
CHnz
1610. kg/m**3      bulk density
6. /m             fracture surface area per unit volume
0.33 m           fracture spacing
13. m            longitudinal matrix dispersivity
13. m            longitudinal fracture dispersivity
30. m            matrix velocity correlation length
10. m            fracture velocity correlation length
10.             matrix tortuosity
1.              fracture tortuosity
1.              matrix/fracture coupling factor
unit # 2... name:
TSw2-3
2300. kg/m**3      bulk density
80. /m            fracture surface area per unit volume
0.025 m          fracture spacing
21. m            longitudinal matrix dispersivity
21. m            longitudinal fracture dispersivity
30. m            matrix velocity correlation length
10. m            fracture velocity correlation length
10.             matrix tortuosity
1.              fracture tortuosity
1.              matrix/fracture coupling factor
unit # 3... name:
TSw1
2300. kg/m**3      bulk density
16. /m            fracture surface area per unit volume
0.13 m           fracture spacing
13. m            longitudinal matrix dispersivity
13. m            longitudinal fracture dispersivity
30. m            matrix velocity correlation length
10. m            fracture velocity correlation length
10.             matrix tortuosity
1.              fracture tortuosity
1.              matrix/fracture coupling factor
unit # 4... name:
PTn
1410. kg/m**3      bulk density
2. /m            fracture surface area per unit volume
1. m             fracture spacing
3.8 m            longitudinal matrix dispersivity
3.8 m            longitudinal fracture dispersivity
30. m            matrix velocity correlation length
10. m            fracture velocity correlation length
10.             matrix tortuosity
1.              fracture tortuosity
1.              matrix/fracture coupling factor
unit # 5... name:
TCw
2290. kg/m**3      bulk density
40. /m            fracture surface area per unit volume
0.05 m           fracture spacing
2.7 m            longitudinal matrix dispersivity
2.7 m            longitudinal fracture dispersivity
30. m            matrix velocity correlation length
10. m            fracture velocity correlation length
10.             matrix tortuosity
1.              fracture tortuosity
1.              matrix/fracture coupling factor

```

Figure 3.21: TRANS input-data file for the waste-repository simulation.

```

***** CONTAMINANT-PROPERTY BLOCK *****
5      # chains
1      # species for chain # 1
3      # species for chain # 2
1      # species for chain # 3
1      # species for chain # 4
1      # species for chain # 5
5      # geologic units (consistency check)
contaminant # 1 chain # 1 species # 1... name:
U-238
6.7E+7 kg      initial inventory
1.42E+17 s     half-life
3.33E-4 Ci/kg  activity
7000. Ci       release limit
5.0E-2 kg/m**3 solubility
1.E-9 m**2/s   diffusion coefficient
5.3E-3 m**3/kg matrix distribution coefficient for unit 1 (CHnz)
0. m           fracture distribution coefficient for unit 1 (CHnz)
1.8E-3 m**3/kg matrix distribution coefficient for unit 2 (TSw2-3)
0. m           fracture distribution coefficient for unit 2 (TSw2-3)
1.8E-3 m**3/kg matrix distribution coefficient for unit 3 (TSw1)
0. m           fracture distribution coefficient for unit 3 (TSw1)
5.3E-3 m**3/kg matrix distribution coefficient for unit 4 (PTn)
0. m           fracture distribution coefficient for unit 4 (PTn)
1.8E-3 m**3/kg matrix distribution coefficient for unit 5 (TCw)
0. m           fracture distribution coefficient for unit 5 (TCw)
contaminant # 2 chain # 2 species # 1... name:
Pu-240
1.4E+5 kg      initial inventory
2.08E+11 s     half-life
2.26E+2 Ci/kg  activity
7000. Ci       release limit
4.3E-4 kg/m**3 solubility
1.E-9 m**2/s   diffusion coefficient
1.4E-1 m**3/kg matrix distribution coefficient for unit 1 (CHnz)
0. m           fracture distribution coefficient for unit 1 (CHnz)
6.4E-2 m**3/kg matrix distribution coefficient for unit 2 (TSw2-3)
0. m           fracture distribution coefficient for unit 2 (TSw2-3)
6.4E-2 m**3/kg matrix distribution coefficient for unit 3 (TSw1)
0. m           fracture distribution coefficient for unit 3 (TSw1)
1.4E-1 m**3/kg matrix distribution coefficient for unit 4 (PTn)
0. m           fracture distribution coefficient for unit 4 (PTn)
6.4E-2 m**3/kg matrix distribution coefficient for unit 5 (TCw)
0. m           fracture distribution coefficient for unit 5 (TCw)
contaminant # 3 chain # 2 species # 2... name:
U-236
2.4E+5 kg      initial inventory
7.54E+14 s     half-life
6.34E-2 Ci/kg  activity
7000. Ci       release limit
5.0E-2 kg/m**3 solubility
1.E-9 m**2/s   diffusion coefficient
5.3E-3 m**3/kg matrix distribution coefficient for unit 1 (CHnz)
0. m           fracture distribution coefficient for unit 1 (CHnz)
1.8E-3 m**3/kg matrix distribution coefficient for unit 2 (TSw2-3)
0. m           fracture distribution coefficient for unit 2 (TSw2-3)
1.8E-3 m**3/kg matrix distribution coefficient for unit 3 (TSw1)
0. m           fracture distribution coefficient for unit 3 (TSw1)
5.3E-3 m**3/kg matrix distribution coefficient for unit 4 (PTn)
0. m           fracture distribution coefficient for unit 4 (PTn)
1.8E-3 m**3/kg matrix distribution coefficient for unit 5 (TCw)
0. m           fracture distribution coefficient for unit 5 (TCw)
contaminant # 4 chain # 2 species # 3... name:
Th-232
7.0E-2 kg      initial inventory
4.42E+17 s     half-life
1.10E-4 Ci/kg  activity
700. Ci        release limit
4.0E-4 kg/m**3 solubility
1.E-9 m**2/s   diffusion coefficient
5.0E-1 m**3/kg matrix distribution coefficient for unit 1 (CHnz)
0. m           fracture distribution coefficient for unit 1 (CHnz)
5.0E-1 m**3/kg matrix distribution coefficient for unit 2 (TSw2-3)
0. m           fracture distribution coefficient for unit 2 (TSw2-3)
5.0E-1 m**3/kg matrix distribution coefficient for unit 3 (TSw1)
0. m           fracture distribution coefficient for unit 3 (TSw1)
5.0E-1 m**3/kg matrix distribution coefficient for unit 4 (PTn)
0. m           fracture distribution coefficient for unit 4 (PTn)

```

Figure 3.21: Continued.

```

5.0E-1 m**3/kg      matrix distribution coefficient for unit 5 (TCw)
0. m                fracture distribution coefficient for unit 5 (TCw)
contaminant # 5 chain # 3 species # 1... name:
C-14
13. kg              initial inventory
1.81E+11 s          half-life
4.45E+3 Ci/kg       activity
7000. Ci            release limit
14. kg/m**3         solubility
1.E-9 m**2/s        diffusion coefficient
0. m**3/kg          matrix distribution coefficient for unit 1 (CHnz)
0. m                fracture distribution coefficient for unit 1 (CHnz)
0. m**3/kg          matrix distribution coefficient for unit 2 (TSw2-3)
0. m                fracture distribution coefficient for unit 2 (TSw2-3)
0. m**3/kg          matrix distribution coefficient for unit 3 (TSw1)
0. m                fracture distribution coefficient for unit 3 (TSw1)
0. m**3/kg          matrix distribution coefficient for unit 4 (PTn)
0. m                fracture distribution coefficient for unit 4 (PTn)
0. m**3/kg          matrix distribution coefficient for unit 5 (TCw)
0. m                fracture distribution coefficient for unit 5 (TCw)
contaminant # 6 chain # 4 species # 1... name:
Tc-99
5.4E+4 kg           initial inventory
6.78E+12 s          half-life
1.70E+1 Ci/kg       activity
700000. Ci          release limit
99. kg/m**3         solubility
1.E-9 m**2/s        diffusion coefficient
0. m**3/kg          matrix distribution coefficient for unit 1 (CHnz)
0. m                fracture distribution coefficient for unit 1 (CHnz)
3.0E-4 m**3/kg      matrix distribution coefficient for unit 2 (TSw2-3)
0. m                fracture distribution coefficient for unit 2 (TSw2-3)
3.0E-4 m**3/kg      matrix distribution coefficient for unit 3 (TSw1)
0. m                fracture distribution coefficient for unit 3 (TSw1)
0. m**3/kg          matrix distribution coefficient for unit 4 (PTn)
0. m                fracture distribution coefficient for unit 4 (PTn)
3.0E-4 m**3/kg      matrix distribution coefficient for unit 5 (TCw)
0. m                fracture distribution coefficient for unit 5 (TCw)
contaminant # 7 chain # 5 species # 1... name:
I-129
1.3E+4 kg           initial inventory
5.02E+14 s          half-life
1.74E-1 Ci/kg       activity
7000. Ci            release limit
130. kg/m**3        solubility
1.E-9 m**2/s        diffusion coefficient
0. m**3/kg          matrix distribution coefficient for unit 1 (CHnz)
0. m                fracture distribution coefficient for unit 1 (CHnz)
0. m**3/kg          matrix distribution coefficient for unit 2 (TSw2-3)
0. m                fracture distribution coefficient for unit 2 (TSw2-3)
0. m**3/kg          matrix distribution coefficient for unit 3 (TSw1)
0. m                fracture distribution coefficient for unit 3 (TSw1)
0. m**3/kg          matrix distribution coefficient for unit 4 (PTn)
0. m                fracture distribution coefficient for unit 4 (PTn)
0. m**3/kg          matrix distribution coefficient for unit 5 (TCw)
0. m                fracture distribution coefficient for unit 5 (TCw)

***** BOUNDARY-CONDITION BLOCK *****
29                  # time snapshots
4                   time conversion number
7                   # contaminants (consistency check)
snapshot # 1
0. yr              problem time
12                 boundary-condition flag
0. kg/m**3         contaminant # 1 lower-boundary matrix conc
0. kg/m**3         contaminant # 1 lower-boundary fracture conc
0. kg/m**2/s       contaminant # 1 upper-boundary matrix conc-flux
0. kg/m**2/s       contaminant # 1 upper-boundary fracture conc-flux
0. kg/m**3         contaminant # 2 lower-boundary matrix conc
0. kg/m**3         contaminant # 2 lower-boundary fracture conc
0. kg/m**2/s       contaminant # 2 upper-boundary matrix conc-flux
0. kg/m**2/s       contaminant # 2 upper-boundary fracture conc-flux
0. kg/m**3         contaminant # 3 lower-boundary matrix conc
0. kg/m**3         contaminant # 3 lower-boundary fracture conc
0. kg/m**2/s       contaminant # 3 upper-boundary matrix conc-flux
0. kg/m**2/s       contaminant # 3 upper-boundary fracture conc-flux

```

Figure 3.21: Continued.

0. kg/m**3	contaminant # 4 lower-boundary matrix conc
0. kg/m**3	contaminant # 4 lower-boundary fracture conc
0. kg/m**2/s	contaminant # 4 upper-boundary matrix conc-flux
0. kg/m**2/s	contaminant # 4 upper-boundary fracture conc-flux
0. kg/m**3	contaminant # 5 lower-boundary matrix conc
0. kg/m**3	contaminant # 5 lower-boundary fracture conc
0. kg/m**2/s	contaminant # 5 upper-boundary matrix conc-flux
0. kg/m**2/s	contaminant # 5 upper-boundary fracture conc-flux
0. kg/m**3	contaminant # 6 lower-boundary matrix conc
0. kg/m**3	contaminant # 6 lower-boundary fracture conc
0. kg/m**2/s	contaminant # 6 upper-boundary matrix conc-flux
0. kg/m**2/s	contaminant # 6 upper-boundary fracture conc-flux
0. kg/m**3	contaminant # 7 lower-boundary matrix conc
0. kg/m**2/s	contaminant # 7 lower-boundary fracture conc
0. kg/m**2/s	contaminant # 7 upper-boundary matrix conc-flux
0. kg/m**2/s	contaminant # 7 upper-boundary fracture conc-flux
snapshot # 2	
1000. yr	problem time
00	boundary-condition flag
snapshot # 3	
2000. yr	problem time
00	boundary-condition flag
snapshot # 4	
3000. yr	problem time
00	boundary-condition flag
snapshot # 5	
4000. yr	problem time
00	boundary-condition flag
snapshot # 6	
5000. yr	problem time
00	boundary-condition flag
snapshot # 7	
6000. yr	problem time
00	boundary-condition flag
snapshot # 8	
7000. yr	problem time
00	boundary-condition flag
snapshot # 9	
8000. yr	problem time
00	boundary-condition flag
snapshot # 10	
9000. yr	problem time
00	boundary-condition flag
snapshot # 11	
10000. yr	problem time
00	boundary-condition flag
snapshot # 12	
15000. yr	problem time
00	boundary-condition flag
snapshot # 13	
20000. yr	problem time
00	boundary-condition flag
snapshot # 14	
25000. yr	problem time
00	boundary-condition flag
snapshot # 15	
30000. yr	problem time
00	boundary-condition flag
snapshot # 16	
35000. yr	problem time
00	boundary-condition flag
snapshot # 17	
40000. yr	problem time
00	boundary-condition flag
snapshot # 18	
45000. yr	problem time
00	boundary-condition flag
snapshot # 19	
50000. yr	problem time
00	boundary-condition flag
snapshot # 20	
55000. yr	problem time
00	boundary-condition flag
snapshot # 21	
60000. yr	problem time
00	boundary-condition flag
snapshot # 22	
65000. yr	problem time
00	boundary-condition flag

Figure 3.21: Continued.

```
snapshot # 23
70000. yr      problem time
00            boundary-condition flag
snapshot # 24
75000. yr      problem time
00            boundary-condition flag
snapshot # 25
80000. yr      problem time
00            boundary-condition flag
snapshot # 26
85000. yr      problem time
00            boundary-condition flag
snapshot # 27
90000. yr      problem time
00            boundary-condition flag
snapshot # 28
95000. yr      problem time
00            boundary-condition flag
snapshot # 29
100000. yr     problem time

***** FILE BLOCK *****
ex3steady.plt  STEADY plot-data file
ex3trans.plt   TRANS plot-data file
ex3trans.lis   output-listing file
200            output-listing control
```

Figure 3.21: Concluded.

The boundary conditions are the same for each contaminant. At the top of the column there is zero flux in both the matrix and the fractures; i.e., no contaminant can cross the top boundary. At the bottom of the column there is zero concentration in both the matrix and the fractures. The zero-concentration boundary implies that any contaminant reaching the bottom boundary is immediately and totally ejected from the mesh, diffusing into the large body of water below the water table. TOSPAC allows specification of both matrix and fracture boundary conditions in order to handle problems where, for example, a contaminant is injected only into a fracture at the top boundary.

The initial condition for each contaminant is zero concentration everywhere. This state is the default initial condition and therefore does not appear as a data block in the transport input-data file.

Section 4.2 contains a more complete discussion of the formats and data requirements for the hydrology and transport input-data files.

Once the input-data files are created, the calculation proceeds as in Chapter 2. TOSPAC is executed and within the TOSPAC SHELL, first STEADY, and then TRANS is executed. On a DEC VAX 8700 computer, STEADY execution takes approximately one minute of computer processor time; the TRANS run takes approximately 40 minutes of computer processor time.

Storage requirements for the output files may be of importance to the user. For the hydrology calculation, the STEADY output-listing file is approximately 340 kilobytes long when results for all mesh points are printed, and the STEADY plot-data file is approximately 400 kilobytes long. For the transport calculation, the TRANS output-listing file is approximately 16 megabytes long when results for all mesh points are printed, and the TRANS plot-data file is 8 megabytes long. The extreme length of the transport files is caused by the large number of mesh points and the number of contaminants. While the output-listing file can be shortened (in the file block for the TRANS input-data file only concentrations at every 200th mesh cell are to be printed out at each time snapshot), the concentration for each contaminant at every mesh point is recorded in the plot-data file to avoid missing potentially significant behavior. Using a mesh with fewer points, more tailored to this problem, would reduce the size of these files.

Figure 3.22 presents a portion of the STEADY output-listing file, showing the second half of the file containing the results of the example computation. Section 4.7.3 contains a discussion of the format of a STEADY output-listing file. The first lines show the boundary conditions. The next line tells us that a total of 354 iterations was performed. Actually, because STEADY solves the problem in piecemeal fashion, this figure is not iterations of the complete mesh; rather, it is iterations of mesh segments of at most 120 mesh points. The second line states that the worst deviation from the correct steady-state flux is only 1.4%, and it occurs at mesh point 2133, corresponding to an elevation of 505.45 m.

The final values of various calculated quantities (pressure head, flux, hydraulic conductivity, etc.) are given next. These values are given for every 200th mesh cell, a user-specified option in the file block of the input-data file. Following this group of results is another collection of calculated quantities (saturation, average linear velocity, etc.) in columns.

The final section of a STEADY output-listing file gives travel-time information for the entire column. The equations used to calculate travel time for steady-state flow are given in Section 2.2.1 of *Volume 1*. A discussion of travel time for this example is given below in the description of Figure 3.35.

A portion of the TRANS output-listing file is presented in Figure 3.23. Section 4.7.10 contains a discussion of the format of this file. The first block shown contains the hydrologic data used by TRANS. Every 200th mesh cell is reported, as well as the mesh points that border the source region

STEADY STATE REACHED AT ITERATION NUMBER 359.
 MAX FLUX DEVIATION= 1.5540 % AT MESH POINT=2112 ELEVATION= 504.92

FINAL CONDITIONS OF MESH

AVERAGE COLUMN SATURATION = 0.998484
 TOTAL VOID VOLUME = 4.623396E+08
 TOTAL WATER VOLUME = 4.619679E+08
 TOTAL AIR VOLUME = 371703
 TOTAL WATER MASS = 4.619679E+11

BOUNDARY CONDITIONS: FLAG = 12
 FLUX = -1.27000E-10
 BOTTOM PRESSURE HEAD = 0.00000E+00

J	UNIT	MAT	FRK	Z	PRES HEAD	%DEVIATION	FLUX	FLXMAT	FLXFRK	HY
2303	5	9	10	530.4	-1.012	0.0000E+00	-1.2700E-10	-8.4059E-12	-1.1859E-10	1.2628E-10
2200	5	9	10	508.3	-1.013	0.4189	-1.2647E-10	-8.4056E-12	-1.1806E-10	1.2646E-10
2051	4	7	8	503.4	-38.82	1.6283E-02	-1.2702E-10	-1.2702E-10	-3.0758E-29	3.5477E-07
2000	4	7	8	485.5	-20.98	1.7043E-02	-1.2698E-10	-1.2698E-10	-1.2241E-26	3.8905E-07
1954	3	5	6	485.3	-0.7888	1.6719E-02	-1.2698E-10	-7.2563E-11	-5.4416E-11	1.2700E-10
1800	3	5	6	427.3	-0.7888	1.9957E-02	-1.2703E-10	-1.8496E-11	-1.0853E-10	1.2703E-10
1600	3	5	6	377.3	-0.7888	1.9957E-02	-1.2703E-10	-1.8496E-11	-1.0853E-10	1.2703E-10
1427	2	3	4	335.2	-0.9522	6.1836E-05	-1.2700E-10	-2.1688E-11	-1.0531E-10	1.2699E-10
1400	2	3	4	328.8	-0.9522	1.8155E-02	-1.2698E-10	-1.8412E-11	-1.0857E-10	1.2698E-10
1200	2	3	4	278.8	-0.9522	1.8155E-02	-1.2698E-10	-1.8412E-11	-1.0857E-10	1.2698E-10
1000	2	3	4	228.8	-0.9522	1.8155E-02	-1.2698E-10	-1.8412E-11	-1.0857E-10	1.2698E-10
800	2	3	4	178.8	-0.9522	1.8155E-02	-1.2698E-10	-1.8412E-11	-1.0857E-10	1.2698E-10
600	2	3	4	136.7	-0.9522	1.8155E-02	-1.2698E-10	-1.8412E-11	-1.0857E-10	1.2698E-10
531	1	1	2	129.5	-1.096	1.7072E-03	-1.2700E-10	-2.0941E-11	-1.0606E-10	1.2700E-10
400	1	1	2	66.75	-1.096	4.8344E-03	-1.2701E-10	-1.8720E-11	-1.0829E-10	1.2701E-10
200	1	1	2	46.75	-1.096	4.8344E-03	-1.2701E-10	-1.8720E-11	-1.0829E-10	1.2701E-10
1	1	1	2	0.0000E+00	0.0000E+00	0.0000E+00	-1.2700E-10	-2.7374E-13	-1.2673E-10	9.2200E-09

J	UNIT	MAT	FRK	SAT	DSAT	SATMAT	SATFRK	VEL	VELMAT	VELFRK
2303	5	9	10	0.9997	4.2653E-04	0.9998	0.3699	-1.5903E-09	-1.0532E-10	-2.5638E-06
2200	5	9	10	0.9997	4.2648E-04	0.9998	0.3694	-1.5837E-09	-1.0532E-10	-2.5659E-06
2051	4	7	8	0.9815	3.1929E-03	0.9815	3.9603E-02	-4.4831E-10	-4.4831E-10	-1.7788E-19
2000	4	7	8	0.9997	8.9276E-05	0.9997	3.9523E-02	-3.5283E-10	-3.5283E-10	-1.9704E-17
1954	3	5	6	1.000	1.0330E-04	1.000	0.5928	-7.6534E-10	-4.3741E-10	-2.7200E-06
1800	3	5	6	1.000	1.0330E-04	1.000	0.5929	-1.2550E-09	-1.8277E-10	-4.7336E-06
1600	3	5	6	1.000	1.0330E-04	1.000	0.5929	-1.2550E-09	-1.8277E-10	-4.7336E-06
1427	2	3	4	0.9999	2.2796E-04	1.000	0.4212	-1.2545E-09	-2.1435E-10	-1.8880E-06
1400	2	3	4	0.9999	2.2796E-04	1.000	0.4211	-1.2541E-09	-1.8197E-10	-1.5803E-06
1200	2	3	4	0.9999	2.2796E-04	1.000	0.4211	-1.2541E-09	-1.8197E-10	-1.5803E-06
1000	2	3	4	0.9999	2.2796E-04	1.000	0.4211	-1.2541E-09	-1.8197E-10	-1.5803E-06
800	2	3	4	0.9999	2.2796E-04	1.000	0.4211	-1.2541E-09	-1.8197E-10	-1.5803E-06
600	2	3	4	0.9999	2.2796E-04	1.000	0.4211	-1.2541E-09	-1.8197E-10	-1.5803E-06
531	1	1	2	0.9999	8.3348E-05	1.000	0.3101	-5.9850E-10	-9.8695E-11	-4.5184E-06
400	1	1	2	0.9999	8.3348E-05	1.000	0.3101	-5.0967E-10	-7.5125E-11	-8.6985E-06
200	1	1	2	0.9999	8.3348E-05	1.000	0.3101	-5.0967E-10	-7.5125E-11	-8.6985E-06
1	1	1	2	1.000	0.0000E+00	1.000	1.000	-5.0956E-10	-1.0985E-12	-2.8684E-06

***** GROUNDWATER TRAVEL TIME *****

START POSITION = 530.40
 END POSITION = 0.00000E+00

AVERAGE FASTEST PARTICLE = 0.10862382E+12 SEC
 COMPOSITE = 0.64642981E+12 SEC
 MATRIX = 0.39362112E+13 SEC (99.87% OF RANGE)
 FRACTURES = 0.18241286E+09 SEC (92.58% OF RANGE)

CALCULATIONAL CUTOFF USED TO DETERMINE SIGNIFICANT FLOW = 0.10000E-04

Figure 3.22: Part of the STEADY output-listing file for the waste-repository simulation.

(mesh cells 1004 and 1024), and the cells at the unit boundaries (mesh cells 1, 530, 1426, 1953, 2050, and 2302). The second block of data reports the transport coefficients used by TRANS for each contaminant (only the first contaminant is shown).

After the vertical ellipsis (used to denote the omission of several fields of data), the results are shown for snapshot 15, occurring at timestep 573, at a time of 9.46728×10^{11} s or 30,000 yr. The timestep length is 1.11132×10^9 s, or approximately 35 yr, between timestep 572 and 573. Shown first are the concentrations in the matrix and fractures for every contaminant. Every 200th mesh cell is shown, mesh cells at the boundaries, the geologic-unit interfaces, and the boundaries of the source region.

Next, data related to the mass conservation in the computation are shown for timestep 573. Mass conservation (also called mass balance) is a measure of the accuracy of the calculation. Of most interest is the final column, showing the percent difference between the mass actually in the problem and the mass that should be in the problem. For ^{238}U and ^{236}U the difference is negligible; for ^{232}Th , ^{14}C , ^{129}I , and ^{99}Tc , the difference is approximately 1%; for ^{240}Pu , the difference is 1.62. Negative values indicate that mass has been lost in the calculation; positive values indicate that mass has been created. The other columns in this block tell where the mass is located; e.g., in the matrix or fracture water, in the source region, adsorbed to the surface of the porous media, etc.

The final group of results is the amount of mass released from the problem domain by timestep 573. The release values are positive: positive values indicate that the contaminant has left the column; negative values indicate that the contaminant has entered the column. Cumulative release is the amount that crosses the boundary—decay is not considered once it is outside the mesh; total release is the actual amount outside the boundary, considering decay. The results show no activity at the upper boundary. For the lower boundary, ^{240}Pu shows no release, but the other contaminants show varying releases; more than 4 kg of both ^{99}Tc and ^{129}I are released. There is more ^{232}Th outside the mesh than crossed the boundary because ^{236}U continued to decay into ^{232}Th outside the mesh.

Figures 3.24 through 3.46 show plots constructed by the TOSPAC OUTPLOT module and are examples of some specific capabilities of OUTPLOT. These plots are not the same set as those presented in *Volume 1*, although there is some duplication. Sections 4.6.3 through 4.6.5 also contains references to these plots. Rather than repeat the discussion given in *Volume 1*, we concentrate on issues of importance to the user: interpretation of the plots and determining correctness of the solution.

The STEADY plots are presented in the order given in the OUTPLOT (STEADY RESULTS) menu. Section 4.6.3 contains a discussion of the STEADY plots available from OUTPLOT, and the following plots are cross-referenced there.

Figure 3.24 presents the mesh/stratigraphy plot. This plot shows the layout of the mesh and the geologic units with respect to elevation. The mesh is shown as a column of rectangles. Each rectangle represents ten mesh points (a user-specified option—with 2303 mesh points, if each rectangle represented a single mesh point, the area would be solid black). Notice that in regions where mesh points are closely spaced the rectangles are thinner. To the left of the mesh the mesh points are numbered by hundreds (a user-specified option). To the right of the mesh are larger rectangles representing geologic units. The unit number, name, and the names of the matrix and fracture materials are given within the appropriate rectangle. The elevation is given to the right of each unit interface. This plot should be compared with the conceptual model given in Figure 3.19.

The characteristic curves for the fracture material used in the TSw2-3 geologic unit is presented in Figure 3.25. These plots can be useful as a check on the input data.

HYDROLOGIC QUANTITIES:

MESH CELL	UNIT #	ELEV	MATRIX MOISTURE	FRACTURE MOISTURE	MATRIX VELOCITY	FRACTURE VELOCITY	ADVECTIVE COUPLING
2302	5	530.4	7.9972E-02	5.1787E-05	-1.0511E-10	-2.2900E-06	-4.5065E-14
2200	5	508.4	7.9972E-02	5.1725E-05	-1.0511E-10	-2.2829E-06	-1.0043E-16
2050	4	503.4	0.3926	1.0666E-06	-3.2352E-10	-2.4893E-23	3.3654E-28
2000	4	485.8	0.3999	1.0671E-06	-3.1756E-10	-1.0101E-20	-4.5050E-27
1953	3	465.3	0.1100	2.4307E-05	-1.6810E-10	-4.4633E-06	-1.0814E-09
1800	3	427.4	0.1100	2.4307E-05	-1.6815E-10	-4.4649E-06	0.0000E+00
1600	3	377.4	0.1100	2.4307E-05	-1.6815E-10	-4.4649E-06	0.0000E+00
1426	2	335.2	0.1100	7.5808E-05	-1.6744E-10	-1.4324E-06	-8.5472E-11
1400	2	328.9	0.1100	7.5807E-05	-1.6742E-10	-1.4321E-06	0.0000E+00
1200	2	278.9	0.1100	7.5807E-05	-1.6742E-10	-1.4321E-06	0.0000E+00
1024	2	234.9	0.1100	7.5807E-05	-1.6742E-10	-1.4321E-06	0.0000E+00
1004	2	229.9	0.1100	7.5807E-05	-1.6742E-10	-1.4321E-06	0.0000E+00
1000	2	228.9	0.1100	7.5807E-05	-1.6742E-10	-1.4321E-06	0.0000E+00
800	2	178.9	0.1100	7.5807E-05	-1.6742E-10	-1.4321E-06	0.0000E+00
600	2	136.8	0.1100	7.5807E-05	-1.6742E-10	-1.4321E-06	0.0000E+00
530	1	129.4	0.2800	1.4266E-05	-6.6859E-11	-7.5902E-06	-1.7758E-11
400	1	96.88	0.2800	1.4266E-05	-6.6861E-11	-7.5906E-06	0.0000E+00
200	1	46.88	0.2800	1.4266E-05	-6.6861E-11	-7.5906E-06	0.0000E+00
1	1	5.0000E-02	0.2800	4.5997E-05	-9.7768E-13	-2.7551E-06	-1.5406E-15

TRANSPORT COEFFICIENTS FOR SPECIES 1 OF DECAY CHAIN 1: U-238

MESH CELL	UNIT #	ELEV	MATRIX RETARD	FRACTURE RETARD	MATRIX DISPERSN	FRACTURE DISPERSN	DISPERSIVE COUPLING
2302	5	530.4	52.54	1.000	1.0000E-10	1.0000E-09	1.2796E-08
2200	5	508.4	52.54	1.000	1.0000E-10	1.0000E-09	1.2796E-08
2050	4	503.4	20.03	1.000	1.0000E-10	1.0000E-09	1.5705E-10
2000	4	485.8	19.69	1.000	1.0000E-10	1.0000E-09	1.5995E-10
1953	3	465.3	38.64	1.000	1.0000E-10	1.0000E-09	2.6034E-09

o
o
o

TIME STEP	0	TIME 0.00000E+00	DELTA TIME 0.00000E+00
BOUNDARY CONDITIONS:	FLAG = 12	SNAPSHOT 1	
1 U-238	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
2 Pu-240	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
3 U-238	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
4 Th-232	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
5 C-14	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
6 Ic-99	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
7 I-129	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00

o
o
o

TIME STEP	576	TIME 9.46728E+11	DELTA TIME 1.11132E+09
BOUNDARY CONDITIONS:	FLAG = 12	SNAPSHOT 15	
1 U-238	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
2 Pu-240	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
3 U-238	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
4 Th-232	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
5 C-14	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
6 Ic-99	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00
7 I-129	BOTTOM: MAT CONC=	0.0000E+00	FRAC CONC= 0.0000E+00

MESH CELL	UNIT #	ELEV	U-238		Pu-240		U-236		Th-232	
			MATRIX CONC	FRACTURE CONC	MATRIX CONC	FRACTURE CONC	MATRIX CONC	FRACTURE CONC	MATRIX CONC	FRACTURE CONC
2302	5	530.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2200	5	508.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2050	4	503.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2000	4	485.8	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1953	3	465.3	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1800	3	427.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1600	3	377.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1426	2	335.2	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1400	2	328.9	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1200	2	278.9	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1024	2	234.9	2.2960E-05	2.2975E-05	4.8944E-10	4.9066E-10	1.3242E-07	1.3250E-07	2.9779E-12	3.0607E-12
1004	2	230.1	5.9632E-05	5.9631E-05	5.3148E-10	5.3251E-10	3.4338E-07	3.4337E-07	2.6573E-12	2.7129E-12
1000	2	228.9	5.7507E-05	5.7508E-05	3.0173E-10	3.0260E-10	3.3088E-07	3.3088E-07	3.5137E-13	3.6266E-13

Figure 3.23: Part of the TRANS output-listing file for the waste-repository simulation.

800	2	178.9	8.7849E-06	8.7862E-06	2.6944E-31	3.0724E-31	4.6114E-08	4.6122E-08	3.3068E-14	3.3077E-14
600	2	136.8	5.0363E-07	5.0379E-07	0.0000E+00	0.0000E+00	2.4440E-09	2.4448E-09	9.9042E-16	9.9085E-16
530	1	129.4	2.5681E-07	2.6646E-07	0.0000E+00	0.0000E+00	1.2305E-09	1.2777E-09	1.0172E-15	7.1411E-16
400	1	96.88	3.9857E-10	4.3566E-10	0.0000E+00	0.0000E+00	1.7722E-12	1.9397E-12	1.1348E-18	1.2553E-18
200	1	46.88	8.5561E-16	1.0067E-15	0.0000E+00	0.0000E+00	3.5783E-18	4.2141E-18	1.3651E-24	1.6225E-24
1	1	5.0000E-02	8.5037E-24	1.0521E-23	0.0000E+00	0.0000E+00	3.4526E-26	4.2748E-26	1.7413E-36	2.0466E-33

MESH CELL	UNIT #	ELEV	C-14		Tc-99		I-129	
			MATRIX CONC	FRACTURE CONC	MATRIX CONC	FRACTURE CONC	MATRIX CONC	FRACTURE CONC
2302	5	530.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2200	5	508.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2050	4	503.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2000	4	485.8	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1953	3	465.3	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1800	3	427.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1600	3	377.4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1426	2	335.2	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1400	2	328.9	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1200	2	278.9	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1024	2	234.9	1.3239E-13	1.3248E-13	1.8850E-08	1.8862E-08	5.0356E-09	5.0388E-09
1005	2	230.1	3.8075E-13	3.8074E-13	5.4033E-08	5.4032E-08	1.4533E-08	1.4532E-08
1000	2	228.9	3.8039E-13	3.8039E-13	5.3911E-08	5.3911E-08	1.4532E-08	1.4532E-08
800	2	178.9	3.7974E-13	3.7974E-13	4.7845E-08	4.7845E-08	1.4531E-08	1.4531E-08
600	2	136.8	3.7966E-13	3.7966E-13	4.0906E-08	4.0906E-08	1.4527E-08	1.4527E-08
530	1	129.4	3.7963E-13	3.7963E-13	4.0255E-08	4.0275E-08	1.4526E-08	1.4526E-08
400	1	96.88	3.7900E-13	3.7900E-13	3.6768E-08	3.6779E-08	1.4499E-08	1.4499E-08
200	1	46.88	3.6543E-13	3.6643E-13	3.0253E-08	3.0265E-08	1.4011E-08	1.4011E-08
1	1	5.0000E-02	1.4612E-15	1.3953E-15	1.0928E-10	1.0441E-10	5.5848E-11	5.3327E-11

MASS CONSERVATION			TIME STEP	573	TIME 9.46728E+11							
CHAIN #	SPECIES # NAME		MATRIX MASS	FRACTURE MASS	ADSORBED MASS	PRECIP MASS	SOURCE MASS	T BDY MASS	B BDY MASS	MASS IN MESH + MASS RELEASED	MASS INJECTED INTO MESH	PERCENT DIFF
1	1	U-238	1.07E+03	7.37E-01	4.03E+04	0.00E+00	6.70E+07	0.00E+00	-5.07E-14	4.14E+04	4.14E+04	-7.70E-04
2	1	Pu-240	2.71E-03	1.87E-06	3.63E+00	0.00E+00	5.97E+03	0.00E+00	0.00E+00	3.63E+00	3.69E+00	-1.62E+00
2	2	U-236	5.98E+00	4.11E-03	2.25E+02	0.00E+00	3.74E+05	0.00E+00	-2.05E-16	2.31E+02	2.31E+02	2.47E-02
2	3	Th-232	1.75E-05	1.22E-08	1.82E-01	0.00E+00	2.94E+02	0.00E+00	-3.90E-21	1.82E-01	1.81E-01	5.72E-01
3	1	C-14	8.51E-05	1.86E-08	0.00E+00	0.00E+00	3.46E-01	0.00E+00	-1.26E-04	2.11E-04	2.14E-04	-1.19E+00
4	1	Tc-99	8.45E+00	2.22E-03	1.76E+01	0.00E+00	4.90E+04	0.00E+00	-4.11E+00	3.02E+01	3.03E+01	-3.27E-01
5	1	I-129	3.26E+00	7.10E-04	0.00E+00	0.00E+00	1.30E+04	0.00E+00	-4.69E+00	7.94E+00	8.02E+00	-9.66E-01

MASS RELEASE			TOP TOTAL	TOP CUMULATIVE	BOTTOM TOTAL	BOTTOM CUMULATIVE
1	1	U-238	0.00E+00	0.00E+00	5.07E-14	5.07E-14
2	1	Pu-240	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2	2	U-236	0.00E+00	0.00E+00	2.05E-16	2.05E-16
2	3	Th-232	0.00E+00	0.00E+00	3.90E-21	0.00E+00
3	1	C-14	0.00E+00	0.00E+00	1.26E-04	4.52E-04
4	1	Tc-99	0.00E+00	0.00E+00	4.11E+00	4.18E+00
5	1	I-129	0.00E+00	0.00E+00	4.69E+00	4.69E+00

o
o
o

Figure 3.23: Concluded.

YUCCA MOUNTAIN EXAMPLE PROBLEM Calculational Mesh

Figure 3.24: Mesh/stratigraphy plot for the waste-repository simulation.

Figure 3.25: Characteristic curves for the fracture material used for unit TSw2-3 in the waste-repository simulation.

To solve a flow problem, TOSPAC uses a composite of the matrix and fracture characteristic curves. The curve of composite hydraulic conductivity versus pressure head for one of the geologic units is presented in Figure 3.26. Composite means the area-weighted average of the matrix and fractures. The plot shows both the characteristic curve for the matrix material and the curve for the fracture material, along with the curve for the composite material.

The curve of composite capacitance versus pressure head for TSw2-3 is presented in Figure 3.27. As with the hydraulic-conductivity plot, the capacitance plot shows both the characteristic curve for the matrix material and the curve for the fracture material, along with the curve for the composite material. Capacitance is not used in a steady-state calculation, as explained in Section 2.2 of *Volume 1*. This plot is included to illustrate capacitance in a geologic unit that has both matrix and fractures; Figure 3.7 illustrates this plot for a geologic unit that is not fractured.

The plots of composite hydraulic conductivity and composite capacitance can be used to interpret results (the capacitance plot is only of use in interpreting transient-flow calculations). STEADY and DYNAMICS solve for pressure head. The user can take the pressure head returned by these modules and determine where on the conductivity and capacitance curves the modules were working. If it is a nonlinear region of the curve, TOSPAC will be less efficient, will require more iterations (and for DYNAMICS, smaller timesteps), and may require a finer mesh-point spacing.

Figure 3.28 shows the plot of pressure head versus elevation for the example problem. Pressure head is the unknown variable in the difference equations in STEADY. Pressure head is calculated using Darcy's law and, in a partially saturated regime, the hydraulic conductivity is dependent on pressure head. Note that the pressure head is approximately -1 m for most of the mesh. From Figure 3.26 it can be seen that -1 m corresponds to a composite hydraulic conductivity of approximately 4 mm/yr (the same as the imposed flux), and that the composite-conductivity curve is very steep in this region. Looking again at Figure 3.27, -1 m corresponds to a capacitance coefficient of approximately $2 \times 10^{-4} \text{ m}^{-1}$, and this value is near a local maximum in a highly nonlinear part of the curve.

Figure 3.29 presents the saturation in the matrix, the fractures, and the composite material versus elevation. For this problem, the matrix-saturation curve appears identical to the composite-saturation curve. The fractures constitute less than 0.01% of the area of the rock; their contribution to the composite saturation is negligible at this scale.

At 4 mm/yr infiltration, the matrix and the composite material of the column appear almost completely saturated. Only near the TCw/P'Tn interface, where the highly conductive P'Tn unit is attempting to drain TCw, is the saturation noticeably less than one. The fractures, on the other hand, approach residual saturation in the highly porous, nonwelded P'Tn, and are at complete saturation at the water table. Most of the geologic units show fractures between 30% and 60% saturated.

The normalized flux versus elevation is presented in Figure 3.30. Normalized flux is the calculated flux in the composite material divided by the imposed flux. Flux is normalized to allow the user to see in a standard way how much the calculated steady-state result differs from the exact result. TOSPAC also allows logarithmic and linear plots of the calculated flux in the composite material, in the matrix material, and in the fractures (Sections 4.3 and 4.6.4). Deviations above the TCw/P'Tn interface and at the bottom boundary are less than 1.5 %, as reported in the STEADY output listing (Figure 3.22). This deviation in this limited region is considered acceptable for this problem.

Figure 3.31 shows the average linear velocity of water in the matrix (the average linear velocity is also called the pore-water velocity). Average linear velocity is calculated by dividing the flux by the area available for flow—the difference of moisture content and residual moisture content ($v = q/(\theta - \theta_r)$).

YUCCA MOUNTAIN EXAMPLE PROBLEM
Composite Hydraulic Conductivity For TSw2-3

Figure 3.26: Composite hydraulic conductivity used for unit TSw2-3 in the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM
Composite Capacitance Coefficients For TSw2-3

Figure 3.27: Composite capacitance coefficients used for unit TSw2-3 in the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM Pressure Head of the Water

Figure 3.28: Pressure-head results for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM Fraction of Pore Space Saturated with Water

Figure 3.29: Saturation profiles for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM
Normalized Composite Flux of Water

Figure 3.30: Normalized flux profile for the waste-repository simulation.

For a given flux, a lower saturation produces a greater average linear velocity. The spikes at the interfaces are caused by changes in the moisture content and changes in the amount of flux within the matrix of each geologic unit. Notice how a sharp decrease in the saturation of TCw near its interface with PTn (Figure 3.29), plus the fact that there is significant flow in the TCw fractures but virtually none in the PTn fractures, causes a velocity spike.

Figure 3.32 presents the average linear velocity of water in the fractures. PTn is the only unit that does not maintain significant flow in the fractures at an infiltration rate of 4 mm/yr. The water velocity in the fractures in the other units is approximately four orders of magnitude higher than the corresponding water velocity in the matrix (Figure 3.31). The area of the fractures, and thus the area available for flow in this case, is approximately four orders of magnitude lower than the area of the matrix.

Examination of Figures 3.31 and 3.32 reveals what appears to be contradictory results. The water velocity in the matrix drops off sharply at the very bottom of the mesh. The bottom boundary condition is held at zero pressure head (the water table), saturating both the matrix and the fractures. Most of the flow occurs in the fractures because of their greater saturated conductivity. Somewhat surprisingly, the water velocity in the fractures also drops off at the bottom of the mesh. The saturated state imposed on the fractures raises the moisture content (the area available for flow) and hence lowers the velocity.

The plots of matrix, fracture, and composite hydraulic conductivity versus elevation are presented in Figure 3.33. Notice that for most of the mesh (units TCw, TSw1, TSw2-3, and CHnz) the composite conductivity equals the flux (4 mm/yr). This condition is called the "characteristic solution" in Section 2.2 of *Volume 1*. The conductivity does not equal the flux immediately above unit interfaces and at the bottom boundary. In these regions, the pressure head is controlled by the characteristic solution in the unit below the interface (or arbitrarily set at the bottom boundary). The characteristic solution is reached over a short distance for most units. The exception is PTn; if the PTn unit were thick enough, the hydraulic conductivity would eventually equal the flux.

Figure 3.34 presents the capacitance coefficient versus elevation. Although capacitance is not a factor in this steady-state problem, it is included here for completeness.

Figure 3.35 presents a bar chart of travel times for a particle of water from the ground surface to the water table. Using the average linear velocity of the water, four different travel times are calculated:

- 1) Minimum travel time: the time it takes a particle of water to cross a distance by the quickest route through either the matrix or fractures.
- 2) Matrix travel time: the time it takes to cross a distance if the particle stays in the matrix.
- 3) Fracture travel time: the time it takes to cross a distance if the particle stays in the fractures.
- 4) Composite travel time: the time it takes to cross distance at the area-weighted average linear velocity in the matrix and the fractures.

Travel time across a cell is calculated by dividing the distance across the cell by the average linear velocity of water in that cell. Using the average linear velocity of water in the matrix returns the travel time in the matrix; using the average linear velocity of water in the fractures returns the travel time in the fractures. To calculate the minimum travel time, the fastest path (matrix or fractures) that supports at least 1% of the total flux is used. (This 1% value is called the computational cutoff value. It

YUCCA MOUNTAIN EXAMPLE PROBLEM
Water Velocity in the Matrix

Figure 3.31: Average linear velocity of water in the matrix for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM Water Velocity in the Fractures

Figure 3.32: Average linear velocity of water in the fractures for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM Hydraulic Conductivity

Figure 3.33: Hydraulic-conductivity profiles for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM Composite Water Capacitance

Figure 3.34: Capacitance-coefficient profiles for the waste-repository simulation.

MILL-TAILINGS AND YUCCA MOUNTAIN EXAMPLE PROBLEMS Groundwater Travel Time Between Top and Bottom

Figure 3.35: Travel time of water for the mill-tailings and waste-repository simulations.

was arbitrarily decided upon after noting that the travel times were insensitive to cutoff values between 0.01% and 10%.) To calculate the composite travel time, the area-weighted average of the velocity in the matrix and the fractures is used. The minimum travel time is an approximation of the worst-case travel time. The composite travel time is an approximation of the travel time of a nonsorbing tracer.

For the travel-time plot, the travel times are calculated between any two locations in the column specified by the user. If the top and bottom are specified (the default), the times plotted are the same as the total travel times in the output-listing file. For the plot in Figure 3.35, travel times for both the potential-repository simulation and the simplified mill-tailings simulation are plotted, showing that multiple STEADY runs can be included on a single plot. This capability is more useful for comparing several similar problems, rather than unrelated problems such as in Figure 3.35. For example, travel times for different stratigraphies could be compared, or travel times for the same stratigraphy with variations in the hydrologic parameters. Section 4.6.3 contains details.

The travel times across all the cells between the particle start position and end position are summed to return the values reported in the output-listing file (Figure 3.22). If the water flow is negligible in the matrix in a cell (i.e., the travel time approaches infinity), then the travel time in that cell is not included in the sum of matrix travel times. Negligible flow is defined as less than 1% of the total flux. Travel time for water in the fractures is similarly constrained. The percentage of the range that actually contributed to the travel-time calculation is listed in parentheses. A percentage less than 100 indicates that there was negligible flow in part of the column.

For this problem, with a computational cutoff of 1%, the minimum groundwater travel time—the approximate worst-case travel time—is 3500 yr. The composite travel time—the approximate travel time of a nonsorbing tracer—is 20,500 yr. The groundwater travel time for flow restricted to the matrix is approximately 125,000 yr; although flow through the matrix is negligible across 0.1% of the column (i.e., flow through the matrix is less than 1% of the total across 0.1% of the column). For flow restricted to the fractures, the travel time is approximately 6 yr; although fracture flow is negligible over 7% of the column.

Figures 3.36 through 3.45 pertain to the transport calculation. Each figure is an example from a category of the OUTPLOT (TRANS RESULTS) menu. Section 4.6.5 contains a discussion of transport plots and these figures are cross-referenced there.

Figure 3.36 shows average linear water velocity versus elevation in both the matrix (solid line) and the fractures (dashed line). The average linear velocity shown in this figure is not the same as the average linear velocity in Figures 3.31 and 3.32, though they are very close most of the time. In the hydrology modules of TOSPAC, the water that represents the residual moisture content (e.g., water molecules held in tension in very small pores) is subtracted from the total moisture content, to yield an effective moisture content. The average linear velocity of water is then calculated by dividing the flux by this effective moisture content: $v = q/(\theta - \theta_r)$. In TRANS, the average linear water velocity is calculated by dividing the flux by the total moisture content: $v = q/\theta$. The residual water is included in the transport velocity calculation because contaminants can diffuse into the residual water from the flowing water and this diffusion can slow the overall progress of the contaminant. Using only the flowing water as the hydrologic background would overestimate the contaminant transport.

Figure 3.37 presents moisture content versus elevation in both the matrix (solid line) and the fractures (dashed line). Moisture content is the product of the saturation and the material porosity. The moisture content shown in this figure is the total moisture content, as used by TRANS to calculate the average linear velocity of water.

YUCCA MOUNTAIN EXAMPLE PROBLEM Effective Water Velocity for Transport

Figure 3.36: Average linear velocity of water (considering the residual saturation) for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM Matrix and Fracture Moisture Contents

Figure 3.37: Moisture-content profiles for the waste-repository simulation.

Figure 3.38 shows the plot of dispersion coefficient versus elevation for ^{99}Tc . The solid line indicates the dispersion coefficient for the matrix water; the dashed line indicates the dispersion coefficient for the fracture water. In TRANS, the dispersion coefficient operates as follows: the greater the dispersion coefficient, the greater the tendency of a concentration front of a contaminant to spread as it moves; hence the sooner the leading edge of the contaminant front reaches the boundary.

The dispersion coefficient for a contaminant in the matrix water is calculated as follows (Equations 3.1-5 and 3.1-16 from *Volume 1*):

$$D_m^i = \frac{D^{*i}}{\tau_m} + \alpha_m |v_m|,$$

where D^{*i} is the diffusion coefficient for a contaminant from the input-data file (Section 4.2.15), τ_m is the tortuosity of the matrix material from the input-data file (Section 4.2.14), α_m is the dispersivity of the matrix material (discussed below), and v_m is the average linear velocity of water in the matrix. Equation 3.1-17 in *Volume 1* gives the dispersion coefficient for fractures, which is similar to the matrix equation. From the discussion for Equation 3.1-51 in *Volume 1*,

$$\alpha_m = \alpha_{ma}[1 - \exp(-\mu l)],$$

where α_{ma} is the matrix dispersivity from the input-data file (Section 4.2.14), μ is one over the matrix-velocity correlation length from the input-data file (Section 4.2.14), and l is distance the contaminant has travelled. TRANS sets α_m and α_f (the dispersivity for the fracture material) to zero upstream from a source region, thereby not allowing dispersion upstream (although diffusion upstream is still allowed). Downstream from a source region, the dispersion coefficient increases as an exponential of the velocity correlation length and the distance traveled until it reaches the dispersivity input variable.

Figure 3.38 reflects zero matrix and fracture dispersivity upstream from a contaminant source, however the dispersion coefficient is not zero because of the diffusion term. Downstream from the source region the dispersion coefficient is shown to increase over distance. Note that below the interface between two geologic units (below the CHnz/TSw2-3 interface in Figure 3.38), the dispersion coefficient changes to its new value by the same exponential function given above.

The dispersion coefficient in the fractures is much greater than in the matrix for two reasons:

- 1) the tortuosity of the fractures is less than that of the matrix, which increases the diffusion term (most noticeably above the source region), and
- 2) in the lower two geologic units, the average linear velocity of water in the fractures is greater than that in the matrix by several orders of magnitude, which increases the hydrodynamic dispersion term (noticeable only below the source region because hydrodynamic dispersion only occurs downstream).

At the bottom boundary, the dispersion coefficient decreases abruptly in response to the decrease in average linear water velocity near the water table (Figure 3.36).

Retardation is a composite of several mechanisms (not all modeled in TRANS) that combine to slow the transport of a solute through porous media. The greater the retardation, the more slowly a contaminant is transported. Figure 3.39 presents a plot of the retardation factor versus elevation for ^{99}Tc . Again, the solid line indicates the retardation in the matrix; the dashed line indicates the retardation in the fractures.

YUCCA MOUNTAIN EXAMPLE PROBLEM Dispersion Coefficients for Tc-99

Figure 3.38: Dispersion-coefficient profiles for ^{99}Tc in the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM Retardation Factors for Tc-99

Figure 3.39: Retardation-factor profiles for ^{99}Tc in the waste-repository simulation.

TRANS calculates retardation factors in the matrix and fractures as follows (from Equations 3.1-12 and 3.1-13 in *Volume 1*):

$$R_m = 1 + \frac{\rho_b K_d}{\theta_m},$$

and

$$R_f = 1 + \frac{\sigma_f K_a}{\theta_f},$$

where ρ_b is the bulk density of a geologic unit (from the input-data file); K_d and K_a are the distribution coefficients for a contaminant in the matrix and fractures, respectively, for a geologic unit (from the input-data file); σ_f is the fracture wall area per unit volume of a geologic unit (from the input-data file); and θ is the moisture content.

A value of 1 for the retardation factor implies no retardation. When $K_d = 0$ or $K_a = 0$, then $R_m = 1$ or $R_f = 1$, respectively. In Figure 3.39, the retardation in the fractures is one (i.e., no retardation) because K_a was set to zero for ^{99}Tc in the TRANS input-data file. ^{99}Tc is also unretarded in the matrix of the nonwelded units, PTn and CHnz, and this condition is reflected in the plot. Because the moisture content is nearly constant in the matrix of the welded units (Figure 3.37), the retardation stays nearly constant. Note that the retardation shown in Figure 3.39 is only the retardation resulting from adsorption and not from any other effects, such as matrix diffusion.

Figure 3.40 presents the plot of the coupling constant versus elevation for ^{99}Tc . The dashed line indicates the strength of the coupling between the fractures and the matrix caused by matrix diffusion. Matrix diffusion is the tendency of the contaminant concentrations in the matrix and the fractures to equilibrate by the process of diffusion. The effect is most apparent when a contaminant being carried rapidly down a fracture is pulled into the matrix. The greater the coupling value, the more quickly the concentrations tend to equilibrate.

The solid line shows the strength of the coupling between the fractures and the matrix caused by advection. This effect takes place most often between a geologic unit where flow is predominantly in the fractures and one where flow is predominantly in the matrix. In the area where water transfers from one system to the other, the advective coupling is strongest, as shown by the spikes in the figure. Where water transfers advectively from fractures to matrix, the spikes are positive; where transfer is from matrix to fractures, the spikes are negative. Because this plot is on a logarithmic scale, only the fracture-to-matrix (positive) spikes are shown.

Both coupling constants are defined in *Volume 1*, Equation 3.1-40. (Advective coupling is represented by Λ_1 ; matrix diffusion coupling is represented by Λ_2 .) How these constants fit in the matrix-fracture coupling term of the transport model is given in Equation 3.1-39 of *Volume 1*.

Figure 3.41 presents a plot of concentration versus elevation for the radionuclide ^{99}Tc . The different curves represent concentrations at different time snapshots. The initial concentration is zero; as time passes the release from the source region increases in proportion to the dissolution of ^{238}U (congruent release). Advection, hydrodynamic dispersion, and diffusion carry the contaminant down the column.

Dispersion occurs only downstream of the source in TRANS as reflected in the plot. Diffusion occurs in both directions; however, the water velocity is sufficient to push the diffusing contaminant back through the source region. Hence, there is little movement of contaminant above the source.

The influence of the different retardation factors of the geologic units is visible in the 20,000-yr time line. The concentration moves downward through CHnz faster than through TSw2-3 (Figure 3.39).

YUCCA MOUNTAIN EXAMPLE PROBLEM
Matrix/Fracture Coupling Rates for Tc-99

Figure 3.40: Matrix/fracture coupling constants for ^{99}Tc in the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM
Tc-99 Concentration in the Matrix Water

Figure 3.41: ^{99}Tc concentration for the waste-repository simulation.

shows that CHnz has a retardation factor of 1 for ^{99}Tc , while TSw2-3 has a retardation factor of approximately 7.3).

The 20,000- and 30,000-yr time lines show the maximum level of ^{99}Tc in the source region. ^{99}Tc concentrations are still increasing, however, below the source region. If the amount of ^{99}Tc leaching from the source were constant, eventually a steady-state plume of ^{99}Tc would form. But after 50,000 yr, radioactive decay has diminished the amount of ^{99}Tc in the waste form. The concentration in the source region begins to decrease, followed by a decrease in the plume concentration. As reflected in the plot, the bottom boundary is set to zero concentration to mimic the mixing of the contaminant in the mass of water below the water table.

Figure 3.42 presents a three-dimensional plot of concentration with respect to elevation and time. The contaminant shown is ^{99}Tc . The concentration is the concentration in the matrix water; at these time scales, with the matrix/fracture coupling multiplier set to one, the concentration in the fracture water would appear identical. This three-dimensional plot allows the user to present an overview of the transport of a contaminant in a single picture. Compare this figure with Figure 3.41, which contains the same information.

Figure 3.43 shows a plot of concentration versus time for ^{99}Tc . The location is the middle of the source region (elevation of 232.5 m). To date, this type of plot has primarily been used to analyze the performance of various source terms. In this case, the concentration of ^{99}Tc rises to a nearly constant value, which decreases slowly because of radioactive decay.

The plot of release versus time for ^{99}Tc across the lower boundary is presented in Figure 3.44. The dashed line shows a running total of the amount in curies of ^{99}Tc that crosses the lower boundary and is removed from the problem. The solid line shows the amount in curies of ^{99}Tc that exists outside the lower boundary. For a contaminant that does not decay, these two curves would be identical. ^{99}Tc decays; therefore, the amount of ^{99}Tc actually outside the boundary is always less than the amount that reached the boundary. The EPA regulations are presently written in terms of the cumulative amount of a contaminant reaching the accessible environment (the dashed line). As Figure 3.44 shows, after 10,000 yr approximately 0.01 Ci of ^{99}Tc has reached the water table (the lower boundary) from the entire potential repository. After 100,000 yr, approximately 1100 Ci of ^{99}Tc has reached the water table, 1000 Ci of which still exists (approximately 100 Ci having been lost because of radioactive decay).

Figure 3.45 presents EPA ratios versus time for the contaminants given in this problem. The EPA ratio for a contaminant is defined as the cumulative release of radioactivity to the accessible environment for the contaminant divided by its EPA limit. The curve defined as TOTAL is the sum of all the EPA ratios plotted. It would represent the EPA sum if all relevant radionuclides were being plotted. (The EPA regulations require consideration of all radionuclides with half-lives greater than 20 yr.) The curves representing the individual contaminants are presented to show the user the contribution of each EPA ratio to the EPA sum. The contaminants shown in the plot are ^{14}C , ^{99}Tc , ^{129}I , ^{238}U , and ^{236}U (^{238}U and ^{236}U are overlaid). The other contaminants have contributions too low to appear on the plot. If the listed contaminants were the only contaminants in the potential repository inventory, including daughter products of contaminants in the inventory, then the EPA sum would be represented by the solid line. Notice that the line is predominantly defined by ^{14}C before approximately 40,000 yr, after which it is predominantly defined by ^{99}Tc . For this contrived problem, the EPA ratios are well below limits prescribed by regulation: at 10,000 yr the sum is four orders of magnitude below regulatory limits.

The OUTPLOT plot-definition file used to define the plots in this section is presented in Figure 3.46.

YUCCA MOUNTAIN EXAMPLE PROBLEM
Tc-99 Concentration in the Matrix Water

Figure 3.42: ⁹⁹Tc concentrations over time and distance for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM
Tc-99 Concentration at Elevation 232.5 m

Figure 3.43: ^{99}Tc concentration in the source region for the waste-repository simulation.

Figure 3.44: ^{99}Tc release at the water table for the waste-repository simulation.

YUCCA MOUNTAIN EXAMPLE PROBLEM
Release from Mesh; Bottom Boundary; Cumulative

Figure 3.45: EPA-ratio plot for the waste-repository simulation.


```

*****
*** TOSPAC OUTPLOT PLOT-DEFINITION FILE ***
*****

***** STEADY PLOT SECTION *****

***** PLOT FILE BLOCK *****
ex3steady.plt          STEADY plot-data filename

***** MESH PLOT BLOCK *****
xaxis lin              elevation axis type
xlimits default        elevation axis limits
box default            mesh points per box
number default         mesh points per label

**** CHARACTERISTIC-CURVE PLOT BLOCK ****
xaxis neglog           pressure-head axis type
xlimits default        pressure-head axis limits
yaxis log              conductivity axis type
ylimits default        conductivity axis limits
yunits mm/yr           use units of mm/yr for conductivity
yfactor 3.156E+10      conversion factor, m/s to mm/yr
zaxis lin              saturation axis type
zlimits default        saturation axis limits
material 4             plot material 4 (TSw2 fractures)

**** COMPOSITE-CONDUCTIVITY PLOT BLOCK ****
xaxis neglog           pressure-head axis type
xlimits default        pressure-head axis limits
yaxis log              conductivity axis type
ylimits default        conductivity axis limits
yunits mm/yr           use units of mm/yr for conductivity
yfactor 3.156E+10      conversion factor, m/s to mm/yr
legend right,top       legend location
unit TSw2-3            plot TSw2-3 curves

**** COMPOSITE-CAPACITANCE PLOT BLOCK ****
xaxis neglog           pressure-head axis type
xlimits default        pressure-head axis limits
yaxis log              capacitance axis type
ylimits default        capacitance axis limits
legend right,top       legend location
unit TSw2-3            plot TSw2-3 curves

***** PRESSURE-HEAD PLOT BLOCK *****
xaxis lin              elevation axis type
xlimits default        elevation axis limits
yaxis lin              pressure-head axis type
ylimits default        pressure-head axis limits
legend none            no legend
orient landscape       plot orientation
mode single            put each STEADY run on a separate plot

***** SATURATION PLOT BLOCK *****
xaxis lin              elevation axis type
xlimits default        elevation axis limits
yaxis lin              saturation axis type
ylimits default        saturation axis type
legend left,top        legend location
orient landscape       plot orientation
mode single            put each STEADY run on a separate plot
plottype all           plot all three saturations

***** NORMALIZED-FLUX PLOT BLOCK *****
xaxis lin              elevation axis type
xlimits default        elevation axis limits
yaxis lin              flux axis type
ylimits default        flux axis limits
legend none            no legend
orient landscape       plot orientation
mode single            put each STEADY run on a separate plot

***** VELOCITY PLOT BLOCK *****
xaxis lin              elevation axis type
xlimits default        elevation axis limits
yaxis neglog           velocity axis type
ylimits default        velocity axis limits
yunits mm/yr           use units of mm/yr for velocity
yfactor 3.156E+10      conversion factor, m/s to mm/yr
legend none            no legend
orient landscape       plot orientation
mode single            put each STEADY run on a separate plot
plottype matrix        plot matrix velocity

```

Figure 3.46: OUTPLOT plot-definition file for the waste-repository simulation.

```

***** VELOCITY PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default   elevation axis limits
yaxis neglog      velocity axis type
ylimits 1.E+0,1.E+6 velocity axis limits
yunits mm/yr      use units of mm/yr for velocity
yfactor 3.158E+10 conversion factor, m/s to mm/yr
legend none       no legend
orient landscape  plot orientation
mode single       put each STEADY run on a separate plot
plottype fracture plot fracture velocity

***** CONDUCTIVITY PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default   elevation axis limits
yaxis log         conductivity axis type
ylimits default   conductivity axis limits
yunits mm/yr      use units of mm/yr for conductivity
yfactor 3.156E+10 conversion factor, m/s to mm/yr
legend left,top   legend location
orient landscape  plot orientation
mode single       put each STEADY run on a separate plot
plottype all      plot all three conductivities

***** CAPACITANCE PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default   elevation axis limits
yaxis log         capacitance axis type
ylimits default   capacitance axis limits
legend none       no legend
orient landscape  plot orientation
mode single       put each STEADY run on a separate plot

***** PLOT FILE BLOCK *****
STEADY.PLT        STEADY plot-data filename
ex3steady.plt    STEADY plot-data filename

***** TRAVEL-TIME PLOT BLOCK *****
xlimits default   elevation limits
yaxis log         time axis type
ylimits default   time axis limits
yunits yr         use units of yr for travel time
yfactor 3.169E-8  conversion factor, sec to yr
file 1            plot travel times for file 1
label Example 1   label for plot
file 2            plot travel times for file 2
label Example 3   label for plot

***** TRANS PLOT SECTION *****
***** PLOT FILE BLOCK *****
ex3trans.plt     TRANS plot-data filename

***** MOISTURE PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default   elevation axis limits
yaxis log         moisture-content axis type
ylimits default   moisture-content axis limits
legend left,center legend location
orient landscape  plot orientation
plottype both     plot both matrix and fracture curves

***** VELOCITY PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default   elevation axis limits
yaxis neglog      velocity axis type
ylimits 1.E-13,1.E-3 velocity axis limits
legend left,top   legend location
orient landscape  plot orientation
plottype both     plot both matrix and fracture curves

***** DISPERSION PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default   elevation axis limits
yaxis log         dispersion axis type
ylimits default   dispersion axis limits
legend right,top  legend location
orient landscape  plot orientation
mode single       put just one species on each plot
plottype both     plot both matrix and fracture curves
species Tc-99     plot Tc-99 dispersion

```

Figure 3.46: Continued.

```

***** RETARDATION PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default    elevation axis limits
yaxis lin          retardation axis type
ylimits default    retardation axis limits
legend left,top    legend location
orient landscape   plot orientation
mode single        put just one species on each plot
plottype both      plot both matrix and fracture curves
species Tc-99      plot Tc-99 retardation

***** COUPLING PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default    elevation axis limits
yaxis log          coupling axis type
ylimits default    coupling axis limits
legend left,top    legend location
orient landscape   plot orientation
mode single        put just one species on each plot
plottype both      plot both advective and diffusive curves
species Tc-99      make plot for Tc-99

***** CVSE PLOT BLOCK *****
xaxis lin          elevation axis type
xlimits default    elevation axis limits
yaxis lin          concentration axis type
ylimits default    concentration axis limits
yunits kg/m**3     concentration units are kg/m**3
legend 15.2,center legend location
orient landscape   plot orientation
mode multi         put all time curves on the same plot
plottype matrix    plot matrix concentration
species Tc-99      plot Tc-99 concentration
snapshot 1         plot snapshot 1 (0 yr)
snapshot 2         plot snapshot 2 (1000 yr)
snapshot 6         plot snapshot 6 (5000 yr)
snapshot 11        plot snapshot 11 (10,000 yr)
snapshot 13        plot snapshot 13 (20,000 yr)
snapshot 15        plot snapshot 15 (30,000 yr)
snapshot 19        plot snapshot 19 (50,000 yr)
snapshot 29        plot snapshot 29 (100,000 yr)

***** 3-D PLOT BLOCK *****
xlimits default    time axis limits
xunits millennia   use millennia for time units
xfactor 3.169E-11  conversion factor, seconds to millennia
ylimits default    elevation axis limits
zlimits default    concentration axis limits
zunits kg/m**3     concentration units are kg/m**3
view default,default,225. viewpoint location
numx default       number of time lines
numy default       number of elevation lines
plottype matrix    plot matrix concentration
species Tc-99      plot Tc-99 concentration

***** CVST PLOT BLOCK *****
xaxis lin          time axis type
xlimits default    time axis limits
xunits millennia   use millennia for time units
xfactor 3.169E-11  conversion factor, seconds to millennia
yaxis lin          concentration axis type
ylimits default    concentration axis limits
yunits kg/m**3     concentration units are kg/m**3
legend left,top    legend location
mode single        put just one elevation on each plot
plottype both      plot both matrix and fracture curves
species Tc-99      plot Tc-99 concentration
elev source        plot concentration at the source

```

Figure 3.46: Continued.

```

***** RELEASE PLOT BLOCK *****
xaxis lin           time axis type
xlimits default    time axis limits
xunits millennia   use millennia for time units
xfactor 3.169E-11  conversion factor, seconds to millennia
yaxis log          release axis type
ylimits default    release axis limits
legend left,top    legend location
mode single        make a separate plot for each species
plottype both      plot both actual and cumulative curves
boundary bottom    plot releases from bottom boundary
release rad        plot releases in terms of radioactivity
species Tc-99      plot Tc-99 releases

***** RELEASE PLOT BLOCK *****
xaxis log          time axis type
xlimits default    time axis limits
xunits millennia   use millennia for time units
xfactor 3.169E-11  conversion factor, seconds to millennia
yaxis log          release axis type
ylimits default    release axis limits
legend left,top    legend location
mode multi         put all species on the same plot
plottype cumulative plot cumulative releases
boundary bottom    plot releases from bottom boundary
release EPA        plot releases in terms of EPA ratio
species all        plot curves for all species

```

Figure 3.46: Concluded.

Chapter 4

GENERAL REFERENCE

TOSPAC (the T^Otal S^Ystem P^Erformance A^Sessment C^Ode) performs calculations modeling the flow of groundwater and the transport of groundwater contaminants. TOSPAC is particularly applicable to modeling groundwater flow in a partially saturated regime through several different media, with contamination from radioactive wastes.

The TOSPAC computer program consists of five major software modules controlled by a sixth module, known as the SHELL (Section 4.1). Each module was developed separately from the others and, with minor programming, can be removed from the SHELL and executed separately. TOSPAC modules are as follows:

- 1) INDATA: the input-driver module, used for the creation and modification of the hydrology and transport input-data files (Section 4.2);
- 2) STEADY: the solver for steady-state groundwater flow (Section 4.3);
- 3) DYNAMICS: the solver for transient groundwater flow (Section 4.4);
- 4) TRANS: the solver for contaminant transport (Section 4.5);
- 5) OUTPLOT: the computer-graphics module, used for plotting the results of a TOSPAC run (Section 4.6).

An overview of the basic structure of TOSPAC is given in Figure 1.2.

Section 4.2, which contains the discussion of the INDATA module, also contains the description of the input data and data requirements.

TOSPAC modules communicate with each other through files. Separate files for hydrology and for transport calculations are designed into TOSPAC to allow the user to make several transport calculations using one hydrology calculation as the transport background. TOSPAC files are described in Section 4.7.

TOSPAC is written in FORTRAN 77 and is portable to most machines with a FORTRAN 77 compiler. TOSPAC does not follow the FORTRAN 77 standard in two major respects. First, standard

FORTRAN 77 limits variable names to a maximum of six characters; however, for understandability, TOSPAC uses variable names which can be longer than six characters. Most FORTRAN 77 compilers allow this exception to the standard. Second, the TOSPAC OUTPLOT module utilizes a proprietary graphics package, CA-DISSPLA (CAI, 1989). The OUTPLOT module, in its present form, can only be executed on computer systems that subscribe to CA-DISSPLA. Contact the authors for potential remedies.

4.1 TOSPAC SHELL

When the user first engages TOSPAC by typing:

```
$ RUN TOSPAC
```

the user enters the TOSPAC SHELL, as indicated by the appearance of the TOSPAC main menu:

```
TOSPAC VERSION 1.10 MAIN MENU
0. STOP
1. INDATA
2. STEADY
3. DYNAMICS
4. TRANS
5. OUTPLOT
```

```
ENTER CHOICE:
```

The TOSPAC SHELL is the basic framework in which the actual TOSPAC modules are embedded. Its purpose is to allow continuity for the user when running TOSPAC. With the SHELL, the user can complete an entire problem without leaving TOSPAC. At the SHELL level, the input-data files necessary for TOSPAC modules are identified and the modules are called. Figure 4.1 shows the primary logical flow within the TOSPAC SHELL.

The TOSPAC modules are for the most part independent of each other and the SHELL. Communication is through files. Section 4.7 contains more information on TOSPAC files.

The calculational modules of TOSPAC can be executed in batch mode by creating a procedure file that supplies the SHELL with the appropriate information. Typically, the procedure file contains a statement to execute TOSPAC, followed by an integer (that corresponds to a TOSPAC module as listed in the TOSPAC main menu), followed by a name of an input-data file for that module, followed by a 0 integer (that corresponds to the STOP in the TOSPAC main menu). The input-data file should contain a file block naming the other necessary files. Appendix A offers a brief description of batch-mode operation of TOSPAC on a DEC VAX computer system.

Figure 4.1: TOSPAC SHELL structure.

4.2 Input Data and the Input-Driver Module (INDATA)

INDATA is the TOSPAC module responsible for creating or modifying the STEADY input-data file, the DYNAMICS input-data file, and the TRANS input-data file. The input file for OUTPLOT, the plot-definition file, is created in the OUTPLOT module (Section 4.6).

TOSPAC input-data requirements are significant. For comprehension, the input data have been first split into three files (STEADY, DYNAMICS, and TRANS input-data files, Section 4.2.2), and then, within each file, into data "blocks" (Section 4.2.4). To simplify data entry, there are numerous default values, all selected by entering a <CR>. Also, there are several data checks.

This section contains a description of the organization, or structure, of the INDATA software (Section 4.2.1), followed by a discussion about running INDATA (Section 4.2.2 for input-data file creation, Section 4.2.3 for input-data file modification). Input data are organized into blocks of information (Section 4.2.4). Sections 4.2.5 through 4.2.18 contain descriptions of data blocks with a discussion of the input-data requirements. A discussion of the format of the input-data files created and modified by INDATA is given in Section 4.7.1.

4.2.1 INDATA Module Structure

Figure 4.2 contains a diagram of the top-level logical flow of INDATA. At the top level, after the variables are initialized, a menu is presented that allows the user to select the creation or modification of STEADY, DYNAMICS, or TRANS input-data files. Within the NAMEIN subroutine, the user names the file to be modified (if applicable), and the file to be created. If the user is modifying a file, the file is copied into a scratch file and only the scratch file is used by INDATA. The INHYDRO subroutine controls data entry for both creation and modification of STEADY and DYNAMICS input-data files; the INTRANS subroutine controls data entry for both creation and modification of TRANS input-data files.

Figure 4.3 contains the logic diagram of the INHYDRO subroutine. Two major flow paths exist: one for creating a new input file (subroutine HCREATE), the other for modifying an existing file (subroutine HMODIFY). The same subroutines are called in either path; however, for creating a file the subroutines are called sequentially, while for modifying a file the subroutines are called from a menu, with control passing back to the menu after the subroutine terminates. After an input-data file has been created or modified, the QUERIES subroutine allows the user to check the file for errors, look at the file, or modify the file. Figure 4.4 contains a similar diagram for the INTRANS subroutine in INDATA.

4.2.2 INDATA Execution (Input-Data File Creation)

INDATA is executed by selecting choice number 1 when presented with the TOSPAC main menu.

Figure 4.2: TOSPAC INDATA module structure.

Figure 4.3: Structure of the INDATA subroutine INHYDRO (for STEADY and DYNAMICS input data).

Figure 4.4: Structure of the INDATA subroutine INTRANS (for TRANS input data)

TOSPAC VERSION 1.10 MAIN MENU

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

ENTER CHOICE: 1

TOSPAC indicates that control is passed to the INDATA module by printing the following message:

TOSPAC MODULE INDATA

INDATA then queries the user for a type of input-data file to create or modify:

INDATA MAIN MENU

- 0. STOP
- 1. CREATE STEADY INPUT-DATA FILE
- 2. CREATE DYNAMICS INPUT-DATA FILE
- 3. CREATE TRANS INPUT-DATA FILE
- 4. MODIFY STEADY INPUT-DATA FILE
- 5. MODIFY DYNAMICS INPUT-DATA FILE
- 6. MODIFY TRANS INPUT-DATA FILE

ENTER CHOICE:

At this point if the user enters a 0, a <CR>, or a CRTLZ, the TOSPAC main menu returns to the screen. If the user enters any character other than those integers shown, the INDATA main menu is rewritten on the user's terminal screen; this procedure is repeated three times before control is returned to the TOSPAC SHELL. If the user selects an integer between 1 and 6 inclusive, control is transferred to the appropriate file-creation or file-modification procedure. The file-modification choices, 4, 5, and 6, are discussed in the next subsection.

If the user enters a choice of 1, the following prompt is issued:

ENTER STEADY INPUT-DATA FILE (DEFAULT=STEADY.DAT):

If the user enters a choice of 2 in response to the INDATA main menu, the following prompt is issued:

ENTER DYNAMICS INPUT-DATA FILE (DEFAULT=DYNAMICS.DAT):

If the user enters a choice of 3 in response to the INDATA main menu, the following prompt appears:

ENTER TRANS INPUT-DATA FILE (DEFAULT=TRANS.DAT):

An acceptable file name is any string of up to 80 characters with no embedded blanks. Of course, the name should be an acceptable file name on the user's computer system. The user *must* enter a file name (or a <CR> for the default name). If the user enters a file name that causes an error, the prompt is repeated. The user is allowed three invalid responses before control is returned to the TOSPAC main menu.

If the user has selected choice 1, 2, or 3, entering the name of a nonexistent file causes creation of that file and continuation with data-entry prompts. If the user has selected choice 1, 2, or 3, and if the user's computer system allows multiple files with the same name (file versions, or cycles), entering the name of an existing file causes creation of a new version of that file. On computer systems that do not allow multiple files with the same name, entering the name of an existing file causes an error message and return to the INDATA main menu.

If the user has selected choice 4, 5, or 6, entering the name of a nonexistent file causes an error message and return to the INDATA main menu. If the user has selected choice 4, 5, or 6, entering the name of an existing file causes INDATA to read that file and proceed with file-modification prompts.

Initially, default names for the input-data files are STEADY.DAT, DYNAMICS.DAT, and TRANS.DAT. If these files have been named previously in the TOSPAC session, the default names are those previous names.

It is only after entry of an input-data file name that the actual execution of INDATA begins. INDATA works primarily by prompting the user; it asks for specific information and the user supplies this information. When a new file is being created, this information is asked for in the same order that it will appear in the new file. When an old file is being modified, a menu is used to select the data block of information within the file that is to be modified.

When the various individual data are entered, they are checked to see if they are within acceptable bounds. After an input-data file is created or modified, the user is queried to see if he or she would like the complete file checked for consistency of the data that must interact.

TOSPAC input-data files are line formatted; i.e., each line is important either as a delimiter or as the carrier for one datum.

The actual query prompts provided by TOSPAC are given in the subsections below dealing with specific data blocks.

Upon completion of data entry for a newly created STEADY, DYNAMICS, or TRANS input-data file, INDATA states:

STEADY INPUT-DATA FILE *file_name* CREATED.

or:

DYNAMICS INPUT-DATA FILE *file_name* CREATED.

or:

TRANS INPUT-DATA FILE *file_name* CREATED.

Then INDATA asks the user the following question:

DO YOU WANT TO HAVE *file_name* CHECKED FOR ERRORS (N OR Y):

If this check is requested, the file is submitted to the actual input subroutine in STEADY, DYNAMICS, or TRANS. If the input-data file passes this check, it will be read successfully by the appropriate calculational module. However, successful reading does not imply successful execution.

Other problems can occur and these are further discussed in Sections 4.3, 4.4, and 4.5. If errors or inconsistencies are found in the file by INDATA, various error messages are displayed on the terminal screen, along with the following message:

**SEVERITY OF ERRORS INDICATES THAT TOSPAC WILL NOT
EXECUTE WITH *file_name*.**

If no errors are found, the following message is printed on the user's terminal:

***file_name* CONTAINS NO OBVIOUS ERRORS.**

After checking the file, or answering no to the checking query, INDATA asks:

DO YOU WANT TO VIEW *file_name* (N OR Y):

Viewing the file allows the user to look at what has been created, a screen of data at a time.

After the user views the file or answers *NO* to the viewing query, INDATA offers one more chance to modify the input-data file:

DO YOU WANT TO MODIFY *file_name* (N OR Y):

Modifying the file causes control to be transferred to the INDATA modification menu (Section 4.2.3).

Remember that the default for these final three questions is *NO*; therefore, a <CR> is the same as answering *NO*. If the user answers *NO* to the last prompt, INDATA is terminated, control is returned to the TOSPAC SHELL, and the TOSPAC main menu is displayed.

4.2.3 INDATA Execution (Input-Data File Modification)

A choice of 4, 5, or 6 in response to the INDATA main menu or a *YES* answer to the modify question after creating a new input-data file, causes transfer of control to the file-modification branch within INDATA.

If the user enters a choice of 4, the following prompts are issued:

**ENTER STEADY INPUT-DATA FILE (DEFAULT=STEADY.DAT):
ENTER NEW STEADY INPUT-DATA FILE (DEFAULT=STEADY.DAT):**

If the user enters a choice of 5 in response to the INDATA main menu, the following prompts are issued:

**ENTER DYNAMICS INPUT-DATA FILE (DEFAULT=DYNAMICS.DAT):
ENTER NEW DYNAMICS INPUT-DATA FILE (DEFAULT=DYNAMICS.DAT):**

If the user enters a choice of 6 in response to the INDATA main menu, the following prompts appear:

**ENTER TRANS INPUT-DATA FILE (DEFAULT=TRANS.DAT):
ENTER NEW TRANS INPUT-DATA FILE (DEFAULT=TRANS.DAT):**

If the user reached the file-modification branch of INDATA by answering *YES* to the modify question after creating a new input-data file, then only the second prompt of the above pairs is issued. It is assumed that the file to be modified is one that was just created.

If the user has selected choice 4, 5, or 6, entering the name of a nonexistent file in response to the first prompt causes an error message and return to the INDATA main menu. If the user has selected choice 4, 5, or 6, entering the name of an existing file causes INDATA to read that file and proceed with file-modification prompts.

Whenever INDATA modifies a file, it creates a new file for the modified version. INDATA always keeps the original file unaltered.

After the new file is named, the TOSPAC INDATA modification menu appears on the terminal screen. If the user is working on a STEADY or DYNAMICS input-data file, the hydrology modification menu appears (for the most part, STEADY input-data files and DYNAMICS input-data files use the same format and data, and thus the same modification menu applies to both):

INDATA HYDROLOGY MODIFICATION MENU

- 0. STOP
- 1. TITLE BLOCK
- 2. CONSTANTS BLOCK
- 3. GEOLOGIC-UNIT BLOCK
- 4. MATERIAL-PROPERTY BLOCK
- 5. MESH BLOCK
- 6. BOUNDARY-CONDITION BLOCK
- 7. INITIAL-CONDITION BLOCK
- 8. FILE BLOCK
- 9. VIEW

ENTER CHOICE:

If the user is working on a TRANS input-data file, the transport modification menu appears:

INDATA TRANSPORT MODIFICATION MENU

- 0. STOP
- 1. TITLE BLOCK
- 2. SOURCE BLOCK
- 3. GEOLOGIC-UNIT OR SATURATED-ZONE BLOCK
- 4. CONTAMINANT-PROPERTY BLOCK
- 5. BOUNDARY-CONDITION BLOCK
- 6. INITIAL-CONDITION BLOCK
- 7. FILE BLOCK
- 8. VIEW

ENTER CHOICE:

Default choice is 0 for both the hydrology and transport modification menus.

For either modification menu, the choice of any of the BLOCK numbers transfers the user to the appropriate block of the input-data file to modify. After that block is modified, the modification menu reappears. Descriptions of each of these data blocks are found in subsequent subsections.

In general, during modification, the defaults for data items are the values from the file being modified, not the generic defaults described in the following subsections.

Choice of VIEW allows the user to examine the input-data file he or she is working on.

Choice of STOP causes the modification section to terminate, and the following set of prompts is displayed:

```
DO YOU WANT TO HAVE file_name CHECKED FOR ERRORS (N OR Y):
DO YOU WANT TO VIEW file_name (N OR Y):
DO YOU WANT TO MODIFY file_name (N OR Y):
```

These prompts are discussed above in Section 4.2.2. If the user answers *NO* to the last prompt, INDATA is terminated and the TOSPAC main menu appears on the screen.

4.2.4 Data Blocks

TOSPAC is input-data intensive. Furthermore, the input data are multidisciplinary, mostly non-intuitive, and esoteric. (It should not escape your attention that computer modeling of groundwater flow with contaminant transport in a partially saturated regime is a difficult problem.) The major obstacle that must be surmounted in order to use TOSPAC effectively is the input data. The data must be available so that the user does not have to invent information; the data must be defined well enough to lead to accurate results; the data and how the data are organized must be understandable in order to avoid misuse.

The input data for TOSPAC are organized in blocks that range from the trivial (e.g., the title block) to the complex (e.g., the material-property block). The purpose of each data block is as follows:

- 1) TITLE BLOCK: identifies a particular calculation; provides labels for computer graphics; and allows the user to enter notes. A title block must be present in all STEADY, DYNAMICS, and TRANS input-data files.
- 2) CONSTANTS BLOCK: specifies constants in the same units as the rest of the input data (TOSPAC works with any units as long as they are self-consistent), and specifies control factors (e.g., the timestep factor). The constants block applies to STEADY and DYNAMICS input-data files.
- 3) GEOLOGIC-UNIT BLOCK: defines stratigraphy and the matrix and fracture hydrologic and transport characteristics of each layer. The geologic-unit block must be in STEADY, DYNAMICS, and TRANS input-data files, although the geologic-unit block for TRANS input-data files contains different data, and may be replaced by a saturated-zone block.
- 4) MATERIAL-PROPERTY BLOCK: defines the hydrologic properties, especially the characteristic curves, of matrix and fracture materials. The material-property block applies only to STEADY and DYNAMICS input-data files.
- 5) MESH BLOCK: defines the calculational mesh for the finite-difference solution method and relates it to the stratigraphy. It applies only to STEADY and DYNAMICS input-data files.
- 6) BOUNDARY-CONDITION BLOCK: specifies hydrologic or transport conditions at the boundary points of the mesh; allows these conditions to change at specified times; and defines the

times when output data are required. A boundary-condition block must be present in all STEADY, DYNAMICS, and TRANS input-data files.

- 7) SOURCE BLOCK: specifies the location of contaminant source (internal to or on the boundary of the calculational mesh); defines the spatial extent of the source region; and defines the type of source term (e.g., congruent leach). The source block applies only to TRANS input-data files.
- 8) SATURATED-ZONE BLOCK: specifies a saturated-zone problem and defines the stratigraphy and the matrix and fracture hydrologic and transport characteristics of each geologic unit. The saturated-zone block is optional in TRANS input-data files; if present, it replaces the geologic-unit block.
- 9) CONTAMINANT-PROPERTY BLOCK: defines the contaminants and the initial inventory. This block is required for TRANS input-data files.
- 10) INITIAL-CONDITION BLOCK: defines the initial pressure-head condition of a dynamic-flow calculation, or defines the initial concentrations of a transport calculation. The initial-condition block applies to DYNAMICS and TRANS input-data files; however, it is optional.
- 11) FILE BLOCK: defines the files to be used or created by STEADY, DYNAMICS, or TRANS (the output-listing file, the plot-data file, or the initial-condition file). The file block applies to all input-data files; however, it is optional.

Each data block consists of a block-identifier line, followed by one or more lines of data, followed by a block terminator. Block terminators include a blank line, another block-identifier line, or an end-of-file.

Data blocks can be located in any order in an input-data file. For a hydrology data file, the following order is recommended:

- 1) TITLE BLOCK
- 2) CONSTANTS BLOCK
- 3) GEOLOGIC-UNIT BLOCK
- 4) MATERIAL-PROPERTY BLOCK
- 5) MESH BLOCK
- 6) BOUNDARY-CONDITION BLOCK
- 7) INITIAL-CONDITION BLOCK (Optional)
- 8) FILE BLOCK (Optional)

For a transport data file, the recommended order is as follows:

- 1) TITLE BLOCK
- 2) SOURCE BLOCK
- 3) GEOLOGIC-UNIT BLOCK (or SATURATED-ZONE BLOCK)
- 4) CONTAMINANT-PROPERTY BLOCK

- 5) BOUNDARY-CONDITION BLOCK
- 6) INITIAL-CONDITION BLOCK (Optional)
- 7) FILE BLOCK (Optional)

Structuring input data into blocks also allows isolation of changes to a basic problem. For instance, imagine that the transport geologic-unit data are suspect. A number of problems could be run, differing only in changes to this block, to help quantify the uncertainty.

The block structure for input data is summarized in Figure 4.5. Each block and the input data it defines is treated in detail in the following subsections.

Figure 4.5: Data blocks.

4.2.5 Title Block (Hydrology and Transport)

The title block is typically the first data block in an input-data file. It is located immediately after the TOSPAC input-data header that INDATA creates. The header—TOSPAC HYDRO INPUT-DATA FILE or TOSPAC TRANS INPUT-DATA FILE, surrounded by a box of stars—is optional.

Within the INDATA module, first, a message is given telling the user the data-block designator:

TITLE BLOCK

The data-block designator is also written to the input-data file, marking the beginning of the title

block. Within the input-data file, the beginning of the title block is indicated by a line of text containing the string "TITLE BLOCK" in any combination of upper-case or lower-case characters.

Next, INDATA prompts for title information:

DEFAULT TITLE: NONE

ENTER PROBLEM TITLE: *This line is an example title that the user can enter*

DEFAULT NOTE: NONE

ENTER NOTES (ENTER A PERIOD (.) IN THE 1ST COLUMN TO STOP NOTES
OR ENTER "DEFAULT" IF YOU WANT THE DEFAULT)...

These lines are an example of notes that the user can enter.

TOSPAC's INDATA module will keep reading in information

until it encounters a line containing only a period in the first column,

so the user can enter almost anything:

\$#!@%&@!!!*

and it will appear in the input-data file as a note.

*So the next line is going to be blank except for a period in
the first column so we can get out of this...*

The title block allows the user to record important information about a particular calculation in a readily retrievable area. This block lets the user identify the calculation at a future date and chronicle the calculation for quality assurance.

The problem title, as defined by the user in the title block, is also used by the OUTPLOT module to label computer graphics.

Figures 2.3, 3.2, and 3.20 present examples of TOSPAC hydrology input-data files. Shown at the top of each file is the optional TOSPAC header, followed by the title block. Figures 2.4 and 3.21 contain examples of TRANS input-data files. The title block for a TRANS input-data file is identical to the title block for a hydrology input-data file.

4.2.6 Constants Block (Hydrology)

The constants block provides the definition of physical constants for the STEADY and DYNAMICS modules of TOSPAC. It also provides program-control parameters for the DYNAMICS module.

The TOSPAC program is unit-independent. The constants block allows the user to enter data (not only these data, but all data used in a given calculation) in whatever units he or she wishes, as long as the data are self-consistent.

For instance, using centimeter-gram-seconds (cgs) units the compressibility of water (Section 4.2.6) is $4.3 \times 10^{-8} \text{ cm}^{-1}$. If the user enters this value, it is up to the user to make sure that *all* data in this input-data file are in cgs units. TOSPAC does not care what units are used—*Système International (SI)*, cgs, foot-pound-second (FPS), cubit-slug-eon—as long as *all* data are in those units for a given calculation. Default values created by TOSPAC are in *SI* meter-kilogram-second (mks) units.

TOSPAC allows the user to place the units after an input value in the input-data file. But TOSPAC does *not* read and understand the units—they are only a note to the user (Section 4.7.1).

The prompts that the INDATA module uses to define the constants block follow. First, a message is given telling the user the data-block designator:

CONSTANTS BLOCK

Then the prompts for input data commence:

ENTER DENSITY OF WATER (DEFAULT=1000. kg/m**3):

The density of water must be a positive real number; the default is 1000 kg/m³ in *SI* units or 1 gm/cm³ in cgs units. The density of water is used in calculating the weight of water in the column.

ENTER COMPRESSIBILITY OF WATER (DEFAULT=4.3E-6 /m):

The compressibility of water is a positive real number; the default is 4.3×10^{-6} in *SI* units. Notice that the standard water compressibility ($\beta_w = 4.4 \times 10^{-10}$ m²/N or m-s²/kg) has been multiplied by the density of water (ρ) and the acceleration caused by gravity (g) in order to get the necessary units:

$$\begin{aligned}\beta'_w &= \beta_w \rho g \\ &= 4.4 \times 10^{-10} \text{ m-s}^2/\text{kg} \times 1000 \text{ kg/m}^3 \times 9.8 \text{ m/s}^2 \\ &= 4.3 \times 10^{-6} \text{ m}^{-1}.\end{aligned}$$

ENTER CROSS-SECTIONAL AREA OF THE COLUMN (DEFAULT=1. m**2):

The cross-sectional area is a positive real number describing the one-dimensional, vertical column being modeled. It is used to calculate the amount of water in the column. The default is 1 m², the unit area.

ENTER TIMESTEP-CONTROL FACTOR (DEFAULT=0.1):

The timestep is controlled by either the time derivative of the hydraulic conductivity or the time derivative of the pressure head, whichever is larger. The timestep-control factor allows scaling the timestep to a particular problem; very nonlinear problems should have smaller factors, and more linear problems should have larger. Section 2.2 of *Volume 1* contains more information. The timestep-control factor is ignored by STEADY calculations.

ENTER IMPLICITNESS FACTOR (DEFAULT=0.5):

The implicitness factor is a real number between 0 and 1, inclusive, that defines where in the timestep the coefficients of the differential equation are to be calculated. For instance, if the timestep is from 0 s to 1 s, an implicitness factor of 0.5 would mean that the hydraulic conductivity and the capacitance and their derivatives should be calculated at 0.5 s. This value is also called the “Crank-Nicholson omega.” If it is set to 0.5, the truncation error for a given timestep is at the minimum, hence the solution is most accurate. However, if the implicitness factor is set to 1, the solution is most stable. Values below 0.5 should not be used. Section 2.2 of *Volume 1* contains more information. The implicitness factor is ignored by STEADY calculations.

An important capability of TOSPAC is calculating groundwater travel times (GWTTs). One method

that TOSPAC uses for this calculation is to track a water particle as it moves through the problem domain. To access this calculation, the starting and ending locations of the particle are specified.

```
ENTER GWTT START POSITION (DEFAULT=TOP):
ENTER GWTT END POSITION (DEFAULT=BOTTOM):
```

Acceptable positions are the words *TOP*, *BOTTOM*, *NONE*, or any real number that corresponds to an elevation in the problem domain. The start position can be either above or below the end position (Section 3.1). The default entries tell TOSPAC to calculate GWTT from the top of the column to the bottom. In the DYNAMICS module of TOSPAC, the GWTT calculation can take excessive of computer time, because the water velocities must be calculated at every time step (without the GWTT calculation, water velocities are only calculated at time snapshots). Entering the word *NONE* in either position causes the GWTT calculation to be circumvented.

The last prompt in the constants block concerns restart of a DYNAMICS calculation (Section 4.4.3).

```
ENTER TIME SNAPSHOT FOR RESTART (DEFAULT=0):
```

The restart number corresponds to the number of the time snapshot from a previous calculation where the present calculation is to be restarted. A restart snapshot can be any integer greater than 0; however, it should be between 0 and the maximum number of time snapshots given in the boundary-condition block (Section 4.2.10). If the restart snapshot is greater than 1, when DYNAMICS executes it reads the plot-data file from a previous execution (named either by default or in the file block—Section 4.2.11) up to the restart number of time snapshots, and begins the new calculation from that time. (Caution—if a pond-drain boundary condition has been used, additional time snapshots may have been automatically inserted into the plot-data file; Sections 4.2.10 and 4.4.3.) The restart number is ignored for a STEADY calculation.

At the conclusion of the constants-block input, INDATA writes a blank-line block terminator on the STEADY and DYNAMICS input-data files.

The constants block is usually located immediately after the title block. It is only used in the STEADY and DYNAMICS input-data files. Figures 2.3, 3.2, and 3.20 contain examples of the constants block.

4.2.7 Geologic-Unit Block (Hydrology)

A geologic unit is a medium through which the groundwater travels. The entire column (that is, the entire calculational mesh) *must* be specified as one or more geologic units in the geologic-unit block.

Through the concept of geologic units, TOSPAC allows the user to take advantage of the composite-porosity model of fractured porous media. The composite-porosity model allows both matrix and fracture materials to be modeled in a one-dimensional column. (The composite-porosity model has the additional advantage of simplifying unsaturated, fractured, porous media enough to allow site-scale calculations.) TOSPAC can return results for both matrix and fracture flow and transport, as well as “composite” flow and transport, using this model. The composite-porosity model is described in Section 2.1 of *Volume 1* and by Peters and Klavetter (1988). If the user is considering using the composite-porosity model, he or she is advised to study it, the assumptions behind it, and its limitations.

A geologic unit can be composed of one or two materials. Typically, an unfractured matrix is represented by a single material, and a fractured matrix is represented by a material for the matrix and a material for the fractures. (It is possible, however, to specify arbitrarily complex materials, and therefore a single material can be given the characteristics of both matrix and fractures. This practice is not recommended, because then TOSPAC cannot return separate matrix and fracture results.) Materials are specified in the material-property block, described in Section 4.2.8.

TOSPAC allows arbitrary configuration of geologic units. Geologic units can differ from one another when their matrices have different properties, when their fractures have different properties, or when they have different geologic-unit properties (e.g., different compressibilities or fracture areas). However, geologic units with identical properties, adjacent or separated by one or more different units, can be specified. This feature may be helpful when specifying a contaminant repository as a geologic unit within another geologic unit.

The geologic-unit block allows stratigraphy to form the basis of hydrologic and transport data: first, because some hydrologic properties (e.g., fracture characteristics) and many transport properties (e.g., densities, dispersions, etc.) are most easily defined at this level of complication; and second, because problem parameters can easily be modified by changing a number (e.g., changing the matrix material in a unit by changing the matrix-material index) while leaving the basic structure of the problem constant.

Also, the steady-state solver (STEADY) attempts to calculate a solution in piecemeal fashion, one geologic unit at a time. For this reason it is recommended (but not required) that a minimum of four mesh cells be included in every geologic unit. Section 4.2.9 contains a discussion of the calculational mesh.

A geologic-unit block is defined as follows (using the INDATA prompts as a framework):

GEOLOGIC-UNIT BLOCK

ENTER # OF GEOLOGIC UNITS (DEFAULT=1):

Next, the number of geologic units to be defined is requested. The number must be an integer between 1 and 20, inclusive. The default value is 1.

INDATA next indicates that it is working on the first unit:

UNIT # 1

Then it reports the default geologic-unit name and asks for the new name:

UNIT # 1 DEFAULT NAME:

ENTER UNIT # 1 NAME:

The name can be any string up to 80 characters long; the default during file creation is a blank name. Geologic-unit names need not be distinct; i.e., although not advised, two different units can have the same name.

ENTER LOWER ELEVATION (DEFAULT=0. m):

ENTER UPPER ELEVATION (DEFAULT=100. m):

The lower elevation of a geologic unit can be any real number. The default is 0 m (e.g., sea level or the

water table). The upper elevation can be any real number greater than the lower elevation; the default is 100 m. TOSPAC assumes that gravity operates from the top of the column to the bottom; the user *cannot* change this orientation.

ENTER MATRIX-MATERIAL INDEX (DEFAULT=1):
ENTER FRACTURE-MATERIAL INDEX (DEFAULT=1):

The matrix-material index is an integer that corresponds to the position of the material in the material-property block (Section 4.2.8). Acceptable inputs are integers between 1 and 40, inclusive. The default is 1 (i.e., the first material specified in the material-property block). The fracture-material index is an integer that also corresponds to the position of the material in the material-property block. The default is again 1.

Note that when the matrix and fractures consist of the same material (the default), the implication is that there are no fractures. Actually, the user can specify a single material in the material-property block that has the characteristics of a composite material (includes both matrix and fracture characteristics in one specification). However, if fractures are to be specified, it is recommended that they be specified in a separate material. TOSPAC gives results for both matrix and fracture flow and transport *only* if the matrix and fractures are specified separately.

ENTER FRACTURE POROSITY (DEFAULT=0.):

The fracture porosity is the fraction of the volume of the unit that is composed of the fracture material (the fractures). TOSPAC multiplies the fracture porosity given in the geologic-unit block by the material porosity of the fracture material given in the material-property block to get the true fracture porosity. For this reason, the porosity for a fracture material given in the material-property block is typically set to one. The fracture porosity can be any real number between 0 and 1, inclusive. The default is 0; i.e., the default is no fractures. Although TOSPAC allows several methods of specifying a matrix-flow-only problem, specifying 0 fracture porosity makes the calculation the most efficient.

ENTER BULK ROCK COMPRESSIBILITY (DEFAULT=0. /m):

The bulk-rock compressibility (α'_b) is the compressibility of the matrix and fractures together (see Equation 2.1-7 in *Volume 1*). The default is 0; i.e., the default is that the bulk rock does not compress. Any nonnegative real number is allowed.

ENTER FRACTURE COMPRESSIBILITY (DEFAULT=0. /m):

The fracture compressibility is the compressibility of the fractures alone ($\partial n_f / \partial \sigma'$ in Equation 2.1-20 of *Volume 1*). The default is 0; i.e., default is that the fractures do not compress. Any nonnegative real number is allowed.

UNIT # 2
UNIT # 2 DEFAULT NAME:
ENTER UNIT # 2 NAME:

o
o
o

And INDATA continues until the specified number of geologic units has been entered. After all the

units have been defined, a blank line signifying block termination is written to the user's terminal and in the hydrology input-data file.

Examples of geologic-unit blocks can be found in Figures 2.3, 3.2, and 3.20. Figure 3.20 shows a geologic-unit block defining five geologic units.

4.2.8 Material-Property Block (Hydrology)

The material-property block defines hydrologic properties of the materials referenced (by index) in the geologic-unit block. A material is the physical medium which constitutes the geologic unit, through which the groundwater passes. Geologic units can comprise one or two materials (typically, the matrix and fractures are defined as two different materials), as discussed in Section 4.2.7.

The material-property block consists of an integer indicating how many materials are in the block, followed by the data for each material. The individual material data consist of a title, a porosity, and characteristic-curve data. Characteristic curves, as used by TOSPAC, are functions of saturation versus pressure head and hydraulic conductivity versus pressure head that describe the hydrologic properties of a porous material. TOSPAC allows characteristic-curve data to be in several different forms: as specified by van Genuchten (1980), or by a table of values, or by a combination of methods. Further information on characteristic curves can be found in Section 2.1 of *Volume 1*.

Within the INDATA module, data entry into the material property block begins with the following:

```
MATERIAL-PROPERTY BLOCK
ENTER # OF MATERIALS (DEFAULT=1):
```

The number of materials is an integer with a value of between 1 and 40, inclusive. This value tells INDATA the number of times it must prompt for material data. INDATA responds:

```
MATERIAL # 1
MATERIAL # 1 DEFAULT NAME:
ENTER MATERIAL # 1 NAME:
```

A material name is a character string of up to 80 characters. Material names need not be distinct; i.e., although not advised, two different materials can have the same name.

```
ENTER POROSITY (DEFAULT=1.):
```

Material porosity (n , n_m , or n_f in various equations in *Volume 1*) is a real number with a value between 0 and 1, inclusive.

Porosity is defined as void volume divided by total material volume. Effective porosity is defined as void volume available for groundwater flow divided by total volume. Effective porosity should be entered here if the total saturation is considered to be one and the residual saturation is considered to be zero (these data are discussed below).

If a TRANS calculation is going to be made with this hydrologic background, it is recommended that the actual porosity be entered here. The residual volume is accessible to dissolved solute, therefore residual-saturation data should be available to TRANS.

TOSPAC multiplies the fracture porosity given in the geologic-unit block (Section 4.2.7) by the material porosity of the fracture material given in the material property block to get the true fracture porosity (n_f). For this reason, the fracture-material porosity given here in the material-property block is typically set to 1.

CHARACTERISTIC-CURVE FLAGS ARE:

1. VAN GENUCHTEN
2. VAN GENUCHTEN TABLE LOOKUP
3. SATURATION DATA TABLE
4. DATA TABLE
5. COMBINATION

ENTER CHARACTERISTIC-CURVE FLAG (DEFAULT=1):

The characteristic-curve flag defines the method used by TOSPAC to evaluate the material characteristic curves. TOSPAC supports five different characteristic-curve formats that are discussed below.

Flag=1 selects the van Genuchten Method (van Genuchten, 1980) with five parameters, as follows:

- 1) S_s , the total saturation: a real number greater than 0 and less than or equal to 1; this parameter is usually set to 1 (except when curve data are based on moisture content— θ , θ_m , or θ_f in *Volume 1*—then this parameter would be set to the value of the effective porosity, and then the porosity parameter, above, would be set to 1).
- 2) S_r , the residual saturation: a real number greater than or equal to 0 and less than 1. When material porosity includes unconnected voids not available to groundwater flow or voids too small to significantly support groundwater flow, then this value is set to the ratio of the volume of voids that do not contribute to groundwater flow over the total volume; otherwise this value is 0.
- 3) α , a curve-fit parameter that approximately indicates the air-entry pressure of the material ($-1/\alpha \approx$ air-entry pressure head). Any positive real number is accepted.
- 4) β , a curve-fit parameter that indicates the steepness of the characteristic curves (both saturation and hydraulic conductivity). Any positive real number greater than 1 is accepted; however, values between 1.5 and 10 are the norm; values larger than 15 can cause floating-point overflow on many computers, and although overflow is screened out in these cases by the STEADY and DYNAMICS modules, a certain degree of imprecision can degrade results.
- 5) K_s , saturated hydraulic conductivity: the STEADY and DYNAMICS modules use this parameter to scale the relative conductivity value returned by the van Genuchten method to the actual conductivity value; i.e., $K = K_s \times K_{relative}$. Any positive real number is accepted. The hydraulic conductivity has the same units as velocity (length over time).

The van Genuchten method is the default. When selected, the following prompts appear on the terminal screen:

ENTER TOTAL SATURATION (DEFAULT=1.):

ENTER RESIDUAL SATURATION (DEFAULT=0.0395):

ENTER ALPHA (DEFAULT=1.2851 /m):

ENTER BETA (DEFAULT=4.23):

ENTER SATURATED HYDRAULIC CONDUCTIVITY (DEFAULT=4.4E-6 m/s):

The default values for each of the van Genuchten parameters correspond to a sand-soil material approximated from Freeze and Cherry (1979). When an input-data file is modified, these defaults can be different than shown.

Flag=2 selects the van Genuchten Table-Lookup Method. The input-data requirements for this method are identical to those for the van Genuchten Method.

The difference between the van Genuchten Method and the van Genuchten Table-Lookup Method follows. The van Genuchten Method uses analytic formulas to calculate saturation, the first and second derivatives of the saturation, hydraulic conductivity, and the first derivative of the conductivity (*Volume 1*). For every iteration, for every mesh point, these equations are solved at each pressure head. These equations contain a number of divisions and exponentiations that are time-consuming to perform. The van Genuchten Table-Lookup Method sets up tables to approximate the analytic formulas. For every iteration, for every mesh point, the tables are searched and a linear interpolation is performed to calculate the hydrologic quantities associated with each pressure head.

The tables are set up so that the error in hydraulic conductivity and in the first derivative of the saturation (an important quantity in calculating the storage capacity) are less than 1%. The tables are searched using a bisection algorithm. (Only the table containing the pressure head, the independent variable, is searched to find the proper table indices and determine the linear-interpolation factor.) The tables contain a minimum of 100 and a maximum of 1000 data points; the number of points is proportional to the magnitude of the β parameter.

The van Genuchten Table-Lookup Method was devised when it was observed that, for a typical DYNAMICS calculation, approximately 80% of the computer processor time was being spent calculating the van Genuchten equations. Computer times for DYNAMICS calculations are decreased by up to a factor of four by using the Table-Lookup Method. Computer times typically increase for STEADY calculations, and therefore, the van Genuchten Table-Lookup Method is not advised for STEADY.

Flag=3 selects the Saturation Data-Table Method. A data table is a list of pairs of numbers that correspond to points on a characteristic curve. A data table should reside in a file that can be accessed by TOSPAC when the STEADY, DYNAMICS, TRANS, or OUTPLOT modules are executed. For the Saturation Data-Table Method, a saturation-curve file (Section 4.7.5) containing one saturation characteristic curve must be present when STEADY or DYNAMICS is executed.

When the Saturation Data-Table Method is selected, the following prompt appears on the terminal screen:

```
SAT-CURVE FILE DEFAULT NAME: SAT.CRV
ENTER SAT-CURVE FILE NAME:
```

The file names are strings of up to 80 characters with no embedded blanks. The user may specify a name for a file that does not yet exist.

A description of the format of a saturation-curve file is given in Section 4.7.5.

TOSPAC uses the saturation data table to calculate a hydraulic-conductivity curve. The calculation is by Mualem (1976), and involves a numerical integration of the saturation curve (TOSPAC uses the simple trapezoidal method). The various derivatives of the saturation and the hydraulic conductivity are calculated as the slopes of these curves (or the slope of the slope, in the case of the second

derivative of the saturation).

When a saturation data table is used by TOSPAC, it is linearly interpolated. This method is fast, but accuracy often depends on the spacing between data points. Therefore, data points should be concentrated in areas of the characteristic curve that show the most change in slope, typically near the air-entry pressure head.

The Saturation Data-Table Method allows the user to prepare characteristic-curve data independent of the methods prescribed by TOSPAC. It further allows the user to use actual data—if there are enough data points and if linear interpolation between the points is satisfactory (i.e., the data are not too noisy). However, because the data tables are linearly interpolated when used by TOSPAC, accuracy is questionable.

An example of a saturation characteristic curve from a data table is given in Figure 4.6 (from Peters *et al.*, 1987).

Flag=4 selects the Data-Table Method. The Data-Table Method is similar to the Saturation Data-Table Method, except that the hydraulic-conductivity data must also be in a file that can be accessed by TOSPAC. Figures 4.6 and 4.7 contain examples of characteristic curves defined by the Data-Table Method.

When the Data-Table Method is selected, the following prompts appear on the terminal screen:

```
SAT-CURVE FILE DEFAULT NAME: SAT.CRV
ENTER SAT-CURVE FILE NAME:
HK-CURVE FILE DEFAULT NAME: HK.CRV
ENTER HK-CURVE FILE NAME:
```

The file names are strings of up to 80 characters with no embedded blanks. The user may specify a name for a file that does not exist yet, although the files must exist when the actual calculation is made.

A description of the format and content of a saturation-curve file is given in Section 4.7.5; a description of a hydraulic-conductivity-curve file is given in Section 4.7.6.

Flag=5 selects the Combination Method. This method allows characteristic curves to be defined by a weighted average of any of the other four methods. Thus, the user can specify “multiple-hump” curves, similar to the multiple humps of the combined matrix-fracture curves.

Multiple-hump curves are useful in describing materials that consist of several separate pore-size distributions (Peters *et al.*, 1987). Multiple-hump curves can also be defined by the Data-Table Method, above. Examples of multiple-hump curves are also given in Figures 4.6 and 4.7.

When the Combination Method is selected, the following prompts appear on the terminal screen:

Figure 4.6: Saturation characteristic curves produced by three different methods.

Figure 4.7: Hydraulic-conductivity characteristic curves produced by three different methods.

```

ENTER # OF CURVES TO COMBINE (DEFAULT=2):
ENTER MATERIAL INDEX (DEFAULT=1):
ENTER FRACTIONAL AREA FOR THIS MATERIAL (DEFAULT=0.5):
ENTER MATERIAL INDEX (DEFAULT=2):
ENTER FRACTIONAL AREA FOR THIS MATERIAL (DEFAULT=0.5):

```

```

o
o
o

```

The defaults specify that the combination material is to be composed of 50% of the first material in the material-property block and 50% of the second material in the material-property block.

A combination material can *only* reference (i.e., can *only* be composed of) materials that precede it in the material-property block. A combination material can reference other combination materials. A combination material cannot reference itself. A material can be referenced by more than one combination material.

The fractional area of a material referenced by the combination material is the ratio of the area of that referenced material to the total area of the combination material. The sum of the fractional areas must equal one.

The characteristic curves for a combination material are calculated as follows. First, the characteristic curves of the contributing materials are examined to find the overall maximum and minimum pressure heads. Using these endpoints, a table of 1000 uniformly-spaced pressure heads is constructed. Finally, at each pressure head in the table, the various hydrologic parameters are calculated for each contributing material; the values are combined according to the fractional area of the contributing material (i.e., an area-weighted average is performed), giving the value for the combination material.

Figure 4.8 contains an example of a material-property block as created by INDATA for a hydrology input-data file. This example shows five different materials, each with characteristic curves defined by a different method. The fifth material is defined by the Combination Method and consists of 25% of the first material and 75% of the second material.

The material-property block appears only in a hydrology input-data file.

4.2.9 Mesh Block (Hydrology)

The mesh block defines the one-dimensional, Eulerian mesh used by the finite-difference method in the calculational modules of TOSPAC.

A mesh is a series of points at which a differential equation is discretized (i.e., approximated by difference equations). The equation parameters are defined at the mesh points, a linear system is set up based on difference equations using these parameters, and when the linear system is solved, values are returned for these mesh points. The mesh points correspond to points in space (elevations, in TOSPAC) and they do not move (this is known as an Eulerian mesh—as opposed to a Lagrangian mesh—to numerical analysts). Often, a mesh is called a logical mesh. A mesh with equally spaced mesh points is called a uniform mesh. Mesh points are sometimes referred to in *Volume 1* as *j*-values, a reference to the array index *j*. The mesh point at the bottom of the mesh corresponds to the lower

```

***** MATERIAL-PROPERTY BLOCK *****
5                                     # MATERIALS
MATERIAL # 1 ...NAME:
Granite
0.04                                MATERIAL EFFECTIVE POROSITY
1                                  CHARACTERISTIC CURVE FIT
1.                                TOTAL SATURATION
0.30                             RESIDUAL SATURATION
0.0155 /m                         ALPHA COEFFICIENT
2.45                             BETA COEFFICIENT
3.e-13 m/s                       SATURATED HYDRAULIC CONDUCTIVITY
MATERIAL # 2 ...NAME:
Sand
0.25                                MATERIAL EFFECTIVE POROSITY
2                                  CHARACTERISTIC CURVE FIT
1.                                TOTAL SATURATION
0.0395                           RESIDUAL SATURATION
1.2851 /m                        ALPHA COEFFICIENT
4.23                             BETA COEFFICIENT
4.4e-6 m/s                       SATURATED HYDRAULIC CONDUCTIVITY
MATERIAL # 3 ...NAME:
Gravel
0.3                                MATERIAL EFFECTIVE POROSITY
3                                  CHARACTERISTIC CURVE FIT
gravel.sat                       SATURATION-DATA FILENAME
MATERIAL # 4 ...NAME:
Loam
0.40                                MATERIAL EFFECTIVE POROSITY
4                                  CHARACTERISTIC CURVE FIT
loam.sat                        SATURATION-DATA FILENAME
loam.hk                         HYDRAULIC-CONDUCTIVITY-DATA FILENAME
MATERIAL # 5 ...NAME:
River-Deposits
0.28                                MATERIAL EFFECTIVE POROSITY
5                                  CHARACTERISTIC CURVE FIT
2                                  # CURVES TO COMBINE
2                                  MATERIAL 1 INDEX
0.25                              MATERIAL 1 FRACTIONAL AREA
3                                  MATERIAL 2 INDEX
0.75                              MATERIAL 2 FRACTIONAL AREA

```

Figure 4.8: A material-property block showing five different ways to specify hydrologic properties.

boundary; the mesh point at the top corresponds to the upper boundary.

A cell or zone is the space between two mesh points. Because there is always a mesh point above and below a cell, the total number of mesh points is always one greater than the total number of cells. Cells and zones, like mesh points, are also mathematical constructs. Neither exists physically. TOSPAC uses cells to define the mesh.

Figure 4.9 shows an example mesh with mesh points and cells superimposed on a given stratigraphy of geologic units.

The mesh construction is very important to TOSPAC; accuracy, efficiency, and usefulness of the results depend a great deal on the mesh structure. An effort has been made to render mesh definition painless—INDATA has an automatic mesh generator—however, for reasons discussed below, the user must know how to construct an adequate mesh.

In general, to construct a mesh, the user makes a one-to-one correspondence between mesh points and elevations. For instance, assign mesh point number 1 to elevation 0; assign mesh point number 2 to elevation 0.43 (or whatever); and so forth. TOSPAC simplifies things, somewhat, by interpolating a uniform spacing over a range of cells: the user specifies 10 cells between elevation 0 and elevation 4.3,

Figure 4.9: Correspondence between mesh points, cells, submeshes, and geologic units.

and TOSPAC then places 11 mesh points between elevation 0 and elevation 4.3: mesh point # 1 → elevation 0, point # 2 → elevation 0.43, point 3 → elevation 0.86, point 4 → elevation 1.62, ..., point 10 → elevation 3.87, point 11 → elevation 4.3. This interpolation range is called a submesh.

The STEADY and DYNAMICS input-data files require, first, the total number of cells, then the total number of submeshes, followed by the definition of each submesh. The definition of a submesh consists of the elevation corresponding to the first mesh point in the submesh, then the elevation corresponding to the last mesh point in the submesh, followed by the number of cells (the number of mesh points minus one) between and including these two elevations.

The prompts that the INDATA module uses to build the mesh block in the hydrology input-data file follow. First, INDATA indicates that it is working on the mesh block:

MESH BLOCK

Then, it determines whether or not to use the automatic mesh generator:

AUTOMATIC MESH GENERATOR (N OR Y):

The automatic mesh generator is discussed later in this subsection. If the automatic mesh generator is *not* specified, INDATA asks for the total number of cells for the entire mesh and the total number of submeshes within the mesh:

ENTER TOTAL # OF CELLS (DEFAULT=200):

ENTER # OF SUBMESHES (DEFAULT=1):

The defaults imply construction of a uniform mesh of 200 cells (201 mesh points) made up of one submesh. The maximum allowable number of cells is 3110; the minimum recommended number of cells is four (actually, four per geologic unit); a more reasonable minimum value is ten per geologic unit. The maximum allowable number of submeshes is the same as the maximum allowable number of cells; and, of course, the minimum is one.

INDATA then prompts for the boundaries of the first submesh (which, in the case of one submesh, is actually the whole mesh):

SUBMESH # 1

ENTER LOWER ELEVATION (DEFAULT=0. m):

ENTER UPPER ELEVATION (DEFAULT=100. m):

ENTER # OF CELLS FOR THIS SUBMESH (DEFAULT=200):

The default values specify that the mesh begins with mesh-point number 1 and ends with mesh-point number 201, and that these mesh points correspond to elevation 0 and elevation 100, respectively. Therefore, each of the 200 cells is 0.5-m long.

If the user had specified several submeshes, INDATA would have continued the submesh data prompting. For instance, consider the following sample session, and assume that in the geologic-unit block the user had specified one geologic unit with a minimum elevation at 3.0 *whatever-units* and a maximum at 3.85 *whatever-units*:

MESH BLOCK

AUTOMATIC MESH GENERATOR (N OR Y): N


```

ENTER TOTAL # OF CELLS (DEFAULT=200): 1000
ENTER # OF SUBMESHES (DEFAULT=1): 3

SUBMESH # 1
ENTER LOWER ELEVATION (DEFAULT=3.0): 3.
ENTER UPPER ELEVATION (DEFAULT=3.85): 3.7
ENTER # OF CELLS FOR THIS SUBMESH (DEFAULT=333): 700

SUBMESH # 2
ENTER LOWER ELEVATION (DEFAULT=3.7): 3.7
ENTER UPPER ELEVATION (DEFAULT=3.85): 3.8
ENTER # OF CELLS FOR THIS SUBMESH (DEFAULT=150): 200

SUBMESH # 3
ENTER LOWER ELEVATION (DEFAULT=3.8): 3.8
ENTER UPPER ELEVATION (DEFAULT=3.85): 3.85
ENTER # OF CELLS FOR THIS SUBMESH (DEFAULT=100): 100

```

In this case, the automatic mesh generator is rejected, and the user asks for 1000 cells to be distributed within three submeshes. INDATA prompts the first submesh with the standard default, which can now be seen to be generated as follows:

- 1) the first lower elevation is taken from the lower elevation of the lowest geologic unit (Section 4.2.7),
- 2) the upper elevation is taken from the upper elevation of the first geologic unit,
- 3) the number of cells is the total number of cells divided by the total number of submeshes.

Note that the submeshes must all fit together. The upper elevation of a submesh must be the same as the lower elevation of the next submesh. When two submeshes meet at an interface between two different geologic units, the mesh point that is placed on the interface is arbitrarily assigned the properties of the geologic unit that appears later in the geologic-unit block. Although it is not required, standard usage normally places a mesh point exactly at the boundary between geologic units.

Some rules with regard to construction of a mesh follow.

- 1) More mesh points, in general, lead to a more accurate solution.
- 2) More mesh points cause longer computer runtimes, for a given problem.
- 3) The more nonlinear the characteristic curves for a given material, the closer together the mesh points should be spaced.
- 4) Mesh points should be spaced closer together where there are changes in the slope of the pressure-head solution (TOSPAC's STEADY and DYNAMICS modules solve for pressure head). The greater the change, the closer the spacing (i.e., the greater the number of cells). These changes are most likely at the interfaces between geologic units (i.e., where material properties change abruptly), and where a pressure-head solution asymptotically approaches a characteristic solution within a given geologic unit.

- 5) Mesh construction is often subjective: if the results produced by a given mesh are unsatisfactory (e.g., if a given steady-state solution has sections in which the flux varies significantly from the input flux), then construct a new mesh. Place mesh points closer together (i.e., add more cells) in the unsatisfactory section. If a section appears particularly stable, the mesh points can be spaced further apart (i.e., delete cells).
- 6) A mesh that generates satisfactory results for steady-state solutions that bound the fluxes specified in a dynamic-flow problem will *not* always suffice for that dynamic-flow calculation.
- 7) A mesh that generates satisfactory results for a steady-state solution that is to be used in a transport problem will *not* always suffice for that transport calculation.
- 8) To check if the mesh-point spacing is influencing the solution, add twice as many mesh points (or perhaps reduce the number of mesh points by half) and rerun the problem; if the same solution is returned, the first mesh was probably satisfactory.

A more rigorous investigation of mesh-point spacing is given in *Volume 1*. Section 2.3 of *Volume 1* contains the discussion of mesh-point spacing for problems involving steady-state and transient flow.

For STEADY calculations, Darcy's Law is examined for length scales in the solution. In the most general situation, *Volume 1* offers Equations 2.3-2 and 2.3-3 as restrictions for selecting appropriate, general mesh-point spacings:

$$\Delta z < \left| \frac{\psi}{1 + q/K} \right|,$$

and

$$\Delta z < \left| \frac{K/K'}{1 + q/K} \right|,$$

where z is elevation and Δz (the change in elevation) is the mesh-point spacing, q is flux, ψ is the pressure head, K is hydraulic conductivity, and K' is the derivative of hydraulic conductivity with respect to pressure head.

These two restrictions work best for the case where the pressure-head solution approaches the characteristic solution in a nonlinear manner, where $\Delta\psi \gg \Delta z$. This situation occurs in a geologic unit that must carry the imposed flux at high pressure heads immediately above a geologic unit that can carry the imposed flux at very low pressure heads; i.e., where the lower unit is applying a pressure to drain the upper unit.

For the special case where the pressure-head solution asymptotically approaches the characteristic solution (the transition point between $\Delta\psi \gg \Delta z$ and $\Delta\psi = 0$) *Volume 1* offers Equation 2.3-7:

$$\Delta z < \left| \frac{q}{K'^c} \right|,$$

where K'^c is the derivative of hydraulic conductivity with respect to the pressure head at the characteristic pressure head (where $K(\psi) = |q|$).

Some users may by now notice that there is a problem with using the above equations to determine the mesh spacing: the solution must be known fairly well in the first place.

Cases exist where a steady-state solution offers no appropriate length scale. Where the pressure-head solution changes in a linear manner, most obviously where $\Delta\psi \approx -\Delta z$ or $\Delta\psi = 0$, any two points can determine a line. The situation $\Delta\psi \approx -\Delta z$ occurs in a geologic unit that can carry the imposed flux at very low pressure heads immediately above a geologic unit that must carry the imposed flux at high pressure heads; i.e., where the lower unit is applying a pressure to dam the upper unit. The $\Delta\psi = 0$ situation occurs at the characteristic solution; i.e., where the hydraulic conductivity equals the flux. (Steady-state solutions in one dimension always reach the characteristic solution if the geologic unit is thick enough.) These situations do not necessarily imply that mesh points can be spaced as far apart as you want. Prudence dictates a reasonable spacing to ascertain that areas where linearity may be violated have not been missed. Also, there could be length scales in the transport solution (the transport calculation would use the same mesh) that should not be overlooked. A discussion of mesh-point spacing for transport calculations is given below.

For DYNAMICS calculations, Equation 2.3-21 in Section 2.3 of *Volume 1* can be used to determine mesh-point spacing in terms of the radii of curvature of the leading and trailing edges of a flux pulse. This equation is as follows:

$$\Delta z < \min \left\{ \left| \frac{q_0}{K'_0 + C_0 v_{fr}} \right|, \left| \frac{q_1}{K'_1 + C_1 v_{fr}} \right| \right\},$$

where z is elevation and Δz is the mesh-point spacing, q is flux, K' is the derivative of hydraulic conductivity with respect to pressure head, C is storage capacity, v_{fr} is the velocity of the flux front, and the subscripts 0 and 1 imply that these parameters occur at the leading and trailing edge of the flux front, respectively. The velocity of the flux front is defined as follows:

$$v_{fr} = \frac{q_1 - q_0}{\theta_1 - \theta_0}.$$

And, as given in Equation 2.3-22 in *Volume 1*, an upper bound on the transient-flow timestep is related to cell size and the velocity of the flux front as follows:

$$\Delta t < \frac{\Delta z}{|v_{fr}|}.$$

In *Volume 1*, Section 3.3 contains a discussion of the bounds on mesh-point spacing for transport problems. Equation 3.3-2 specifies the following:

$$\Delta z < |D/v|,$$

where D is the diffusion/dispersion coefficient and v is the average linear velocity of the water (although this v is not the average linear velocity of the water used in the hydrology discussion. This velocity is q/θ , not $q/(\theta - \theta_r)$; i.e., the residual saturation is not removed from consideration).

In addition, the TRANS solution has an accuracy bound that is of interest to mesh-point spacing. This bound is given in Equation 3.3-3 in *Volume 1*, as follows:

$$\ell < |v|t + Dt/\Delta z,$$

with ℓ being the distance below the repository or the boundary where a contaminant is being introduced, and v is assumed to be negative (downward). This expression gives the region where the numerical transport solution for a simple problem is expected to be accurate. Notice that the region expands linearly with time. If the user is interested in the amount of contaminant reaching the lower boundary, then ℓ is known, and the time that it takes for an accurate solution at that boundary can be calculated. If the accuracy time is greater than the time of interest to the user, the user can decrease Δz .

The above mesh-spacing equations have been reproduced here so that they might be readily available to the user. The user is strongly advised to read and understand the discussion in *Volume 1* before attempting to construct a mesh (before attempting to solve a problem), and before attempting to use these equations.

INDATA also includes an automatic mesh generator that the user can utilize for producing a mechanical, first attempt at a mesh. It is activated by answering *YES* to the INDATA prompt:

MESH BLOCK

AUTOMATIC MESH GENERATOR (N OR Y): Y

INDATA responds with the following prompt:

ENTER STARTING # OF CELLS (DEFAULT=200):

The user enters the number of cells that would correspond to a uniform mesh for a typical problem. Cell size can be fairly large for a STEADY calculation, because difficult areas will be addressed separately. Cell size should be fairly small for a DYNAMICS calculation. This cell size is called the standard cell size in the remainder of this discussion. INDATA now prompts:

LOWER UNIT # 1

ENTER # OF 1%-SPACED CELLS (DEFAULT=0):

ENTER # OF 10%-SPACED CELLS (DEFAULT=0):

UPPER UNIT # 1

ENTER # OF 1%-SPACED CELLS (DEFAULT=0):

ENTER # OF 10%-SPACED CELLS (DEFAULT=0):

INDATA's automatic mesh generator starts with the bottom geologic unit, places the appropriate number of standard-sized cells in the unit, then goes back and fills in the given number of very fine cells (1% cells, i.e., cells that are one-hundredth the size of the standard-sized cells) at the bottom boundary. It then fills in the given number of 10% cells (i.e., cells that are one-tenth the size of the standard-sized cells) immediately following the 1% cells. It then jumps to the top of the unit and places the given number of 1% and 10% cells next to this border.

When the automatic mesh generator is done with the first geologic unit, it has created as many as five submeshes. If 1% cells have been specified at the bottom, the first submesh begins at the bottom boundary and places the specified number of 1% cells there. If 10% cells have been specified at the

bottom, the second submesh begins either at the bottom boundary or where the 1% cells left off and inserts the specified number of 10% cells. The third submesh consists of the standard-sized cells, and runs from where the bottom 10% cells left off and concludes where the upper 10% cells begin.

If no 1% or 10% cells are specified at either the top or the bottom of the unit—this case is the default—then the unit is filled with a uniform mesh of the standard-sized cells. Almost. The standard-sized cells will not always fit exactly into the unit, so they are scaled somewhat. Note that this scaling means that a stratigraphy of several geologic units will usually have slightly different standard-sized cells in each unit.

If the user has specified more than one geologic unit in the geologic-unit block (Section 4.2.7), the automatic mesh generator continues to prompt for information:

```

LOWER UNIT # 2
ENTER # OF 1%-SPACED CELLS (DEFAULT=0):
ENTER # OF 10%-SPACED CELLS (DEFAULT=0):
UPPER UNIT # 2
ENTER # OF 1%-SPACED CELLS (DEFAULT=0):
ENTER # OF 10%-SPACED CELLS (DEFAULT=0):

LOWER UNIT # 3
ENTER # OF 1%-SPACED CELLS (DEFAULT=0):
ENTER # OF 10%-SPACED CELLS (DEFAULT=0):
UPPER UNIT # 3
ENTER # OF 1%-SPACED CELLS (DEFAULT=0):
ENTER # OF 10%-SPACED CELLS (DEFAULT=0):

```

```

o
o
o

```

When the automatic mesh generator has received information for all the geologic units, it signals:

AUTOMATIC MESH GENERATOR WORKING...

The automatic mesh generator allows a different number of 1% and 10% cells in each geologic unit because hydrologic properties of the units vary and, at times, vastly dissimilar units abut. At these interfaces, a greater number of 1% and 10% cells should be entered. When hydrologically similar units abut, it may not be necessary to enter any 1% cells—or any 10% cells, either.

The reason that the automatic mesh generator allows a different number of 1% and 10% cells at the bottom of a geologic unit as compared with the top is more complicated. With a steady-state hydrology, the higher up in a unit, the more the pressure head has approached the characteristic solution for that unit (again, details are in *Volume 1*); i.e., the more regular and less nonlinear it has become. Thus, mesh points can be spaced farther apart and still accurately track this behavior. Unfortunately, with a dynamic hydrology, this condition does not hold. But dynamic instabilities must usually be controlled by reducing the size of the standard-sized cells, and hence, the user still may be able to specify many fewer 1% and 10% cells at the top of a geologic unit.

```

***** MESH BLOCK *****
38      TOTAL # CELLS
5      # SUBMESHES
SUBMESH # 1:
0.000000E+00    LOWER ELEVATION
1.000000        UPPER ELEVATION
10           # CELLS
SUBMESH # 2:
1.000000        LOWER ELEVATION
11.00000       UPPER ELEVATION
10           # CELLS
SUBMESH # 3:
11.00000       LOWER ELEVATION
94.50000      UPPER ELEVATION
8            # CELLS
SUBMESH # 4:
94.50000      LOWER ELEVATION
99.50000      UPPER ELEVATION
5            # CELLS
SUBMESH # 5:
99.50000      LOWER ELEVATION
100.0000     UPPER ELEVATION
5            # CELLS

```

Figure 4.10: Mesh block generated by the automatic mesh generator.

If the user intends to use the mesh for a transport calculation, it is recommended that the source-region boundaries fall exactly on mesh points (Section 4.2.13). There are three possible courses of action:

- 1) If the automatic mesh generator is to be used, it is advised to define the source region as a geologic unit (Section 4.2.7).
- 2) If the automatic mesh generator is *not* to be used, construct a special submesh for the source region and define the submesh boundaries to coincide with the source region boundaries.
- 3) Or, whether or not the automatic mesh generator is used, the user can construct a mesh, compute the elevations to mesh points around the source region, and then use the closest desirable elevations as the boundaries for the source region. (TRANS makes this approximation automatically if the source boundaries do not correspond to mesh points.)

Figure 4.10 presents an example of a mesh block created by the automatic mesh generator for the mill-tailings example in Chapter 2. The block was created with the following commands.

```

MESH BLOCK
AUTOMATIC MESH GENERATOR (N OR Y): Y

ENTER STARTING # OF CELLS (DEFAULT=200): 10

LOWER UNIT # 1
ENTER # OF 1%-SPACED CELLS (DEFAULT=0): 10
ENTER # OF 10%-SPACED CELLS (DEFAULT=0): 10

```

```
UPPER UNIT # 1
ENTER # OF 1%-SPACED CELLS (DEFAULT=0): 5
ENTER # OF 10%-SPACED CELLS (DEFAULT=0): 5
```

Figure 4.11 shows a plot of the mesh produced by this mesh block. The mesh is for one geologic unit having a total of 38 cells (39 mesh points) in five different submeshes, beginning at the bottom boundary with ten cells of 1% size, followed by ten cells of 10% size, followed by eight cells of standard size, followed by five cells of 10% size, and ending at the upper boundary with five cells of 1% size. Notice that the number of standard-sized cells was reduced from ten to eight when the smaller cells were fit into the mesh.

The mesh block occurs only in a hydrology input-data file; further examples can be seen in Figures 2.3, 3.2, and 3.20.

4.2.10 Boundary-Condition Block (Hydrology)

Boundary conditions are algebraic constraints applied to values of a differential equation. In general, boundary conditions can be satisfied at discrete points for the purpose of yielding a unique solution to the differential equation.

For a TOSPAC hydrology calculation, the boundary conditions are two values assigned to the outermost mesh points of a finite-difference mesh that allows these points to be fully defined. These values can, with certain restrictions, be specified either in terms of pressure head or flux (in a one-dimensional calculation, flux equals Darcy velocity, percolation rate, and rate of infiltration).

The boundary-condition block serves several purposes:

- 1) defines boundary conditions, of course,
- 2) defines times when boundary conditions can change (DYNAMICS only), and
- 3) defines times when results are written to the output-listing file and the plot-data file (DYNAMICS only).

The boundary-condition block is organized according to "time snapshots." Time means problem time—time simulated in a calculation—not real time. Snapshot means a peek at the results the problem has generated at that specific time.

At least one time snapshot must be defined. If only one time snapshot is defined, the problem is a steady-state-flow problem. If STEADY is executed with an input-data file that contains more than one time snapshot, only the first is considered. A transient-flow calculation is specified by entering more than one time snapshot. If DYNAMICS is executed with an input-data file that only contains one time snapshot, execution terminates after printing out the initial conditions. Both STEADY and DYNAMICS can run any hydrology input-data file (as long as the boundary conditions are appropriate, as discussed below).

A time snapshot is defined by a begin time, a boundary condition, and the parameters for the boundary condition. At any time snapshot the user is allowed to set or change boundary conditions. A boundary condition is active from the time of the snapshot where it is defined to the time of the next

Figure 4.11: Mesh/stratigraphy plot of the mesh defined in Figure 4.10.

snapshot. The last snapshot specifies the end time of the calculation. (For STEADY, which allows only one time snapshot, the last snapshot is also the first.) The last snapshot of a DYNAMICS calculation does not require a boundary condition.

For a DYNAMICS calculation, intermediate results are produced at every time snapshot. STEADY calculations generate only final results. Results are written into the output-listing file and plot-data file (Section 4.7). These results can be used for computer graphics by the OUTPLOT module, and the STEADY results can be used by TRANS to define the hydrologic background for a transport calculation.

The more time snapshots that are defined in a transient-flow calculation, the better the resolution in the OUTPLOT computer graphics routines, and the better the ability of the user to understand the details of the calculation. However, the more time snapshots, the bigger the output files (the output-listing file, in particular, but also the plot-data file). The number of time snapshots may be dictated by the user's disk space. Section 3.2 contains a discussion of the size of the output files generated during the execution of the waste-repository example problem.

Within the INDATA module, the prompts for data begin with the block identifier and proceed as follows:

BOUNDARY-CONDITION BLOCK

INDATA next queries for the number of time snapshots the user wishes to define:

ENTER # OF TIME SNAPSHOTS (DEFAULT=1):

The number of time snapshots must be an integer between 0 and 100, inclusive.

For the boundary-condition block alone, for time-snapshot times alone, INDATA incorporates a method for converting a variety of time units into other standard time units. The conversion is specified through a menu:

```
TIME CONVERSION MENU
0. NO CONVERSION
1. NO CONVERSION (SECONDS ASSUMED)
2. CONVERT HOURS TO SECONDS
3. CONVERT DAYS TO SECONDS
4. CONVERT YEARS TO SECONDS
5. NO CONVERSION (YEARS ASSUMED)
6. CONVERT SECONDS TO YEARS
7. CONVERT HOURS TO YEARS
8. CONVERT DAYS TO YEARS
ENTER CHOICE (DEFAULT=1): 4
```

This entry requires explanation. As mentioned previously, TOSPAC input data can be in any units as long as the data are self-consistent. Thus, the user can enter time data in any units (e.g., seconds, minutes, hours, fortnights, eons, etc.) as long as all time-dependent input data are based on the same scale (e.g., hydraulic conductivity must be in cubits per eon if the units are cubits-tonnes-eons). This freedom is cumbersome when entering very long times in seconds, or very short times in years. If the user wishes to enter time in the units he or she chose originally, e.g., seconds for *SI* units, then the user can enter a choice of 0, 1 (the default), or 5 (if the time units were years). If the user wishes to enter

time in a different unit, then the user can select the appropriate choice and enter the appropriate integer.

The time conversion number carries over to the OUTPLOT module, where the default time-related messages—axis labels and legend labels—will be determined from the response to the time-conversion menu.

For instance, groundwater in a partially saturated regime often moves very slowly, and the user may have entered all input data in *SI* units, but would rather define the time snapshots in years rather than seconds. In the above example, choice 4 is entered to produce this conversion. When the calculation is complete and the OUTPLOT module of TOSPAC is run to create plots of the results, the default time units on the plots will be in years.

If the time units everywhere in the input-data file are self-consistent, a choice of 0 could be entered. The disadvantage to this choice is that when OUTPLOT produces the plots for this calculation, it would use the word UNITS as the default time-unit message. If time units were in seconds everywhere in the input-data file, a choice of 1 could be entered (or the default <CR>), and then the time-snapshot times should be entered in seconds. The time-message default in OUTPLOT will then be seconds. If the time units everywhere in the input-data file were in years, a choice of 5 could be entered, and then the time-snapshot times should be entered in years. The time-message default in OUTPLOT will then be years.

Once the user selects a time conversion, he or she *must* enter *all* times for the time snapshots in the boundary-condition block in the selected units.

INDATA now prompts for data for each time snapshot as follows:

```
SNAPSHOT # 1
ENTER TIME (DEFAULT=0. yr):
```

Time can be any real number. However, time must always be greater than the time given for the preceding time snapshot. The default value for time always begins at zero—in this case, 0 yr, because a time-conversion choice of 4 (above) indicated that the time snapshots were being entered in years. For subsequent prompts the default becomes two times the time entered for the previous snapshot. For instance, if the user enters 1 for the time of the first snapshot, the next time prompt will have a default time of 2; if the user enters a value of 60, the next default will be 120; etc.

The remainder of the time-snapshot data are dependent on the type of boundary condition specified. The prompt for the boundary-condition flag and the prompts resulting from a boundary-condition flag of 12 are as follows:

```
BOUNDARY-CONDITION FLAGS ARE 2 DIGITS (LOWER/UPPER):
0. USE PREVIOUS BOUNDARY CONDITION
1. PRESSURE-HEAD BOUNDARY
2. FLUX BOUNDARY
3. POND-DRAIN BOUNDARY (UPPER ONLY)
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=12):
ENTER LOWER-BOUNDARY PRESSURE HEAD (DEFAULT=0. m):
ENTER UPPER-BOUNDARY FLUX (DEFAULT=0. m/s):
ENTER MAX POND HEIGHT (DEFAULT=0. m):
```

		SECOND DIGIT UPPER BOUNDARY FLAG				
		0	1	2	3	
FIRST DIGIT LOWER BOUNDARY FLAG	0	00 PREVIOUS LOWER PREVIOUS UPPER	01 PREVIOUS LOWER PRESSURE-HEAD UPPER	02 PREVIOUS LOWER FLUX UPPER	03 PREVIOUS LOWER POND-DRAIN UPPER	NOT ALLOWED FOR FIRST TIME SNAPSHOT
	1	10 PRESSURE-HEAD LOWER PREVIOUS UPPER	11 PRESSURE-HEAD LOWER PRESSURE-HEAD UPPER	12 PRESSURE-HEAD LOWER FLUX UPPER	13 PRESSURE-HEAD LOWER POND-DRAIN UPPER	
	2	20 FLUX LOWER PREVIOUS UPPER	21 FLUX LOWER PRESSURE-HEAD UPPER	22 FLUX LOWER FLUX UPPER	23 FLUX LOWER POND-DRAIN UPPER	THE ONLY FLAG PRESENTLY ALLOWED FOR STEADY!
		NOT ALLOWED FOR FIRST TIME SNAPSHOT		ALSO REQUIRES MAX POND HEIGHT		

Figure 4.12: Boundary-condition flags for STEADY and DYNAMICS.

The boundary-condition flag is a two-digit number that specifies the type of boundary condition. The first digit specifies the type of boundary condition at the lower boundary; the second digit specifies the upper boundary. The allowable digits and the corresponding types of boundary conditions are as follows:

Flag Digit=0 the previously defined boundary-condition type (the first time snapshot has no previously defined boundary condition, so entering a 0 is not allowed there),

Flag Digit=1 a boundary condition defined by a constant pressure head,

Flag Digit=2 a boundary condition defined by a constant flux, and

Flag Digit=3 a boundary-condition defined by a pressure head that decreases over time, simulating a pond draining into the column.

Information about boundary-condition flags used by STEADY and DYNAMICS is summarized in Figure 4.12.

A boundary defined by a pressure head (flag 1) is a real number that specifies a constant pressure head

at the boundary mesh point. Values greater than the air-entry pressure head of the material or materials assigned to this mesh point imply a saturated condition. Values less than the air-entry pressure head imply an unsaturated condition at the top of the column.

A flux-defined boundary (flag 2) is a real number corresponding to a constant rate of infiltration or exfiltration. A *negative* value implies a *downward* flux. A negative flux at the upper boundary means that water is entering the column at the top; a negative flux at the lower boundary means that water is leaving the column at the bottom. A positive flux at the upper boundary means that water is exiting the column at the top; a positive flux at the lower boundary means that water is entering the column at the bottom.

When a boundary condition is entered as a flux, STEADY and DYNAMICS convert it to a pressure head. (Both the STEADY and the DYNAMICS modules solve a problem for pressure head; i.e., the difference equations are written so that pressure head is the unknown variable, and saturation, velocity, etc., are calculated from the computed pressure head.)

A maximum-pond-height prompt appears only with boundary-condition flags 21 and 22—the conditions determined by flux at the upper boundary. The maximum pond height is a method for limiting the amount of water allowed into a column. The physical interpretation is that water above the maximum pond height would run off. If the specified flux is greater than the saturated hydraulic conductivity at the top of the column, the water will pond until it reaches the maximum pond height. At this point, the flux boundary condition terminates and a pressure-head boundary condition supplants it. The pressure-head boundary condition is equal to the maximum pond height, because pond height translates directly into pressure head (a pond 20 m deep has a pressure head of 20 m at the pond bottom).

Specification of a pond-drain boundary (flag 3) begins with a nonnegative real number corresponding to an initial pond height (depth). The initial pond height is the same value as the pressure head at the top of the column. As the problem progresses, DYNAMICS decreases this value to simulate water entering the column. (The pressure-head boundary condition can also be used to simulate a pond at the top of the column; however, it is a pond of constant height—the water draining into the column is constantly being replaced.) The pond-drain boundary condition is only valid at the upper boundary.

A pond-drain boundary also includes parameters for a flux boundary condition; if and when the pond-drain pressure head is decreased to a negative value (i.e., the pond has completely drained), the pond-drain condition reverts to the flux-defined condition. At the time when the pond-drain pressure head is decreased to a negative value, a new time snapshot is automatically formed in the plot-data and the output-listing files, and a message is written to the user's terminal. The presence of this new time snapshot has consequences in two areas: to correctly plot and label time snapshots when using the OUTPLOT module (Section 4.6.4 contains a discussion of using OUTPLOT for DYNAMICS results); and, to correctly determine the restart number for restarting a DYNAMICS calculation (Sections 4.2.6 and 4.4.3).

The solution method currently used in STEADY (see *Volume 1*) only allows boundary conditions of type 12: a pressure-head lower boundary and a flux upper boundary. In addition, two other restrictions on STEADY boundary conditions are enforced:

- 1) the flux must be nonpositive: $q \leq 0$, and
- 2) the flux must not exceed the saturated hydraulic conductivity of any of the units: $|q| \leq K_s$.

These requirements are not unduly restrictive, as most problems of interest satisfy them. A typical STEADY problem specifies the position of the water table at the bottom of the column by setting the pressure head, and specifies the infiltration rate into the top of the column by setting the flux. STEADY ignores the entries for time and maximum pond height that are produced with boundary-condition type 12.

The INDATA-produced defaults for a boundary-condition type 12 specify a flux of zero at the top of the column and a pressure head of zero at the bottom. This case corresponds to a hydrostatic or no-flow condition, with the water table at the bottom.

DYNAMICS does not enforce the above restrictions, but the user must be careful in specifying the boundary conditions. If outflow is specified at a boundary (i.e., $q > 0$ at the top boundary, or $q < 0$ at the bottom boundary), there may be no mathematical solution to the problem if there is not enough water present to support the outflux. In such a case, DYNAMICS might execute, but could return an incorrect solution. When the water content is depleted to the point that there is not enough water present to flow out at the rate specified, the DYNAMICS solution will develop a discontinuity at the boundary and the effective boundary condition will be no flow, rather than the outflow specified.

If flux exceeds the saturated conductivity in a DYNAMICS calculation, a perched water zone will develop. The DYNAMICS solution should be correct in such a case, but it might require very small timesteps.

After the first time snapshot, the default for the boundary-condition flag changes to 00: the boundary conditions are to be the same as previously specified. All boundary-condition flags are acceptable input for a dynamic-flow problem, except that the first time snapshot cannot have 0 for either digit.

An example of the INDATA prompts for a DYNAMICS run with several time snapshots follows.

BOUNDARY-CONDITION BLOCK

ENTER # TIME SNAPSHOTS (DEFAULT=1): 7

TIME CONVERSION MENU

- 0. NO CONVERSION
- 1. NO CONVERSION (SECONDS ASSUMED)
- 2. CONVERT HOURS TO SECONDS
- 3. CONVERT DAYS TO SECONDS
- 4. CONVERT YEARS TO SECONDS
- 5. NO CONVERSION (YEARS ASSUMED)
- 6. CONVERT SECONDS TO YEARS
- 7. CONVERT HOURS TO YEARS
- 8. CONVERT DAYS TO YEARS

ENTER CONVERSION NUMBER (DEFAULT=1): 1

SNAPSHOT # 1

ENTER TIME (DEFAULT=0. s): 0.

BOUNDARY-CONDITION FLAGS ARE 2 DIGITS (LOWER/UPPER):

- 0. USE PREVIOUS BOUNDARY CONDITION
- 1. PRESSURE-HEAD BOUNDARY
- 2. FLUX BOUNDARY
- 3. POND-DRAIN BOUNDARY (UPPER ONLY)

```

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=12): 12
ENTER LOWER-BOUNDARY PRESSURE HEAD (DEFAULT=0. m): 20. m
ENTER UPPER-BOUNDARY FLUX (DEFAULT=0. m/s): -1. m/s
ENTER MAX POND HEIGHT (DEFAULT=0. m): 1. m

SNAPSHOT # 2
ENTER TIME (DEFAULT=0. s): 3.16E+7 s
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 22
ENTER LOWER-BOUNDARY FLUX (DEFAULT=0. m/s): -1. m/s
ENTER UPPER-BOUNDARY FLUX (DEFAULT=0. m/s): -1. m/s
ENTER MAX POND HEIGHT (DEFAULT=0. m): 1. m

SNAPSHOT # 3
ENTER TIME (DEFAULT=6.32E+7 s): 3.16E+8 s
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 11
ENTER LOWER-BOUNDARY PRESSURE HEAD (DEFAULT=0. m): -3. m
ENTER UPPER-BOUNDARY PRESSURE HEAD (DEFAULT=0. m): 100. m

SNAPSHOT # 4
ENTER TIME (DEFAULT=6.32E+8 s): 3.16E+9 s
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 21
ENTER LOWER-BOUNDARY FLUX (DEFAULT=0. m/s): 5. m/s
ENTER UPPER-BOUNDARY PRESSURE HEAD (DEFAULT=0. m): 0. m

SNAPSHOT # 5
ENTER TIME (DEFAULT=6.32E+9 s): 3.16E+10 s
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 13
ENTER LOWER-BOUNDARY PRESSURE HEAD (DEFAULT=0. m): 0. m
ENTER UPPER-BOUNDARY FLUX (DEFAULT=0. m/s): 0. m/s
ENTER MAX POND HEIGHT (DEFAULT=0. m): 5. m

SNAPSHOT # 6
ENTER TIME (DEFAULT=6.32E+10 s): 3.16E+11 s
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 00

SNAPSHOT # 7
ENTER TIME (DEFAULT=6.32E+11 s): 3.16E+12 s

```

This example shows a request for seven time snapshots, defining the following calculation:

- 1) The first snapshot begins at the initial problem time of 0 s. The initial conditions of the problem are written to the output-listing file and the plot-data file. Boundary-condition flag 12 (the default) is operable: a pressure-head lower boundary and a flux upper boundary. As specified, the lowermost mesh point is to be assigned a value of 20 m of pressure head. The uppermost mesh point is to be assigned a pressure-head value that corresponds to an influx of 1 m/s. A maximum pond height of 1 m is specified. If the column will not accept an influx of 1 m/s (either because it exceeds the saturated hydraulic conductivity of the upper geologic unit, or because water cannot exit the column fast enough), then the upper boundary condition will become a pressure head of 1 m.
- 2) The second snapshot is to occur at 1 yr (3.16×10^7 s). At this time a change in the boundary

condition is specified. Intermediate results are written to the output-listing file and the plot-data file, and then the boundary-condition flag is set to number 22: flux lower and flux upper boundary. The lower condition is specified as an outflux of 1 m/s and the the upper boundary condition is specified as an influx of 1 m/s. If this specification is left on long enough, and if the column can accept a flux of this magnitude, the water flow should go to steady state. If the column cannot accept a flux this large, a maximum pond height of 1 m is specified.

- 3) The third snapshot is to occur at 10 yr (3.16×10^8 s). Intermediate results are written to the output-listing and the plot-data files. Again the boundary conditions are changed; the boundary-conditions flag is now number 11: pressure-head lower and upper boundaries. The lower boundary is specified as -3 m pressure head, which means that water will probably be drained from the column to maintain this negative pressure head. The upper boundary is specified as 100 m pressure head, which means that water will be forced into the column as if from the bottom of a 100-m-deep pond.
- 4) The fourth snapshot is to occur at 100 yr (3.16×10^9 s). Intermediate results are written to the output-listing and the plot-data files, and the boundary-condition type is now changed to number 21. The lower boundary is specified as 5 m/s flux, which means that water is forced into the column from the bottom. The upper boundary is specified as 0 m pressure head, which means that the water table is at the top of the column.
- 5) The fifth snapshot is to occur at 1000 yr (3.16×10^{10} s). Intermediate results are written to the output-listing file and the plot-data file. A pond has been placed at the top of the column, and it will begin to drain into the column until the boundary condition is changed or until a steady state is reached (in this case, steady state would be a hydrostatic condition). The lower boundary is specified as 0 m pressure head, which means that the water table is now at the bottom of the column.
- 6) The sixth snapshot is to occur at 10,000 yr (3.16×10^{11} s). Again, intermediate results are written to the output-listing file and the plot-data file, but this time the boundary conditions are not changed. The boundary condition for this snapshot is specified as flag number 00: use the same boundary conditions as those specified for the immediately preceding (fifth) time snapshot. The pond-drain boundary condition is still active and the pond continues to drain.
- 7) The final snapshot is to occur at 100,000 yr (3.16×10^{12} s). This snapshot marks the end of the calculation; at this point, the final results are written to the output-listing file and the plot-data file. No new boundary conditions are specified.

Figure 4.13 presents an example of the boundary-condition block for a DYNAMICS input-data file created by INDATA in response to the above prompts.

4.2.11 File Block (Hydrology and Transport)

The file block defines the files to be used or created during execution of STEADY, DYNAMICS, or TRANS. The file block also allows the user to control the amount of results written to the output-listing file. The main purpose of the file block is to provide an audit trail between the input-data file and the output files that result from its use.

In INDATA, when a STEADY input-data file is being created, the file-block prompts are as follows:

FILE BLOCK

```

***** BOUNDARY-CONDITION BLOCK *****
7          # TIME SNAPSHOTS
1          TIME CONVERSION NUMBER
SNAPSHOT # 1
0.         PROBLEM TIME
12         BOUNDARY-CONDITION FLAG
20. m      LOWER-BOUNDARY PRESSURE HEAD
1. m/s     UPPER-BOUNDARY FLUX
1. m       MAX POND HEIGHT
SNAPSHOT # 2
3.16E+7 s  PROBLEM TIME
22         BOUNDARY-CONDITION FLAG
-1. m/s    LOWER-BOUNDARY FLUX
-1. m/s    UPPER-BOUNDARY FLUX
1. m       MAX POND HEIGHT
SNAPSHOT # 3
3.16E+8 s  PROBLEM TIME
11         BOUNDARY-CONDITION FLAG
-3. m      LOWER-BOUNDARY PRESSURE HEAD
100. m     UPPER-BOUNDARY PRESSURE HEAD
SNAPSHOT # 4
3.16E+9 s  PROBLEM TIME
21         BOUNDARY-CONDITION FLAG
5. m/s     LOWER-BOUNDARY FLUX
0. m       UPPER-BOUNDARY PRESSURE HEAD
SNAPSHOT # 5
3.16E+10 s PROBLEM TIME
13         BOUNDARY-CONDITION FLAG
0. m       LOWER-BOUNDARY PRESSURE HEAD
0. m/s     UPPER-BOUNDARY FLUX
5. m       MAX POND HEIGHT
SNAPSHOT # 6
3.16E+11 s PROBLEM TIME
00         BOUNDARY-CONDITION FLAG
SNAPSHOT # 7
3.16E+12 s PROBLEM TIME

```

Figure 4.13: DYNAMICS boundary-condition block example.

```

STEADY SOLUTION FILE DEFAULT NAME: STEADY.PSI
ENTER STEADY SOLUTION FILE NAME:
PLOT-DATA FILE DEFAULT NAME: STEADY.PLT
ENTER PLOT-DATA FILE NAME:
OUTPUT-LISTING FILE DEFAULT NAME: STEADY.LIS
ENTER OUTPUT-LISTING FILE NAME:
ENTER OUTPUT-LISTING CONTROL (DEFAULT=1):

```

The first three prompts ask for the name of the indicated output file to be created. The file names are strings of up to 80 characters with no embedded blanks. If the user does not want one or more of these files to be created, the user should respond with the word *NONE* to the prompt.

The final prompt asks for a control number for the output-listing file. The control number must be a nonnegative integer. Control number 0 means do not create the file (as does the word *NONE* in response to the prompt for the file name). Control number 1 means to write results for all mesh points onto the file. Control number *N* means to restrict the results written onto the file, as follows: write results for the mesh points at the boundaries and geologic-unit interfaces; write results for every mesh point that is a multiple of *N*; and, in the case of a TRANS run with an internal source, write results for the top and bottom mesh points of the source region.

In INDATA, when a DYNAMICS input-data file is being created, the prompts for the file block are as follows:

```
FILE BLOCK
INITIAL-CONDITION FILE DEFAULT NAME: STEADY.PSI
ENTER INITIAL-CONDITION FILE NAME:
PLOT-DATA FILE DEFAULT NAME: DYNAMICS.PLT
ENTER PLOT-DATA FILE NAME:
OUTPUT-LISTING FILE DEFAULT NAME: DYNAMICS.LIS
ENTER OUTPUT-LISTING FILE NAME:
ENTER OUTPUT-LISTING CONTROL (DEFAULT=1):
```

The prompts are the same as those issued for a STEADY input-data file, except that the first prompt is worded differently. The first prompt is for a file containing the pressure-head data to be assigned to the mesh as an initial condition. A STEADY solution file can be used for an initial-condition file, or the user can create the file by other means. DYNAMICS has provision for an initial-condition block (Section 4.2.12) which allows several methods of defining an initial condition. If a DYNAMICS input-data file contains both a file block and an initial-condition block, the initial-condition block overrides the initial-condition-file specification in the file block. In this case, therefore, the following is recommended: if the initial-condition block also specifies an initial-condition file, then the same initial-condition-file name should be entered in both the file block and the initial-condition block; and if the initial-condition block specifies a different method for defining the initial condition, then the word *NONE* should be given as the initial-condition-file name in the file block.

In INDATA, when a TRANS input-data file is being created, the prompts for the file block are as follows:

```
FILE BLOCK
STEADY PLOT-DATA FILE DEFAULT NAME: STEADY.PLT
ENTER STEADY PLOT-DATA FILE NAME:
TRANS PLOT-DATA FILE DEFAULT NAME: TRANS.PLT
ENTER TRANS PLOT-DATA FILE NAME:
OUTPUT-LISTING FILE DEFAULT NAME: TRANS.LIS
ENTER OUTPUT-LISTING FILE NAME:
ENTER OUTPUT-LISTING CONTROL (DEFAULT=1):
```

The prompts are similar to those given for STEADY and DYNAMICS input-data files. Only the first prompt asks for a different file. TRANS expects a hydrology plot-data file (presently only from STEADY) as input, unless a saturated-zone block is present. If the word *NONE* is entered in response to the hydrology plot-data-file name and a saturated-zone block is *not* present, TOSPAC will prompt for a file name when TRANS is executed.

Figure 3.21 gives an example of a file block in a TRANS input-data file. Notice that the control number for the output-listing file is 200. In Figure 3.23, the resulting TRANS output-listing file is shown. In the section where concentrations are listed by mesh point, only the concentrations for the following mesh points have been written:

- 1) boundary mesh points,
- 2) mesh points at interfaces between geologic units,
- 3) every 200th mesh point, and

- 4) the top and bottom mesh points of the source region.

The file block is optional. If no file block is present in an input-data file when one of the calculational modules is executed, TOSPAC prompts the user for file information. Besides Figure 3.21, examples of file blocks can be found in Figures 2.3, 2.4, 3.2, and 3.20.

4.2.12 Initial-Condition Block (Hydrology)

An initial condition is a set of values assigned to a calculational mesh before attempting a solution. For the DYNAMICS module, which solves for pressure head, the initial condition consists of the set of pressure-head values at each mesh point before a calculation begins.

STEADY *calculates its own initial condition*. Therefore, the hydrology initial-condition block is only used by DYNAMICS. When creating a STEADY input-data file, INDATA will not prompt for an initial-condition block. If an initial-condition block appears in a steady-state input-data file, it is ignored during execution of STEADY.

If the input-data file specifies a dynamic-flow calculation and the initial-condition block does not exist, DYNAMICS will first attempt to open and read the initial-condition file specified in the file block. If no file block is present, DYNAMICS will attempt to open and read the STEADY solution file (the file of pressure-head values created by STEADY, default name STEADY.PSI); if the STEADY solution file is not then found, an error results.

INDATA prompts for initial-condition data as follows:

INITIAL-CONDITION BLOCK

INITIAL-CONDITION FLAGS ARE:

1. FILE-DEFINED PRESSURE HEADS
2. HYDROSTATIC (NO FLOW)
3. CONSTANT PRESSURE HEAD

ENTER INITIAL-CONDITION FLAG (DEFAULT=1):

Three different methods of defining an initial pressure head are allowed:

Flag=1 file: each mesh point is assigned a pressure-head value read from a file previously created by the STEADY module or by the user.

Flag=2 hydrostatic: pressure heads are calculated for each mesh point so that a no-flow condition results.

Flag=3 constant: each mesh point is assigned a specified constant pressure head.

The default initial-condition flag is number 1: read the pressure-head values from a file. This default is used because STEADY creates a file of pressure-head values (the STEADY solution file, default name STEADY.PSI), and many interesting dynamic-flow problems involve perturbations of steady-state flows. If an initial-condition flag of 1 is specified, INDATA generates one other prompt:

INITIAL-CONDITION FILE DEFAULT NAME: STEADY.PSI

ENTER INITIAL-CONDITION FILE NAME:

The initial-condition-file name is a string of up to 80 characters with no embedded blanks. STEADY.PSI is the default name for the pressure-head file created by the STEADY module. If the user ran STEADY previously during this run, the default would be whatever name the user specified upon entry into STEADY. Section 4.7.2 contains a description of contents and format of the initial-condition file.

If an initial-condition flag of 2 is selected, INDATA again generates one other prompt:

ENTER PRESSURE HEAD AT LOWER BOUNDARY (DEFAULT=0. m):

The pressure head at the first mesh point (the bottom of the mesh) is used to calculate the pressure heads for all the mesh points so that a hydrostatic condition begins the dynamic-flow calculation. The equation used to determine the hydrostatic condition is as follows: $\psi = \psi_1 - z$. Note that the bottom pressure head need not be the same as the pressure head specified in the first boundary condition (if one is specified). The default lower pressure head of 0 specifies the water table at the bottom boundary.

If an initial-condition flag of 3 is selected, INDATA again generates one other prompt:

ENTER CONSTANT PRESSURE HEAD (DEFAULT=0. m):

This constant pressure head will be assigned to every mesh point at the beginning of a dynamic-flow calculation. The default is a condition of incipient saturation. It should be noted that a constant pressure head across the mesh results in an initial downward flow because of gravity. If the user starts a dynamic-flow calculation with a constant pressure head of 0, an upper-boundary-condition flux of 0, and a lower-boundary-condition pressure head of zero, the column drains until it reaches a hydrostatic condition identical to that which can be specified with a number 2 initial-condition flag.

An example of an initial-condition block in a DYNAMICS input-data file can be found in Figure 3.2.

4.2.13 Source Block (Transport)

The source (also called the source term) is the origin of the contamination in a transport problem. The source is composed of the following parts:

- 1) the initial location of the contaminants in the geologic stratigraphy of a transport problem (this location can also be called the source region);
- 2) the initial inventory, or amount, of the contaminant; and
- 3) the method by which the contaminants are released from the source region.

The source block includes information on location and method of release. Because a large number of contaminants can be included in one problem, the initial inventory of a contaminant is defined in the contaminant-property block, Section 4.2.16. TOSPAC presently allows only one source region interior to the mesh and one method of release in a given problem.

INDATA begins prompting for a source block by first identifying the block, then asking for release-model information:

SOURCE BLOCK

SOURCE FLAGS ARE:

0. SOURCE SET BY BOUNDARY CONDITION
1. INTERIOR, CONGRUENT-LEACH SOURCE
2. INTERIOR, SOLUBILITY-LIMIT SOURCE
3. INTERIOR, FILE-DEFINED SOURCE
4. INTERIOR, SAND91-0155 SOURCE

ENTER SOURCE FLAG (DEFAULT=0):

The source-term flag can take on five values, as follows:

Flag=0 source region is exterior to the mesh with the source term set in the boundary condition (this flag is the default).

Flag=1 source region is interior to the mesh with the source term based on a congruent-leach model.

Flag=2 source region is interior to the mesh with the source term based on a solubility-limited-leach model.

Flag=3 source region is interior to the mesh with the source term defined in a file.

Flag=4 source region is interior to the mesh with the source term based on a series of analytic formulas.

In the congruent-leach model, the rate of release for all contaminants is dependent on the solubility limit of the first contaminant defined in the contaminant-property block. For example, the congruent-leach model is used in the problem given in Section 3.2, where the solubility of the first contaminant, ^{238}U , controls the release rates for all the other contaminants. The congruent-leach source term used is described in detail in *Volume 1*. Note one peculiarity of TOSPAC's congruent-leach source is that a container lifetime of 3000 yr is implicit.

In the solubility-limited-leach model the rate of release of each contaminant is determined by its own solubility limit. If there is only one contaminant, the congruent-leach model and the solubility-limited-leach model are similar, but the solubility-limited-leach model has greater releases at early times (because of the container lifetime in the congruent-leach source). The SAND91-0155 source model is a parametric model allowing greater flexibility in specifying how the radionuclides are released from the engineered-barrier system (Wilson, 1991).

If the source-term flag is specified as 0, the prompting begins as follows:

ENTER AREA OF REPOSITORY (DEFAULT=1. m**2):

If the source-term flag is specified as 1, 2, 3, or 4, the next two prompts are:

ENTER ELEVATION OF SOURCE LOWER BOUNDARY (DEFAULT=0. m):

ENTER ELEVATION OF SOURCE UPPER BOUNDARY (DEFAULT=0. m):

Source boundary elevations must be real numbers and must be less than the maximum elevation and greater than the minimum elevation of the mesh. The lower boundary of the source must be below the upper boundary. A source region must encompass at least one cell; hence, the upper and lower boundaries cannot be at the same elevation.

As discussed in the geologic-unit block (Section 4.2.7) and the mesh block (Section 4.2.9), the source-boundary elevations should fall exactly on mesh points. Whether these elevations and points coincide cannot be determined at the time INDATA is creating the transport input-data file. If TRANS attempts to run with these elevations and points out of alignment, TRANS puts the source boundaries at nearby mesh points, perhaps changing the problem in an undesirable way. TRANS issues a warning message to alert the user to the situation.

An interior source region *cannot* include either the lower or upper boundary mesh point. Furthermore, source regions that begin only one cell in from either boundary can cause large errors in the mass balance; therefore, it is recommended that several cells be inserted between a source region and a mesh boundary.

INDATA continues by prompting for information concerning the physical layout of the contaminant in the source region—i.e., the repository:

```
ENTER AREA OF REPOSITORY (DEFAULT=1. m**2):  
ENTER FRACTION OF REPOSITORY AREA COVERED BY CONTAMINANT (DEFAULT=1.):
```

The area of the repository is requested when the source-term flag is 1, 2, 3, or 4. The fraction of the repository area covered by contaminant is prompted for when the source-term flag is 1, 2, or 4; however, this input is not used when the source-term flag is 4.

The initial inventory of a contaminant is defined in the contaminant-property block; the default values are in terms of total moles (Section 4.2.16). This total amount of contaminant is considered to be spread out, according to the fraction of the repository area covered, over the area of the repository.

If the source-term flag is 3, the prompt for fraction of the repository area is replaced with the following prompt:

```
SOURCE-FILE DEFAULT NAME: TRANS.SRC  
ENTER SOURCE-FILE NAME:
```

The source-file name is a string of up to 80 characters with no embedded blanks. The file must exist on the user's computer system at the time TRANS is executed or TRANS will terminate with an error. The content and format of the TRANS source file is described in Section 4.7.8.

If the source-term flag is 4, the following additional prompts are generated.

```
ENTER MEAN CANISTER LIFETIME (DEFAULT=0. s):  
ENTER MEAN CLADDING LIFETIME (DEFAULT=0. s):  
ENTER BEGINNING OF RESATURATION (DEFAULT=0. s):  
ENTER END OF RESATURATION (DEFAULT=0. s):  
ENTER TIMESCALE FOR RELEASES FROM STRUCTURAL METALS (DEFAULT=0. s):  
ENTER TIMESCALE FOR RELEASES FROM CLADDING (DEFAULT=0. s):  
ENTER TIMESCALE FOR RELEASES FROM FUEL MATRIX (DEFAULT=0. s):  
ENTER ALTERATION TIMESCALE (DEFAULT=0. s):
```

ENTER FRACTION OF C-14 INVENTORY IN STRUCTURAL METALS (DEFAULT=0.):
 ENTER FRACTION OF C-14 INVENTORY IN CLADDING (DEFAULT=0.):
 ENTER FRACTION OF C-14 INVENTORY AVAILABLE FOR QUICK RELEASE (DEFAULT=0.):
 ENTER FRACTION OF MO-93 INVENTORY IN STRUCTURAL METALS (DEFAULT=1.):
 ENTER FRACTION OF ZR-93 INVENTORY IN CLADDING (DEFAULT=0.):
 ENTER GAP/GRAIN-BOUNDARY FRACTION (DEFAULT=0.):

These prompts should be reasonably self-explanatory, but details of how the parameters are used in calculating source releases may be found in Wilson (1991). It is of interest to note that the congruent-leach source is a special case of the SAND91-0155 source, obtained with the following parameter values:

- Mean canister lifetime: 3000 yr (a canister life of 3000 yr is programmed into the congruent-leach source term).
- Mean cladding lifetime: 0.
- Beginning of resaturation: 0.
- End of resaturation: 0.
- Release timescales (all four of them):

$$t_r = \frac{M_U}{|q|f_c A_{r,p} S_U}$$

where M_U is the mass of uranium in the inventory (from the contaminant-property block, the inventory of ^{238}U), q is the volume flux of water (from the STEADY boundary-condition block, the upper-boundary flux), f_c is the fraction of the repository covered by contaminant (from the source block, above), $A_{r,p}$ is the repository area (from the source block, above), and S_U is the solubility of uranium (from the contaminant-property block).

- Fraction of ^{14}C inventory in structural metals: any value.
- Fraction of ^{14}C inventory in cladding: any value.
- Fraction of ^{14}C inventory available for quick release: 0.
- Fraction of ^{93}Mo inventory in structural metals: any value.
- Fraction of ^{93}Zr inventory in cladding: any value.
- Gap/grain-boundary fraction: 0.

The correspondence between the congruent-leach source and the SAND91-0155 source with the above parameter values is not exact for low-solubility nuclides, because solubility is handled differently in the two sources (see *Volume 1* and Wilson, 1991).

An example of the source block for a source interior to the mesh is given in Figure 3.21. An example of the source block for a source exterior to the mesh (i.e., on the boundary) is given in Figure 2.4.

4.2.14 Geologic-Unit Block (Transport)

The geologic-unit block is used to assign transport-specific data to the geologic units defined in the hydrology input-data file. Much of the discussion in this section requires knowledge of the hydrology geologic-unit block, and the user should read Section 4.2.7. The purpose for having separate geologic-unit blocks for hydrology and transport input-data files is to allow multiple transport problems to be based on a single hydrology problem.

The geologic-unit block is only required if TRANS is executed using a hydrologic background from a STEADY calculation (using a STEADY plot-data file). TRANS can be executed independent of STEADY; in this case, the user supplies the hydrologic parameters – the water velocities and moisture contents – for each geologic unit. The user-supplied parameters must be given in a saturated-zone block (Section 4.2.15), which replaces the geologic-unit block.

The number of geologic units *must* be the same in the transport geologic-unit block as in the hydrologic geologic-unit block. Furthermore, they *must* be in the same order, because the properties are mapped first unit to first unit, second unit to second unit, etc. TOSPAC does not ascertain that the geologic units are the same; this consistency is required of the user.

A discussion of geologic-unit input data required by TRANS follows. The user is also advised to read Section 3.1 of *Volume 1* to gain understanding of the significance of these data in a transport calculation and how the limitations of the TOSPAC transport model have influenced the choices in these data.

An INDATA session for constructing a geologic-unit block begins with a query to determine the problem domain.

UNSATURATED- OR SATURATED-ZONE PROBLEM (U OR S):

Selection of the saturated-zone problem leads to creation of a saturated-zone block (Section 4.2.15). Selection of the unsaturated-zone problem leads to creation of a geologic-unit block.

Construction of the TRANS geologic-unit block begins identically to the creation of a hydrology geologic-unit block (Section 4.2.7 contains details):

GEOLOGIC-UNIT BLOCK

ENTER # OF GEOLOGIC UNITS (DEFAULT=1):

UNIT # 1

UNIT # 1 DEFAULT NAME: NONE

ENTER UNIT # 1 NAME:

The unit names can be different from the names given in the hydrology input-data file; however, it is recommended that they be the same.

Then, INDATA prompts reflect transport-specific data:

ENTER BULK DENSITY (DEFAULT=2000. kg/m**3):

Bulk density is the density of a unit volume (remember, the user defines the units) of a geologic unit;

both matrix and fractures are included. It is used in the calculation of the retardation factor, along with the moisture content and the contaminant-dependent distribution coefficient (*Volume 1*). The default value is for a generic rock in *SI* units. For reference, the density of water in *SI* units is 1000 kg/m³; in cgs units it is 1 gm/cm³. Any real number greater than zero is accepted as input.

Next, prompts are issued for various fracture characteristics of the unit:

ENTER FRACTURE SURFACE AREA PER UNIT VOLUME (DEFAULT=0. m):
ENTER FRACTURE SPACING (DEFAULT=0. m):

The fracture surface area per unit volume is the amount of fracture wall area in a unit volume of rock; it is used in calculating the fracture retardation factor. The fracture spacing is the average distance between fractures, center to center; it is used in the calculation of the matrix/fracture coupling (discussed below). For simple planar fractures, these two numbers are related: if $2a$ is the fracture spacing, then the fracture surface area per unit volume is given by $\sigma_f = 1/a$. Note that in the TRANS input-data file in Figure 3.21, the fracture surface area per unit volume is always two divided by the fracture spacing, because the only data available are for fracture spacings. The defaults of 0 imply no fractures. Real numbers greater than or equal to 0 are acceptable input.

Next, INDATA prompts for information used in calculating hydrodynamic dispersion:

ENTER LONGITUDINAL MATRIX DISPERSIVITY (DEFAULT=0. m):
ENTER LONGITUDINAL FRACTURE DISPERSIVITY (DEFAULT=0. m):

The matrix and fracture longitudinal dispersivities are the rates of contaminant hydrodynamic dispersion downstream through the geologic unit. Although the defaults have been set to 0, these defaults are *not conservative*. It is highly recommended that the user make an effort to use actual dispersivities. If the data do not exist, an alternative is to use some value proportional to the distance a contaminant travels in the unit, e.g., one tenth of the unit thickness. Any real number greater than or equal to 0 is accepted as input.

The next prompts are related to the statistical variability of the water velocity within the geologic unit:

ENTER MATRIX-VELOCITY CORRELATION LENGTH (DEFAULT=0. m):
ENTER FRACTURE-VELOCITY CORRELATION LENGTH (DEFAULT=0. m):

Correlation length also is used to calculate hydrodynamic dispersion; the shorter the correlation length, the smaller the distance over which the velocity is variable, and the more quickly contaminants are dispersed. The default of 0 is the most conservative case, implying that the contaminants reach their maximum rate of dispersion immediately. Any real number greater than or equal to 0 is accepted as input. Section 3.1.3 of *Volume 1* contains a description of the dispersion model used in TRANS and how the dispersivities and correlation lengths are used.

The last prompts for this data block concern the path that a contaminant must take as it is transported:

ENTER MATRIX TORTUOSITY (DEFAULT=1.):
ENTER FRACTURE TORTUOSITY (DEFAULT=1.):

Tortuosity is a dimensionless measure of the "crookedness" of paths through a geologic unit; i.e., the amount of twisting and turning involved in passing from pore to pore down through the unit.

Tortuosity is used in calculating molecular diffusion in both the matrix/fracture coupling effect and the vertical-transport diffusion/dispersion term. Tortuosity can be any number greater than or equal to 1. The default values of 1 are conservative (i.e., straight paths).

The final transport-related prompt for the geologic-unit block is as follows:

ENTER MATRIX/FRACTURE COUPLING FACTOR (DEFAULT=1.):

The matrix/fracture coupling factor describes the amount of contaminant that is transferred from fractures to matrix, or vice versa, by means of diffusion (a process often called matrix diffusion). The matrix/fracture coupling factor is an adjustment to the strength of this coupling. This factor can be any nonnegative real number. The larger the factor, the stronger the coupling. The default value of 1 is the standard matrix/fracture coupling as defined in *Volume 1*. The default value is actually quite strong; contaminants cannot be transported down the fractures very far before being pulled into the matrix. In *Volume 1*, a coupling factor of 1 is used for the strongly coupled cases; a coupling factor of 10^{-4} is used for the weakly coupled cases. A coupling factor of 0 implies no coupling; e.g., as if the fractures were lined with a deposit impermeable to the contaminant. A coupling factor of 0 is probably conservative; however a coupling factor of 1 is probably more accurate for most circumstances.

A portion of the INDATA terminal session for creating the geologic-unit block shown in Figure 3.21 follows:

GEOLOGIC-UNIT BLOCK

ENTER # OF GEOLOGIC UNITS (DEFAULT=1): 5

UNIT # 1

UNIT # 1 DEFAULT NAME: NONE

ENTER UNIT # 1 NAME: *CHnz*

ENTER BULK DENSITY (DEFAULT=2000. kg/m**3): *1610. kg/m**3*

ENTER FRACTURE SURFACE AREA PER UNIT VOLUME (DEFAULT=0. /m): *6. /m*

ENTER FRACTURE SPACING (DEFAULT=0. m): *0.33 m*

ENTER LONGITUDINAL MATRIX DISPERSIVITY (DEFAULT=0. m): *13. m*

ENTER LONGITUDINAL FRACTURE DISPERSIVITY (DEFAULT=0. m): *13. m*

ENTER MATRIX-VELOCITY CORRELATION LENGTH (DEFAULT=0. m): *30. m*

ENTER FRACTURE-VELOCITY CORRELATION LENGTH (DEFAULT=0. m): *10. m*

ENTER MATRIX TORTUOSITY (DEFAULT=1.): *10.*

ENTER FRACTURE TORTUOSITY (DEFAULT=1.): *1.*

ENTER MATRIX/FRACTURE COUPLING FACTOR (DEFAULT=1.):

UNIT # 2

UNIT # 2 DEFAULT NAME: NONE

ENTER UNIT # 2 NAME: *TSw2-3*

ENTER BULK DENSITY (DEFAULT=2000. kg/m**3): *2300. kg/m**3*

ENTER FRACTURE SURFACE AREA PER UNIT VOLUME (DEFAULT=0. /m): *80. /m*

ENTER FRACTURE SPACING (DEFAULT=0. m): *0.025 m*

ENTER LONGITUDINAL MATRIX DISPERSIVITY (DEFAULT=0. m): *21. m*

ENTER LONGITUDINAL FRACTURE DISPERSIVITY (DEFAULT=0. m): *21. m*

ENTER MATRIX-VELOCITY CORRELATION LENGTH (DEFAULT=0. m): *30. m*

ENTER FRACTURE-VELOCITY CORRELATION LENGTH (DEFAULT=0. m): *10. m*

ENTER MATRIX TORTUOSITY (DEFAULT=0.): *10.*

ENTER FRACTURE TORTUOSITY (DEFAULT=0.): *1.*

ENTER MATRIX/FRACTURE COUPLING FACTOR (DEFAULT=1.):

UNIT # 3

UNIT # 3 DEFAULT NAME: NONE

ENTER UNIT # 3 NAME: *TSw1*

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o

o

Examples of geologic-unit blocks in TRANS input-data files are given in Figures 2.4 and 3.21.

4.2.15 Saturated-Zone Block (Transport)

The saturated-zone block is used to assign hydrologic and transport data to the geologic units. The purpose of a saturated-zone block is to allow transport calculations in the saturated zone. The saturated-zone block is based on the TRANS geologic-unit block; much of the discussion in this section requires knowledge of the TRANS geologic-unit block, and the user should read Section 4.2.14. The saturated-zone block is identical to the geologic-unit block, except that it contains seven more items of data. The saturated-zone block replaces the geologic-unit block.

The TRANS module of TOSPAC can solve transport problems in either the unsaturated or the saturated zone, but not both at the same time. (STEADY and DYNAMICS can only solve problems in the unsaturated zone.) The geologic-unit block is required if TRANS is executed using a hydrologic background from a STEADY calculation, (using a STEADY plot-data file). For a saturated-zone problem, the user can supply the necessary parameters--the water velocities, moisture contents, and calculational mesh--for each geologic unit using a saturated-zone block.

Initially, INDATA asks for the type of problem.

UNSATURATED- OR SATURATED-ZONE PROBLEM (U OR S):

Specifying an unsaturated-zone problem causes creation of a geologic-unit block (Section 4.2.14). Specifying a saturated-zone problem causes creation of a saturated-zone block. Construction of the TRANS saturated-zone block begins similarly to the creation of a TRANS geologic-unit block (Section 4.2.14).

SATURATED-ZONE BLOCK

ENTER # OF GEOLOGIC UNITS (DEFAULT=1):

UNIT # 1

UNIT # 1 DEFAULT NAME: NONE

ENTER UNIT # 1 NAME:

INDATA next begins to prompt for the data for one geologic unit at a time. First, INDATA prompts for the size of a geologic unit.

ENTER START LOCATION (DEFAULT=0. m):

ENTER END LOCATION (DEFAULT=100. m):

Boundary locations correspond to the lower and upper elevations of a geologic unit in a hydrology geologic-unit block. In the convention adopted for TOSPAC, the problem domain stretches from left to right, with left corresponding to lower and right corresponding to upper. However, flow can be in either direction and contaminants can be injected anywhere in the mesh. Acceptable entries are any real numbers. If more than one geologic unit has been specified, the boundaries of geologic units must abut.

ENTER NUMBER OF CELLS (DEFAULT=500):

The number of cells is used by TRANS to determine a simple calculational mesh. The cells will be of uniform size, situated between the boundaries of the geologic unit. The number of cells must be an integer greater than four.

Next, INDATA prompts for the hydrologic parameters.

ENTER MATRIX WATER VELOCITY (DEFAULT=0. m/s):

ENTER FRACTURE WATER VELOCITY (DEFAULT=0. m/s):

ENTER MATRIX MOISTURE CONTENT (DEFAULT=0.):

ENTER FRACTURE MOISTURE CONTENT (DEFAULT=0.):

The water velocity can be any real number. The defaults are no-flow conditions for a diffusion-only problem. The moisture content is the same as the (effective) porosity in a saturated-zone problem. The moisture content can be any number between 0 and 1, inclusive. The defaults imply an impermeable medium; no solution is possible if both moisture-content defaults are selected.

The remainder of the data required for a geologic unit is exactly the same as that required for the geologic-unit block: bulk density, fracture surface area, fracture spacing, longitudinal dispersivities, velocity correlation lengths, tortuosities, and matrix/fracture coupling factor. Descriptions of these data are given in Section 4.2.14.

No examples of saturated-zone blocks are contained in this User's Guide; the block is identical to a TRANS geologic-unit block, except the block header states SATURATED-ZONE, and each geologic unit has the seven additional items of data discussed above.

4.2.16 Contaminant-Property Block (Transport)

The contaminant-property block defines the transport-specific characteristics of the contaminants. Many contaminant properties needed as input for TOSPAC can be found in the *CRC Handbook of Chemistry and Physics* (Weast, 1990-91).

TOSPAC presently only handles water-soluble contaminants, including radionuclides. (Nonpolar contaminants--most gases, oils, gasoline, glycerines, etc.--are transported by a mechanism known as two-phase flow, which is not incorporated into TOSPAC's flow solvers. Colloids, or particles suspended in groundwater, might be added to TOSPAC's transport solver at a later date.)

The contaminant-property block is organized by chains and species. The organization was developed specifically for radionuclide contaminants. A chain is a series of species (or isotopes, or nuclides), related to each other by radioactive decay. For groundwater contaminants, the radioactive decay is the process by which one isotope changes into another: for instance, beta decay (a neutron changing into a proton and an electron), or alpha decay (loss of an alpha particle--two protons and two neutrons--a

helium nucleus). As an example, the plutonium isotope with a molecular weight of 240 (^{240}Pu) undergoes an alpha decay to become the uranium isotope with a molecular weight of 236 (^{236}U), which undergoes another alpha decay to become the thorium isotope with a molecular weight of 232 (^{232}Th). In this case ^{240}Pu , ^{236}U , and ^{232}Th form a single chain of three species. ^{240}Pu is referred to as the parent, ^{236}U and ^{232}Th are the daughters (note that ^{236}U is also the parent of ^{232}Th).

Radioactive decay changes one isotope into another as an exponential function of time. This function of time is characterized by a half-life: the time it takes half of the parent to decay into a daughter.

Some radionuclides have daughters that are not of consequence in many problems. For instance, these daughters might not be radioactive or toxic, or they might decay too fast to be of significance. Further, many contaminants are not radioactive.

To digress for a moment, if a nonradioactive contaminant breaks down chemically (perhaps by a biological agent) into another contaminant of concern, it may be possible to model it using chains and species. Such a contaminant could be described as having a "half-life," in the sense that its amount may decrease as an exponential function of time. If it changes according to some other function of time (e.g., linear), it could *not* be modeled effectively by the present version of TOSPAC.

Many contaminants of interest are described by chains containing only one species. Tracers are a special class of contaminant that should be modeled in TOSPAC by a chain consisting of a single species.

The INDATA module begins prompting for contaminant properties by announcing the data block and asking for the number of chains:

```
CONTAMINANT-PROPERTY BLOCK
ENTER # OF CHAINS (DEFAULT=1):
```

The number of chains must be an integer greater than 0.

INDATA now begins asking for information concerning each chain:

```
ENTER # OF SPECIES FOR CHAIN # 1 (DEFAULT=1):
```

The number of species must be an integer greater than 0. The total number of species in all chains must be no more than 50. Notice that the default is for one chain with one species (i.e., one contaminant). If more than a single chain has been specified, the prompt for the number of species is repeated, once for each chain:

```
ENTER # OF SPECIES FOR CHAIN # 2 (DEFAULT=1):
ENTER # OF SPECIES FOR CHAIN # 3 (DEFAULT=1):
```

```
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o
o
```

If a contaminant occurs in two chains, TRANS treats it as two different contaminants and, it must be entered twice in the contaminant-property block.

In order to allow each block in a TRANS input-data file to be self-contained (for modifying and for a

consistency check), the number of geologic units must be reentered:

ENTER # OF GEOLOGIC UNITS (DEFAULT=1):

INDATA now indicates that it is asking for data concerning the first chain, first species:

CONTAMINANT # 1 CHAIN # 1 SPECIES # 1
CONTAMINANT # 1 DEFAULT NAME: NONE
ENTER CONTAMINANT # 1 NAME:

The name can be any character string up to 80 characters long. The name need not be unique, although it is so recommended. The default name is a blank string.

INDATA next begins prompting for specific contaminant data as follows:

ENTER INITIAL INVENTORY (DEFAULT=0. mol):

The initial inventory is the amount of contaminant contained in the entire source region—the entire repository—at the beginning of the problem. It should be a real number greater than or equal to 0. An initial inventory of 0 mol (the default) implies that the source is exterior to the mesh, as in the example problem given in Section 2, or that this species is a daughter-product in this chain. If a contaminant occurs in two chains, then it must be entered twice in the contaminant-property block, and the initial inventory must be divided between the chains.

The default units, moles, are *SI*; one mole is Avogadro's number of molecules (6.02×10^{23}). To convert one mole of a contaminant to kilograms, take the product of its molecular weight and 0.001 g/kg. For example, one mole of UO_2 is 0.270 kg—270 g (238 g for ^{238}U , plus 32 g for $^{16}\text{O}_2$) times 0.001 g/kg. It is not advised to use mass-concentration units (e.g., kg/m³), because using mass-concentration units with chains, the decay equations in TRANS are inaccurate.

ENTER HALF-LIFE (DEFAULT=INFINITY):

The half-life, as mentioned above, is the time it takes for one-half of a given contaminant to change into another substance or isotope. Half-life usually only applies to radioactive isotopes, but the TRANS module of TOSPAC allows any contaminant to have a half-life. Be careful, however, because TRANS computes the amount of contaminant present at any given time by an exponential-decay equation (Bateman equation), and thus for nonradioactive contaminants, decay must be exponential for this calculation to be accurate.

The default (the word *INFINITY*, in any combination of uppercase or lowercase characters) implies that the contaminant remains immutable (does not decay) for the time span of the problem. For a contaminant that does decay, the half-life should be a real number strictly greater than 0.

Note that, as currently programmed, TOSPAC does *not* allow two nuclides in the same chain to have the same half-life. If two nuclides in the same chain are given the same half-life, an error message results. The reason for this restriction is that the algorithm used for solving the decay equations involves dividing by the differences of the decay rates.

ENTER ACTIVITY (DEFAULT=0. Ci/mol):
ENTER RELEASE LIMIT (DEFAULT=0. Ci):

Activity only applies to a radioactive contaminant and is defined in terms of curies per mole of the radionuclide. Curies is not an *SI* unit; the *SI* units for radioactivity is the becquerel (Bq), representing one nuclear transformation per second. To convert Ci to Bq, multiply by 3.7×10^{10} Bq/Ci. An activity of 0 (the default) implies that the contaminant is not radioactive.

Release limit is a quantity defined by the EPA specifically for radioactive-waste repositories. The release limit is presently a function of the total amount of heavy metal in the inventory of the repository, following 40 CFR 191 (EPA, 1985).

Activity and release limit are *not* used in the calculational module TRANS. Rather, they are only used by OUTPLOT in construction of the EPA-ratio plot (Section 4.6.5). Therefore, the user can select the default values even for radioactive contaminants and not affect the accuracy of the results.

ENTER SOLUBILITY (DEFAULT=0. mol/m**3):

The solubility is the amount of contaminant that water can hold in solution at complete saturation at the problem temperature (remember, TOSPAC only performs isothermal calculations, and thus a constant problem temperature is implied). Solubility should be a real number greater than or equal to 0. If 0 (the default) is entered *no* transport occurs. (TOSPAC presently handles neither colloid transport nor two-phase flow.)

ENTER DIFFUSION COEFF (DEFAULT=0. m**2/s):

The diffusion coefficient is a scaling factor for the molecular diffusion of a contaminant that sees a concentration gradient. It must be a real number greater than or equal to 0. If 0 (the default) is entered, no diffusion occurs (although hydrodynamic dispersion can still occur; Section 4.2.14).

ENTER MATRIX DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m**3/mol):

ENTER FRACTURE DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m):

ENTER MATRIX DISTRIB COEFF FOR UNIT # 2 (DEFAULT=0. m**3/mol):

ENTER FRACTURE DISTRIB COEFF FOR UNIT # 2 (DEFAULT=0. m):

ENTER MATRIX DISTRIB COEFF FOR UNIT # 3 (DEFAULT=0. m**3/mol):

ENTER FRACTURE DISTRIB COEFF FOR UNIT # 3 (DEFAULT=0. m):

o

o

o

TRANS uses the distribution coefficient to determine the retardation of a contaminant during transport (*Volume 1*). The amount of a contaminant adsorbed onto a material is proportional to the concentration of that material in the surrounding water; the distribution coefficient is part of the constant of proportionality. In effect, the distribution coefficient tells how much contaminant adsorbs on a given material. For the fluid in the matrix, the adsorbed amount per unit volume is given by the product of the bulk density of the matrix (ρ_b), the matrix distribution coefficient (K_d), and the radionuclide concentration in the matrix water (C_m)— $\rho_b K_d C_m$; for the fluid in the fractures, the adsorbed amount per unit volume is given by the product of the surface area of the fracture (σ_f), the fracture distribution coefficient (K_a), and the radionuclide concentration in the fracture water (C_f)— $\sigma_f K_a C_f$.

Two distribution coefficients must be entered for *each* geologic unit specified in the transport geologic-unit block. Distribution coefficients must be real numbers greater than or equal to 0. The

default value, 0, means that no contaminant is adsorbed—the conservative case.

Figures 2.4 and 3.21 show TRANS input-data files containing contaminant-property blocks. A portion of the INDATA session for creating the contaminant-property block shown in Figure 3.21 follows.

CONTAMINANT-PROPERTY BLOCK

```

ENTER # OF CHAINS (DEFAULT=1): 5
ENTER # OF SPECIES FOR CHAIN # 1 (DEFAULT=1): 1
ENTER # OF SPECIES FOR CHAIN # 2 (DEFAULT=1): 3
ENTER # OF SPECIES FOR CHAIN # 3 (DEFAULT=1): 1
ENTER # OF SPECIES FOR CHAIN # 4 (DEFAULT=1): 1
ENTER # OF SPECIES FOR CHAIN # 5 (DEFAULT=1): 1
ENTER # OF GEOLOGIC UNITS (DEFAULT=5): 5

CONTAMINANT # 1 CHAIN # 1 SPECIES # 1
CONTAMINANT # 1 DEFAULT NAME: NONE
ENTER CONTAMINANT # 1 NAME: U-238
ENTER INITIAL INVENTORY (DEFAULT=0. mol): 6.7E+7 kg
ENTER HALF-LIFE (DEFAULT=INFINITY): 1.42E+17 s
ENTER ACTIVITY (DEFAULT=0. Ci/mol): 3.33E-4 Ci/kg
ENTER RELEASE LIMIT (DEFAULT=0. Ci): 7000. Ci
ENTER SOLUBILITY (DEFAULT=0. mol/m**3): 5.0E-2 kg/m**3
ENTER DIFFUSION COEFF (DEFAULT=0. m**2/s): 1.E-9 m**2/s
ENTER MATRIX DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m**3/kg): 5.3E-3 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m): 0. m
ENTER MATRIX DISTRIB COEFF FOR UNIT # 2 (DEFAULT=0. m**3/kg): 1.8E-3 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 2 (DEFAULT=0. m): 0. m
ENTER MATRIX DISTRIB COEFF FOR UNIT # 3 (DEFAULT=0. m**3/kg): 1.8E-3 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 3 (DEFAULT=0. m): 0. m
ENTER MATRIX DISTRIB COEFF FOR UNIT # 4 (DEFAULT=0. m**3/kg): 5.3E-3 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 4 (DEFAULT=0. m): 0. m
ENTER MATRIX DISTRIB COEFF FOR UNIT # 5 (DEFAULT=0. m**3/kg): 1.8E-3 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 5 (DEFAULT=0. m): 0. m

CONTAMINANT # 2 CHAIN # 2 SPECIES # 1
CONTAMINANT # 2 DEFAULT NAME: NONE
ENTER CONTAMINANT # 2 NAME: Pu-240
ENTER INITIAL INVENTORY (DEFAULT=0. mol): 1.4E+5 kg
ENTER HALF-LIFE (DEFAULT=INFINITY): 2.08E+11 s
ENTER ACTIVITY (DEFAULT=0. Ci/mol): 2.26E+2 Ci/kg
ENTER RELEASE LIMIT (DEFAULT=0. Ci): 7000. Ci
ENTER SOLUBILITY (DEFAULT=0. mol/m**3): 4.3E-4 kg/m**3
ENTER DIFFUSION COEFF (DEFAULT=0. m**2/s): 1.E-9 m**2/s
ENTER MATRIX DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m**3/kg): 1.4E-1 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 1 (DEFAULT=0. m): 0. m
ENTER MATRIX DISTRIB COEFF FOR UNIT # 2 (DEFAULT=0. m**3/kg): 6.4E-2 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 2 (DEFAULT=0. m): 0. m
ENTER MATRIX DISTRIB COEFF FOR UNIT # 3 (DEFAULT=0. m**3/kg): 6.4E-2 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 3 (DEFAULT=0. m): 0. m
ENTER MATRIX DISTRIB COEFF FOR UNIT # 4 (DEFAULT=0. m**3/kg): 1.4E-1 m**3/kg
ENTER FRACTURE DISTRIB COEFF FOR UNIT # 4 (DEFAULT=0. m): 0. m

```

ENTER MATRIX DISTRIB COEFF FOR UNIT # 5 (DEFAULT=0. m**3/kg): $6.4E-2$ m**3/kg
 ENTER FRACTURE DISTRIB COEFF FOR UNIT # 5 (DEFAULT=0. m): 0. m

CONTAMINANT # 3 CHAIN # 2 SPECIES # 2
 CONTAMINANT # 3 DEFAULT NAME: NONE
 ENTER CONTAMINANT # 1 NAME: U-236
 ENTER INITIAL INVENTORY (DEFAULT=0. mol): $2.4E+5$ kg

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This example consists of definitions for five contaminant chains, each containing a single species, except for the second chain which contains three species. These contaminants are being used in a stratigraphy of five geologic units, hence the ten prompts (each unit has a matrix and a fracture material) for the distribution coefficients. Note that with the multiplicative effect of chains, species, and units, a contaminant-property block can end up being quite sizeable. Also note that mass-concentration units are used in this example, in complete disregard of our previous advice.

4.2.17 Boundary-Condition Block (Transport)

The boundary-condition block in a transport input-data file is used to define boundary conditions, times when boundary conditions can change, and times when results are output for graphics. The transport boundary-condition block is similar to the hydrology boundary-condition block, and the user is advised to read Section 4.2.10.

The transport boundary-condition block is organized according to time snapshots, just as the hydrology boundary-condition block is. At every time snapshot, intermediate results are written into the TRANS output-listing file and the TRANS plot-data file.

The boundary-condition block contains an entry specifying the number of time snapshots to be defined, followed by a time-conversion number. Then, each time snapshot contains a time value accompanied by the boundary condition. The boundary condition specified at a given time snapshot begins at that time snapshot and ends at the next time snapshot. The last time snapshot specifies the end time of the calculation and does not require a boundary-condition definition. At every time snapshot, the user is allowed to change boundary conditions.

Within the INDATA module, the prompts for data begin with the transport boundary-condition block identifier:

BOUNDARY-CONDITION BLOCK

The first INDATA prompt of the boundary-condition block is for the number of time snapshots:

ENTER # OF TIME SNAPSHOTS (DEFAULT=1):

The number of time snapshots must be an integer between 1 and 100, inclusive. The more time snapshots that are defined, the better the resolution in the OUTPLOT computer graphics routines, especially the three-dimensional graphs, and the better the ability of the user to understand the details of the calculation. However, the more time snapshots, the bigger the output files (Section 3.2 and

Section 4.2.10).

As with the boundary-condition block for DYNAMICS input-data files, INDATA allows the user to convert time units to a more appropriate scale.

```
TIME CONVERSION MENU
0. NO CONVEPSION
1. NO CONVERSION (SECONDS ASSUMED)
2. CONVERT HOURS TO SECONDS
3. CONVERT DAYS TO SECONDS
4. CONVERT YEARS TO SECONDS
5. NO CONVERSION (YEARS ASSUMED)
6. CONVERT SECONDS TO YEARS
7. CONVERT HOURS TO YEARS
8. CONVERT DAYS TO YEARS
ENTER CHOICE (DEFAULT=1):
```

A discussion of time-unit conversion is contained in Section 4.2.10.

In order for blocks of TRANS data to be self-consistent for modifying and error checking, the number of contaminants entered in the contaminant-property block must also be entered in the boundary-condition block. The number of boundary conditions at any given time snapshot depends on the number of contaminants.

ENTER # OF CONTAMINANTS (DEFAULT=1):

INDATA now prompts for time-snapshot data as follows:

```
SNAPSECT # 1
ENTER TIME (DEFAULT=0 s):
```

Time can be any real number. The typical starting time is 0; therefore, the first default for time is 0. Time units for the default are determined by the user's response to the time-conversion menu. Subsequent defaults for time are the times of the previous snapshots multiplied by two.

At each snapshot, a boundary condition can be defined. INDATA begins prompting for this information as follows:

```
BOUNDARY-CONDITION FLAGS ARE 2 DIGITS (LOWER/UPPER):
1. USE PREVIOUS BOUNDARY CONDITION
2. CONCENTRATION BOUNDARY
3. CONCENTRATION-FLUX BOUNDARY
4. ZERO-CONCENTRATION-GRADIENT BOUNDARY
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=12):
```

The boundary-condition flag consists of two digits. The first digit indicates the boundary condition at the lower boundary; the second indicates the condition at the upper boundary. A boundary-condition flag can be one of the following:

Flag Digit=0 Use previously defined boundary condition. Of course, this flag is not allowed for the first boundary-condition definition.

Flag Digit=1 Define the boundary by setting a constant concentration for a contaminant.

Flag Digit=2 Define the boundary by setting a constant concentration flux for a contaminant.

Flag Digit=3 Define the boundary by setting the first spatial derivative of the concentration of a contaminant to 0.

Any boundary condition can be composed of any combination of two of these digits. Information about boundary-condition flags used by TRANS is summarized in Figure 4.14.

		SECOND DIGIT UPPER BOUNDARY FLAG				
		0	1	2	3	
FIRST DIGIT LOWER BOUNDARY FLAG	0	00 PREVIOUS LOWER PREVIOUS UPPER	01 PREVIOUS LOWER CONCENTRATION UPPER	02 PREVIOUS LOWER FLUX UPPER	03 PREVIOUS LOWER ZERO-GRADIENT UPPER	} NOT ALLOWED FOR FIRST TIME SNAPSHOT
	1	10 CONCENTRATION LOWER PREVIOUS UPPER	11 CONCENTRATION LOWER CONCENTRATION UPPER	12 CONCENTRATION LOWER FLUX UPPER	13 CONCENTRATION LOWER ZERO-GRADIENT UPPER	
	2	20 FLUX LOWER PREVIOUS UPPER	21 FLUX LOWER CONCENTRATION UPPER	22 FLUX LOWER FLUX UPPER	23 FLUX LOWER ZERO-GRADIENT UPPER	
	3	30 ZERO-GRADIENT LOWER PREVIOUS UPPER	31 ZERO-GRADIENT LOWER CONCENTRATION UPPER	32 ZERO-GRADIENT LOWER FLUX UPPER	33 ZERO-GRADIENT LOWER ZERO-GRADIENT UPPER	
		} NOT ALLOWED FOR FIRST TIME SNAPSHOT				

Figure 4.14: Boundary-condition flags for TRANS.

During the period between one time snapshot and another, *all contaminants will have the same boundary-condition type*. For instance, suppose boundary-condition flag 11 is specified; each contaminant can have different concentration values at the boundaries, but the boundary conditions will only be concentration-defined boundaries.

For the first time snapshot, the default value for the boundary-condition flag is 12; i.e., the lower

boundary is defined with a concentration and the upper boundary is defined with a concentration flux. After the first time snapshot, the default value for the boundary-condition flag is changed to 00; i.e., the same boundary condition as previously specified.

A concentration-defined boundary (flag 1) must be a nonnegative real number.

A boundary defined by concentration flux (flag 2) is a real number corresponding to a flux of contaminant across a boundary. A negative value implies a downward flux; therefore, a negative flux at the upper boundary means that contaminant is entering the column at the top; a negative flux at the lower boundary means that contaminant is leaving the column at the bottom. The signs of the concentration-flux values are consistent with the groundwater-flux signs (Section 4.2.10).

Because concentration-flux boundaries can be defined as an influx or an outflux, if an outflux is specified, care must be taken to assure that there is enough contaminant in the mesh to support an outflux. The situation is analogous to an outflux boundary for a water-flow problem (Section 4.2.10); however, if the outflux is excessive, TRANS produces negative concentrations. Negative concentrations are nonphysical.

Entering the boundary condition as a flux is most useful in the case where the repository is on the boundary (the source region is outside the boundary), and in the case where an impermeable or semi-permeable barrier to a contaminant is on the boundary (e.g., in modeling a laboratory experiment).

A boundary defined by a zero concentration gradient (flag 3) requires no additional input from the user: the value is assumed to be 0. Computationally, with this boundary condition the concentration at the boundary is simply set equal to the concentration at the first mesh cell in from the boundary.

A zero-concentration-gradient boundary condition is useful for modeling the situation in which the contaminant is quickly swept away outside the boundary. In such a situation, a zero-concentration boundary condition could also be used but, if the concentration is expected to go from some positive value to zero in a very small region near the boundary, the zero-concentration-gradient boundary condition can be used to avoid having to model the boundary layer where concentration is rapidly varying. Also, this boundary condition can be used if diffusion and dispersion have both been set to zero, whereas, in such a case, a concentration or flux boundary condition may produce a discontinuity, causing the amount of contaminant mass crossing the boundary to be estimated incorrectly.

The INDATA prompts for boundary-condition flag 12 (the initial default) follow. Prompts for the other boundary-condition types are similar, except that no prompts are given for zero-concentration-gradient boundary conditions.

```
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):
```

The default values for boundary-condition flag 12 specify a concentration flux of zero at the top of the column and a concentration of zero at the bottom. This situation corresponds to no contaminant

entering or leaving the top boundary, but whatever contaminant reaches the bottom boundary leaves, keeping the concentration equal to zero at the boundary.

An example of an INDATA session for creating a boundary condition block with several time snapshots follows. One contaminant chain is assumed to be specified in the contaminant property block; the chain consists of two species.

BOUNDARY-CONDITION BLOCK

ENTER # OF TIME SNAPSHOTS (DEFAULT=1): 11

TIME CONVERSION MENU

- 0. NO CONVERSION
 - 1. NO CONVERSION (SECONDS ASSUMED)
 - 2. CONVERT HOURS TO SECONDS
 - 3. CONVERT DAYS TO SECONDS
 - 4. CONVERT YEARS TO SECONDS
 - 5. NO CONVERSION (YEARS ASSUMED)
 - 6. CONVERT SECONDS TO YEARS
 - 7. CONVERT HOURS TO YEARS
 - 8. CONVERT DAYS TO YEARS
- ENTER CHOICE (DEFAULT=1): 4

ENTER # OF CONTAMINANTS (DEFAULT=2): 2

SNAPSHOT # 1

ENTER TIME (DEFAULT=0. yr): 0. yr

BOUNDARY-CONDITION FLAGS ARE 2 DIGITS (LOWER/UPPLR):

- 0. USE PREVIOUS BOUNDARY CONDITION
- 1. CONCENTRATION BOUNDARY
- 2. CONCENTRATION-FLUX BOUNDARY
- 3. ZERO-CONCENTRATION-GRADIENT BOUNDARY

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=12): 11

ENTER CONTAMINANT # 1

LOWER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3): 0. mol/m**3

ENTER CONTAMINANT # 1

LOWER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3): 3 mol/m**3

ENTER CONTAMINANT # 1

UPPER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3): 10. mol/m**3

ENTER CONTAMINANT # 1

UPPER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3): 100. mol/m**3

ENTER CONTAMINANT # 2

LOWER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3):

ENTER CONTAMINANT # 2

LOWER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):

ENTER CONTAMINANT # 2

UPPER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3):

ENTER CONTAMINANT # 2

UPPER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):

SNAPSHOT # 2

ENTER TIME (DEFAULT=0. yr): 1. yr

```

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 12
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3): 20. mol/m**3
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3): 20. mol/m**3
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s): 1. mol/m**2/s
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s): 1. mol/m**2/s
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):

SNAPSHOT # 3
ENTER TIME (DEFAULT=2. yr): 10. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 13
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3): 20. mol/m**3
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3): 20. mol/m**3
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):

SNAPSHOT # 4
ENTER TIME (DEFAULT=20. yr): 100. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 21
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s): 0. mol/m**2/s
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s): 3. mol/m**2/s
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3): 10. mol/m**3
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3): 100. mol/m**3
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):

SNAPSHOT # 5
ENTER TIME (DEFAULT=200. yr): 1000. yr

```

```

ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 22
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s): 0. mol/m**2/s
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s): 3. mol/m**2/s
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s): 1. mol/m**2/s
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s): 1. mol/m**2/s
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):

SNAPSHOT # 6
ENTER TIME (DEFAULT=2000. yr): 10000. yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 23
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s): 0. mol/m**2/s
ENTER CONTAMINANT # 1
  LOWER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s): 3. mol/m**2/s
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):
ENTER CONTAMINANT # 2
  LOWER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):

SNAPSHOT # 7
ENTER TIME (DEFAULT= 20000. yr): 1.E+5 yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 31
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3): 10. mol/m**3
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3): 100. mol/m**3
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY MATRIX CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY FRACTURE CONC (DEFAULT=0. mol/m**3):

SNAPSHOT # 8
ENTER TIME (DEFAULT=200000. yr): 2.E+5 yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 32
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s): 1. mol/m**2/s
ENTER CONTAMINANT # 1
  UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s): 1. mol/m**2/s
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY MATRIX CONC-FLUX (DEFAULT=0. mol/m**2/s):

```

```
ENTER CONTAMINANT # 2
  UPPER-BOUNDARY FRACTURE CONC-FLUX (DEFAULT=0. mol/m**2/s):
```

```
SNAPSHOT # 9
ENTER TIME (DEFAULT=400000. yr): 3.E+5 yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 33
```

```
SNAPSHOT # 10
ENTER TIME (DEFAULT=600000. yr): 4.E+5 yr
ENTER BOUNDARY-CONDITION FLAG (DEFAULT=00): 00
```

```
SNAPSHOT # 11
ENTER TIME (DEFAULT=800000. yr): 5.E+5 yr
```

This example shows a request for 11 time snapshots, defining the following calculation. Notice that we have asked TOSPAC to convert the snapshot times from years to seconds so that we could enter the time in years.

- 1) The first snapshot starts at time 0. The initial condition for the problem will be output at this time to the output-listing file and the plot-data file. The problem starts with boundary-condition type 11: both lower and upper boundaries defined by concentration. As specified, for the first contaminant the lowermost mesh point is assigned a value of 0 concentration in the matrix and 3 mol/m³ concentration in the fractures. The uppermost mesh point is assigned a concentration value of 10 mol/m³ in the matrix and 100 mol/m³ in the fractures. The other contaminant is assigned the default values: zero concentration at both boundaries. Note that these concentration values are maintained at the boundaries throughout the timestep. If the amount of contaminant coming from the interior of the mesh is too little to cause this concentration, contaminant is supplied from outside the mesh. If the amount of contaminant coming from the interior of the mesh is more than these values, contaminant is removed from the mesh. These boundary conditions are to be in effect until the next time snapshot.
- 2) The second snapshot occurs at 1 yr. Notice that the default time is 0 yr, which is twice the immediately preceding time. The boundary condition is now changed to type 12: concentration lower boundary and concentration-flux upper boundary. For the first contaminant, the lower boundary condition is specified as 20 mol/m³ concentration in both the matrix and fractures; the upper boundary condition is specified as an outflux of 1 mol/m²/s. Note that the outflux boundary condition only makes sense if there is sufficient contaminant in that part of the mesh. Again, the contaminants in chain number 2 are assigned the default values.
- 3) The third snapshot is to occur at 10 yr. The boundary-condition type is 13: concentration lower boundary and zero-concentration-gradient upper boundary. The lower boundary is specified as 20 moles/m³ in the matrix and the fractures. The contaminants in chain number 2 are assigned the default values. The upper boundary is not explicitly assigned any values because the zero-concentration-gradient condition automatically assigns a value of 0 to the first spatial derivative.
- 4) The fourth snapshot is to occur at 100 yr. Boundary-condition flag 21, concentration-flux lower and concentration upper boundary, is requested. The lower boundary is specified as an influx of 0 mol/m²/s for the matrix, and an influx of 3 mol/m²/s for the fractures. The upper boundary is assigned a concentration of 10 mol/m³ for the matrix and 100 mol/m³ for the fractures. Once more, the contaminants in chain number 2 are assigned the default values.

- 5) The fifth snapshot is to occur at 1000 yr. The boundary-condition type is 22: concentration-flux lower and upper boundaries. The lower boundary is specified the same as in the fourth snapshot (we could have entered a 0 digit for the lower boundary-condition type). The first contaminant is assigned a concentration outflux of $1 \text{ mol/m}^2/\text{s}$ for the matrix and the fractures at the upper boundary. The second contaminant is assigned the default values.
- 6) The sixth snapshot is to occur at 10,000 yr. The boundary-condition type is 23: concentration-flux lower boundary and zero-concentration-gradient upper boundary. For the first contaminant, the lower boundary is assigned a concentration-influx of $0 \text{ mol/m}^2/\text{s}$ for the matrix and $3 \text{ mol/m}^2/\text{s}$ for the fractures. The second contaminant is assigned the default value of $0 \text{ mol/m}^2/\text{s}$. Note that zero flux implies an impermeable barrier. Again, the zero-concentration-gradient boundary requires no additional input from the user.
- 7) The seventh snapshot is to occur at 100,000 yr. The boundary-condition type is 31: zero-concentration-gradient lower boundary and concentration upper boundary. The lower boundary is specified implicitly. The upper boundary is specified the same as in the first and fourth snapshots (note that we could not have entered a 0 digit for the upper boundary-condition type because the upper boundary is specified differently from the immediately preceding snapshot).
- 8) The eighth snapshot is to occur at 200,000 yr. The boundary-condition type is 32: zero-concentration-gradient lower boundary and concentration-flux upper boundary. The lower boundary is specified implicitly. The upper boundary is specified the same as in the second and fifth snapshots.
- 9) The ninth snapshot is to occur at 300,000 yr. Boundary-condition type 33, zero concentration gradient at both boundaries, is requested. The lower and upper boundaries are specified implicitly, and thus no boundary-condition values are listed for this snapshot.
- 10) The tenth snapshot is to occur at 400,000 yr. The boundary conditions are not changed at this timestep: they remain the same as those specified for the immediately preceding (ninth) time snapshot.
- 11) The final snapshot is to occur at 500,000 yr. This snapshot marks the end of the calculation; at this point, the final results are written to the output-listing file and the plot-data file. No boundary conditions are necessary and none are specified.

Figure 4.15 presents an example of the transport input-file boundary-condition block created by INDATA in response to the above prompts. Figures 2.4 and 3.21 show the boundary-condition blocks in two TRANS input-data files.

4.2.18 Initial-Condition Block (Transport)

An initial condition for a transport calculation consists of assigning concentration values for all contaminants to the calculational mesh before attempting a solution. The initial-condition block is optional. If the initial-condition block does not exist, TRANS defaults to a constant zero initial concentration at all mesh points for all chains and species.

Supplying an initial-condition concentration is useful in relaxation problems. For instance, assume that a dissolved contaminant is buried underground; it has a given concentration in the immediate area and zero concentration elsewhere. Assume no other source. How it is transported is a relaxation problem.


```

***** BOUNDARY-CONDITION BLOCK *****
10 # TIME SNAPSHOTS
4 TIME CONVERSION NUMBER
2 # CONTAMINANTS (CONSISTENCY CHECK)

SNAPSHOT # 1
0 yr
11
0 mol/m**3
3 mol/m**3
10 mol/m**3
100 mol/m**3
0 mol/m**3
0 mol/m**3
0 mol/m**3
0 mol/m**3
SNAPSHOT # 2
1 yr
12
20 mol/m**3
20 mol/m**3
1 mol/m**2/yr
1 mol/m**2/yr
0 mol/m**3
0 mol/m**3
0 mol/m**2/s
0 mol/m**2/s
SNAPSHOT # 3
10 yr
13
20 mol/m**3
20 mol/m**3
0 mol/m**3
0 mol/m**3
SNAPSHOT # 4
100 yr
21
0 mol/m**2/s
3 mol/m**2/s
10 mol/m**3
100 mol/m**3
0 mol/m**2/s
0 mol/m**2/s
0 mol/m**3
0 mol/m**3
SNAPSHOT # 5
1000 yr
22
0 mol/m**2/s
3 mol/m**2/s
1 mol/m**2/s
1 mol/m**2/s
0 mol/m**2/s
0 mol/m**2/s
0 mol/m**2/s
0 mol/m**2/s
SNAPSHOT # 6
10000 yr
23
0 mol/m**2/s
3 mol/m**2/s
0 mol/m**2/s
0 mol/m**2/s
SNAPSHOT # 7
1.E+5 yr
31
10 mol/m**3
100 mol/m**3
0 mol/m**3
0 mol/m**3
SNAPSHOT # 8
2.E+5 yr
32
1 mol/m**2/s
1 mol/m**2/s
0 mol/m**2/s
0 mol/m**2/s
SNAPSHOT # 9
3.E+5 yr
33
SNAPSHOT # 10
4.E+5 yr
00
SNAPSHOT # 11
5.E+5 yr

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 LOWER-BDRY MATRIX CONC
CONTAMINANT # 1 LOWER-BDRY FRACTURE CONC
CONTAMINANT # 1 UPPER-BDRY MATRIX CONC
CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC
CONTAMINANT # 2 LOWER-BDRY MATRIX CONC
CONTAMINANT # 2 LOWER-BDRY FRACTURE CONC
CONTAMINANT # 2 UPPER-BDRY MATRIX CONC
CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 LOWER-BDRY MATRIX CONC
CONTAMINANT # 1 LOWER-BDRY FRACTURE CONC
CONTAMINANT # 1 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 2 LOWER-BDRY MATRIX CONC
CONTAMINANT # 2 LOWER-BDRY FRACTURE CONC
CONTAMINANT # 2 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC-FLUX

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 LOWER-BDRY MATRIX CONC
CONTAMINANT # 1 LOWER-BDRY FRACTURE CONC
CONTAMINANT # 2 LOWER-BDRY MATRIX CONC
CONTAMINANT # 2 LOWER-BDRY FRACTURE CONC

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 LOWER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 1 LOWER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 1 UPPER-BDRY MATRIX CONC
CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC
CONTAMINANT # 2 LOWER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 2 LOWER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY MATRIX CONC
CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 LOWER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 1 LOWER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 1 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 2 LOWER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 2 LOWER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC-FLUX

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 LOWER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 1 LOWER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 1 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 2 LOWER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 2 LOWER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC-FLUX

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 UPPER-BDRY MATRIX CONC
CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC
CONTAMINANT # 2 UPPER-BDRY MATRIX CONC
CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC

PROBLEM TIME
BOUNDARY-CONDITION FLAG
CONTAMINANT # 1 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY MATRIX CONC-FLUX
CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC-FLUX

PROBLEM TIME
BOUNDARY-CONDITION FLAG

PROBLEM TIME
BOUNDARY-CONDITION FLAG

PROBLEM TIME

```

Figure 4.15: TRANS boundary-condition block example.

INDATA prompts for initial-condition data as follows:

INITIAL-CONDITION BLOCK

INITIAL-CONDITION FLAGS ARE:

- 0. ZERO CONCENTRATION, ALL CONTAMINANTS, ALL MESH POINTS
- 1. CONSTANT CONCENTRATIONS
- 2. FILE-DEFINED CONCENTRATIONS

ENTER INITIAL-CONDITION FLAG (DEFAULT=0):

Using the initial-condition flag, three different methods of defining an initial concentration are possible:

Flag=0 zero: zero concentrations are assigned to all contaminants at every mesh point.

Flag=1 constant: a constant concentration is assigned to each species at every mesh point. (The constant can be different for different species, and the concentrations in the matrix and the fractures can be different.)

Flag=2 file: each mesh point is assigned a concentration value from a file previously created by the user.

If an initial-condition flag of 0 is specified, INDATA generates no further prompts for this data block. The default initial condition is to assign constant concentration values of 0 at each mesh point.

If an initial-condition flag of 1 is selected, INDATA generates the following series of prompts:

```
ENTER # OF CONTAMINANTS (DEFAULT=1):
ENTER CONTAMINANT # 1 INITIAL MATRIX CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 1 INITIAL FRACTURE CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 2 INITIAL MATRIX CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 2 INITIAL FRACTURE CONC (DEFAULT=0. mol/m**3):
ENTER CONTAMINANT # 3 INITIAL MATRIX CONC (DEFAULT=0. mol/m**3):
```

```
o
o
o
```

This constant concentration will be assigned to every mesh point at the beginning of a transport calculation. The default value of 0 implies a condition of no contaminant in the column. Concentration values must be nonnegative.

If an initial-condition flag of 2 is specified, INDATA generates one prompt:

```
INITIAL-CONDITION FILE DEFAULT NAME: TRANS.CON
ENTER INITIAL-CONDITION FILE NAME:
```

The initial-condition-file name is a string of up to 80 characters with no embedded blanks. TRANS.CON is the default name for the initial-condition file; therefore, if the user would like to use the default, he or she must create a file named TRANS.CON before running the TRANS module. The contents and format of the initial-condition file are given in Section 4.7.9.

An example INDATA session for the construction of a transport initial-condition block follows. Notice

that two chains are specified in the contaminant-property block: the first chain consists of one species, the second consists of two species.

INITIAL-CONDITION BLOCK

INITIAL-CONDITION FLAGS ARE:

0. ZERO CONCENTRATION, ALL CONTAMINANTS, ALL MESH POINTS

1. CONSTANT CONCENTRATIONS

2. FILE-DEFINED CONCENTRATIONS

ENTER INITIAL-CONDITION FLAG (DEFAULT=0): 1

ENTER # OF CONTAMINANTS (DEFAULT=1): 3

ENTER CONTAMINANT # 1 INITIAL MATRIX CONC (DEFAULT=0. mol/m**3): 0.01 mol/m**3

ENTER CONTAMINANT # 1 INITIAL FRACTURE CONC (DEFAULT=0. mol/m**3):

ENTER CONTAMINANT # 2 INITIAL MATRIX CONC (DEFAULT=0. mol/m**3): 0.5 mol/m**3

ENTER CONTAMINANT # 3 INITIAL FRACTURE CONC (DEFAULT=0. mol/m**3): 0.5 mol/m**3

ENTER CONTAMINANT # 3 INITIAL MATRIX CONC (DEFAULT=0. mol/m**3):

ENTER CONTAMINANT # 3 INITIAL FRACTURE CONC (DEFAULT=0. mol/m**3):

In this example, the first contaminant has a concentration of 0.01 in the matrix and a concentration of 0 in the fractures assigned to every mesh point. The second contaminant has a concentration of 0.5 assigned in both matrix and fractures. The third contaminant has a concentration of 0 assigned in both matrix and fractures (the default).

Figure 4.16 presents the initial-condition block of a transport input-data file created by the above INDATA session.

```

***** INITIAL-CONDITION BLOCK *****
1      INITIAL-CONDITION FLAG
3      # CONTAMINANTS (CONSISTENCY CHECK)
0.01 mol/m**3  CONTAMINANT # 1 UPPER-BDRY MATRIX CONC
0. mol/m**3    CONTAMINANT # 1 UPPER-BDRY FRACTURE CONC
0.5 mol/m**3   CONTAMINANT # 2 UPPER-BDRY MATRIX CONC
0.5 mol/m**3   CONTAMINANT # 2 UPPER-BDRY FRACTURE CONC
0. mol/m**3    CONTAMINANT # 3 UPPER-BDRY MATRIX CONC
0. mol/m**3    CONTAMINANT # 3 UPPER-BDRY FRACTURE CONC

```

Figure 4.16: TRANS initial-condition block example.

4.3 Steady-State-Flow Hydrology Module (STEADY)

The TOSPAC module to solve for steady-state water flow is called STEADY. The module uses a finite-difference method, differenced across three mesh points, to solve a conservation-of-mass form of Darcy's Law (Section 2.2 of *Volume 1*).

In one dimension, a steady-state solution can be obtained by treating the problem as an initial value problem (IVP) and integrating with respect to pressure head. STEADY treats the problem as a boundary value problem (BVP) in order to be consistent with TOSPAC's dynamic-flow and transport solvers.

As discussed in Section 4.2.10, STEADY is restricted to a flux upper-boundary condition and a pressure-head lower-boundary condition (boundary-condition flag 12). Furthermore, STEADY can only solve for downward flow (negative flux).

This section contains a discussion about the structure of the STEADY module (Section 4.3.1), followed by a discussion of how to execute STEADY (Section 4.3.2).

4.3.1 STEADY Module Structure

Figure 4.17 contains a diagram of the top-level logical flow of STEADY. STEADY begins by reading the hydrology input-data file (default name STEADY.DAT) in subroutine SINPUT, and initializing various parameters in subroutine SINTLZ. SINTLZ includes a first estimate of upper and lower bounds for the pressure-head solution, and a calculation of various dependent variables, such as saturation, hydraulic conductivity, and flux. The initial estimate of a solution is the lower bound on the pressure head in some units, and the upper bound in others. (*Volume 1* contains the reasons behind using upper and lower bounds.) The initial boundary conditions are then calculated in subroutine PHBND. STEADY concludes the setup section of the program by writing out all the data it is using to the output-listing file and the plot data file in subroutine SINWRITE.

The calculational section of STEADY consists of one major loop. The calculational mesh is broken into parts, working from the bottom up, each consisting of a single geologic unit or of 100 mesh-point sections (if the geologic unit comprises more than 120 mesh points). The difference equations (*Volume 1*) are used in subroutine PICARD to construct a tridiagonal matrix $\mathbf{A}$ and an inhomogeneous vector $\mathbf{b}$ —i.e., the linear system, $\mathbf{A} \cdot \mathbf{p} = \mathbf{b}$, where the pressure-head vector $\mathbf{p}$ is the unknown. The initial estimate of a pressure-head solution is used to construct $\mathbf{A}$ and $\mathbf{b}$. The unknown vector $\mathbf{p}$ contains the refined estimate of the pressure-head solution once the linear system is solved. The linear system is solved in subroutine TRIDG. Note that the three-point differencing used in PICARD results in a matrix with three diagonal bands, a relatively easy linear system to solve (*Volume 1*).

The solution of the linear system returns a better estimate of the pressure-head vector. Not only must this estimate be computed and recomputed over and over again (a process called iteration) until it converges to an acceptable answer, but because of the numerics, it is not guaranteed to converge! In subroutine ADJBND, the pressure-head solution is checked to determine if it falls between the upper and lower bounds; if not, it is adjusted. Furthermore, the two previous pressure-head estimates are used to determine whether or not the solution is oscillating between the two bounds. If it is, the bounds are arbitrarily collapsed, and the solution is considered unacceptable from that mesh point upwards (the discussion of subroutine REBND, below, discusses what happens in this case).

Figure 4.17: TOSPAC STEADY module structure.

Subroutine GETCRV calculates the hydraulic conductivity (based on the pressure-head solution) necessary to reset the difference equations. GETCRV also calculates other dependent variables, such as matrix and fracture saturation. A call to PHBND reasserts the pressure-head (lower) boundary and recalculates a pressure head for the flux (upper) boundary.

The solution is then checked for convergence. Convergence is reached when the pressure head at any mesh point varies from the pressure head calculated during the previous iteration by less than a factor of 0.01 (one-hundredth --surprisingly, tighter tolerances do not help). If the pressure-head solution has not converged, STEADY goes back to PICARD and begins a new iteration. If the pressure-head solution has converged, but the bounds have been tampered with, STEADY cuts off the part of the solution that was acceptable, calculates new bounds for the remainder, and goes back to PICARD to begin a new iteration. This process takes place in subroutine REBND. If the pressure-head solution has converged and the bounds have not been tampered with in ADJBND, STEADY continues to calculate the solution for the next geologic unit.

When the pressure head has been computed for each geologic unit, various other dependent variables are calculated (flux, velocity) in subroutine GETOUT. The solution and the dependent variables are written to the output-listing file and the plot-data file in subroutine SITWRITE. Travel times are calculated and written to the output-listing file in subroutine TTOUT. And finally, the pressure-head solution for the entire mesh is written to the STEADY solution file.

4.3.2 STEADY Execution

STEADY is executed by selecting choice number 2 when presented with the TOSPAC main menu:

```
TOSPAC VERSION 1.10 MAIN MENU
```

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

```
ENTER CHOICE: 2
```

TOSPAC indicates that it is executing STEADY with the following:

```
TOSPAC MODULE STEADY
```

At this point, TOSPAC asks for the name of the input-data file:

```
ENTER STEADY INPUT-DATA FILE (DEFAULT=STEADY.DAT):
```

If the input-data file does not exist, an error message results and the prompt is repeated for a maximum of three times, after which control is returned to the TOSPAC main menu.

If the input-data file exists, TOSPAC reads it, and informs the user:

```
READING INPUT-DATA FILE input-data_file_name.
```

If the input-data file contains errors or inconsistencies, one or more error messages will appear on the terminal screen. Any error causes the interruption of STEADY; control is then returned to the TOSPAC SHELL and the TOSPAC main menu appears on the terminal screen.

If the input-data file does not contain a file block (Section 4.2.11), TOSPAC prompts for the names of the three STEADY output files:

```
ENTER STEADY SOLUTION FILE (DEFAULT=STEADY.PSI):  
ENTER STEADY OUTPUT-LISTING FILE (DEFAULT=STEADY.LIS):  
ENTER STEADY PLOT-DATA FILE (DEFAULT=STEADY.PLT):
```

Default file names are discussed in Section 4.7.

If a file block is present in the input-data file, STEADY creates the files named in the file block:

```
CREATING STEADY SOLUTION FILE  solution_file_name.  
CREATING STEADY PLOT-DATA FILE  plot-data_file_name.  
CREATING STEADY OUTPUT-LISTING FILE  output-listing_file_name.
```

After the input and output file names are defined and if the input-data file contains no errors or inconsistencies, STEADY enters the calculation loop with the following report:

INITIALIZING VARIABLES...

BEGINNING STEADY-STATE FLOW CALCULATION...

```
ITERATION =    1  WORKING ON UNIT #  1  
ITERATION =   10  WORKING ON UNIT #  1  
ITERATION =   20  WORKING ON UNIT #  1  
ITERATION =   30  WORKING ON UNIT #  1
```

○
○
○

The iteration status report is written at least every ten iterations. STEADY calculates the steady-state flow for one geologic unit at a time, beginning with the bottom unit, and every time STEADY begins working on another geologic unit, another iteration status report is written. Thus, the user can keep track of how the calculation is proceeding.

STEADY allows a maximum of 5000 iterations per calculation. If 5000 iterations have occurred and no solution has been reached, an error message is written to the screen, and STEADY is interrupted, with control returning to the TOSPAC SHELL. Usually, an inordinant number of iterations indicates a fault with the spacing of the mesh points in the calculational mesh. It is advised that the user modify the mesh block in the hydrologic input-data file, then rerun STEADY.

As STEADY terminates execution, the deviation between the calculated flux and the imposed flux is computed. If the flux deviation does not exceed 10% at any mesh point, STEADY writes the following message to the user's terminal:

MAX FLUX DEVIATION= ?????? % AT MESH POINT= ??? ELEVATION= ????.

where the question marks are replaced by appropriate numbers. If the flux deviation is greater than 10% at more than a single mesh point, a line reporting the flux deviation is written for each of the mesh points exceeding 10% deviation.

FLUX DEVIATION= ?????? % AT MESH POINT= ??? ELEVATION= ????.

FLUX DEVIATION= ?????? % AT MESH POINT= ??? ELEVATION= ????.

FLUX DEVIATION= ?????? % AT MESH POINT= ??? ELEVATION= ????.

o

o

o

If STEADY calculates a solution in less than 5000 iterations, the following message is displayed:

NORMAL STEADY TERMINATION

If STEADY takes more than 5000 iterations to calculate a solution (or if errors are found in the input data) the following message is displayed:

ABNORMAL STEADY TERMINATION

At this point, control is returned to the TOSPAC SHELL and the TOSPAC main menu appears on the user's terminal.

It must be stressed that just because STEADY has reached a solution, whether or not termination is normal, it does not mean that the solution is acceptable. The solution calculated by STEADY may vary significantly from steady state. Mathematically, steady-state flow in one dimension requires the flux (or Darcy velocity or percolation rate or rate of infiltration) to be a constant. The acceptability of a solution, i.e., the amount that the calculated flux deviates from the imposed flux, depends on the application. To improve the solution, refine the mesh—add mesh points in the areas where the flux is unacceptable—then rerun STEADY. Sometimes, calculating an acceptable solution may involve several iterations where the mesh is refined and STEADY is rerun. Equations providing guidance on acceptable mesh-point spacings for steady-state calculations are offered in Section 4.2.9 of this Guide, and Section 2.3 of *Volume 1*.

4.4 Transient-Flow Hydrology Module (DYNAMICS)

The TOSPAC module to calculate dynamic, or transient, water flow is called DYNAMICS. The module uses a finite-difference method, differenced across three mesh points, to solve the Richards' Equation. Richards' Equation is similar to the conservation-of-mass form of Darcy's law, except that where Darcy's law states that the divergence of the flux equals zero, Richards' Equation states that the divergence of the flux changes with time and with the capacitance (storage capacity) of the material carrying the flow.

The difference equations in DYNAMICS are very similar to the difference equations in the steady-state-flow solver, STEADY. DYNAMICS can use a STEADY solution as an initial condition.

This section contains a discussion of the structure of the DYNAMICS module (Section 4.4.1), a discussion of how to execute DYNAMICS (Section 4.4.2), and a discussion of the capability to restart a DYNAMICS calculation (Section 4.4.3).

4.4.1 DYNAMICS Module Structure

Figure 4.18 contains a diagram of the top-level logic flow of the DYNAMICS module. DYNAMICS begins by reading the hydrology input-data file (default name DYNAMICS.DAT) in subroutine SINPUT, and initializing various parameters in subroutine DINTLZ. In DINTLZ the default initial condition—the initial pressure head at each mesh point—is read (unless it was defined in SINPUT), and the initial calculation of various dependent variables, such as saturation, hydraulic conductivity, and flux takes place. The initial boundary conditions are then calculated in subroutine PHBND, and the initial water mass and average saturation are calculated in subroutine AVESAT. DYNAMICS then writes out the setup data it is using to the output-listing file (default name DYNAMICS.LIS) and the plot-data file (default name DYNAMICS.PLT), in subroutine DINWRITE.

The calculational section of DYNAMICS, as in STEADY, consists of one major loop. The loop begins with the calculation of a timestep in subroutine TMCNTL. Each iteration has a timestep. The problem time starts at the first time (usually 0) defined in the boundary-condition block in the input-data file, and as the calculation progresses, it is the sum of all the preceding timesteps.

The timestep is added onto the problem time in subroutine DDCNTL. The new problem time is checked to determine if a time snapshot has been met or if the maximum time has been exceeded; if yes, various flags are set to output results, change boundary conditions, or, eventually, to halt the problem. With this bookkeeping taken care of, DYNAMICS begins the solution.

The Picard difference equations (*Volume 1*) are implemented in subroutine PICARD to construct a tridiagonal matrix $\mathbf{A}$ and an inhomogenous vector $\mathbf{b}$; i.e., the linear system, $\mathbf{A} \cdot \mathbf{p} = \mathbf{b}$, where the pressure-head vector $\mathbf{p}$ is the unknown. The first time through the loop, the initial-condition pressure head is used to construct $\mathbf{A}$ and $\mathbf{b}$. The linear system is solved in subroutine TRIDG. (Note that, as in STEADY, the three-point differencing used in PICARD results in a matrix with three diagonal bands, a relatively easy linear system to solve.)

After the Picard linear system is solved, the unknown vector $\mathbf{p}$ contains the initial estimate of the pressure-head solution at the new problem time. DYNAMICS then uses Newton's Method to converge to a more accurate, and more stable, solution. Coverage is assumed when the pressure head at each

Figure 4.18: TOSPAC DYNAMICS module structure.

mesh point changes less than a factor of 10^{-6} from the previous iteration. Newton's Method is programmed in subroutine NEWTON. This linear system is also solved in subroutine TRIDG.

If more than ten iterations of Newton's Method are needed to meet the convergence criterion, the timestep is stopped. The calculation is backed up to the previous time and is repeated with a smaller timestep.

With the new pressure-head values, new saturation and hydraulic conductivity values are calculated in subroutine GETCRV. In subroutine PHBND, pressure-head boundary conditions are reasserted and, for flux boundary conditions, new boundary pressure heads are calculated.

At the end of the loop, if a time-snapshot flag is set, output data are calculated. With pressure heads and conductivities at all mesh points at the new problem time, the flux and average linear velocities are calculated in subroutine GETOUT. The water mass and saturation of the column are calculated in AVESAT. Then the pressure-head solution and the dependent variables are written to the output-listing file and the plot-data file in subroutine DITWRITE. Then the termination flag is checked. If the flag is not set, the calculation continues. If the flag is set, then the calculational loop halts, and the DYNAMICS module terminates.

4.4.2 DYNAMICS Execution

DYNAMICS is executed by selecting choice number 3 when presented with the TOSPAC main menu:

TOSPAC VERSION 1.10 MAIN MENU

- 0. STOP
- 1. INDATA
- 2. STEADY
- 3. DYNAMICS
- 4. TRANS
- 5. OUTPLOT

ENTER CHOICE: 3

TOSPAC indicates that it is executing DYNAMICS with the following:

TOSPAC MODULE DYNAMICS

At this point, TOSPAC asks for the name of the input-data file.

ENTER DYNAMICS INPUT-DATA FILE (DEFAULT=DYNAMICS.DAT):

If the input-data file does not exist, an error message results and the prompt is repeated for a maximum of three times, after which control is returned to the TOSPAC main menu.

If the input-data file exists, TOSPAC reads it, and informs the user:

READING INPUT-DATA FILE *input-data_file_name*.

If the input-data file contains errors or inconsistencies, one or more error messages will appear on the

terminal screen. Any error causes the interruption of DYNAMICS; control is then returned to the TOSPAC SHELL and the TOSPAC main menu appears on the terminal screen.

If the input-data file does not contain a file block (Section 4.2.11), TOSPAC prompts for the names of the files:

```
ENTER DYNAMICS INITIAL-CONDITION FILE (DEFAULT=STEADY.PSI):
ENTER DYNAMICS OUTPUT-LISTING FILE (DEFAULT=DYNAMICS.LIS):
ENTER DYNAMICS PLOT-DATA FILE (DEFAULT=DYNAMICS.PLT):
```

File-name defaults are handled similarly to the method used by STEADY. Section 4.2.2 contains a discussion of file-name defaults. Section 4.2.2 also contains a discussion of creating multiple files with the same name.

If the input-data file does contain a file block, DYNAMICS prints out the names of the output files when they are created:

```
CREATING DYNAMICS PLOT-DATA FILE plot-data_file_name.
CREATING DYNAMICS OUTPUT-LISTING FILE output-listing_file_name.
```

If the initial condition is specified by file, TOSPAC indicates when the file is being read:

```
READING DYNAMICS INITIAL-CONDITION FILE initial-condition_file_name.
```

As with the input-data file, if the initial-condition file contains errors or inconsistencies, an error message results and control is returned to the TOSPAC SHELL.

After the input and output file names are defined and if no errors have been registered, DYNAMICS enters the calculation loop with the following report:

INITIALIZING VARIABLES...

BEGINNING TRANSIENT FLOW CALCULATION...

SNAPSHOT 1... TIME(UNITS) = ????

ITERATION =	1	STEP(UNITS) =	????	TIME(UNITS) =	????
ITERATION =	10	STEP(UNITS) =	????	TIME(UNITS) =	????
ITERATION =	20	STEP(UNITS) =	????	TIME(UNITS) =	????
ITERATION =	30	STEP(UNITS) =	????	TIME(UNITS) =	????

○
○
○

ITERATION =	??	STEP(UNITS) =	????	TIME(UNITS) =	????
-------------	----	---------------	------	---------------	------

SNAPSHOT 2... TIME(UNITS) = ????

ITERATION =	??	STEP(UNITS) =	????	TIME(UNITS) =	????
ITERATION =	??	STEP(UNITS) =	????	TIME(UNITS) =	????

○
○
○

where the question marks are replaced by appropriate numbers and the word UNITS is replaced by appropriate time units (deduced from the time-conversion menu). The iteration status report is written every ten iterations of the main calculational loop, or when a time snapshot is reached. The status is reported at the end of the tenth time iteration: STEP is the amount of time that the tenth iteration stepped; TIME is the problem time at the end of that tenth iteration. The snapshot status message is written when the boundary conditions defined by the time snapshot take effect, at which point the results are written to the output-listing and plot-data files.

Dynamic-flow calculations begin at the time of the first time snapshot, usually time 0. DYNAMICS has an automatic timestep control that adjusts the timestep for every iteration, including the first. The automatic timestep control allows each timestep to increase a maximum of 1.5 times the previous timestep; and it allows each timestep to decrease a maximum of 0.667 times the previous timestep. If the automatic timestep controller calculates a timestep less than 0.667 times the previous timestep, an instability is indicated. At this point, DYNAMICS backs up and recalculates the previous iteration with a reduced timestep. DYNAMICS then uses this reduced timestep as the maximum allowable for five more iterations. DYNAMICS also backs up in this manner when more than ten Newton iterations are needed for convergence in a given timestep. When the timestep causes the problem time to exceed a snapshot time, the timestep is adjusted (in TMCNTL) so that the problem time is equal to the snapshot time.

The timestep is presently based on the quantities $K/\dot{K}$ and $\psi/\dot{\psi}$, multiplied by the timestep factor. The first iteration uses a Courant condition to determine the timestep, because the time derivatives of K and ψ are not yet available to DYNAMICS. If DYNAMICS spends a significant amount of time backing up and recalculating timesteps, it may be necessary to rerun the calculation with a smaller timestep factor.

When the problem time reaches the time of the final snapshot, the calculation ceases and the following message appears on the user's terminal:

NORMAL DYNAMICS TERMINATION

Control is then returned to the TOSPAC SHELL and the TOSPAC main menu appears on the user's terminal.

As with STEADY, it must be stressed that a DYNAMICS solution may not be acceptable. And unfortunately, there is no foolproof independent check on the solution (remember, in STEADY the flux should equal a constant). The user should check the flux plots for evidence of instability or nonphysical behavior. The user should check the mass balance reported in the output-listing file; very little extraneous mass should be created or lost by the calculation. Other ways of checking a solution are possible. The user is advised to read the description of the mathematical model in DYNAMICS in *Volume 1*. Section 3.1 of this User's Guide offers information on checking the accuracy of a calculation.

4.4.3 DYNAMICS Restart Capability

The purpose of the restart capability is to reduce the cost of a DYNAMICS calculation by allowing the user to extend a previous calculation or to change a previous calculation without recalculating all of the results.

Restart capability is accessed through the restart-snapshot datum in the constants block of a hydrology input-data file (Section 4.2.6). If the restart snapshot is specified to be 0 or 1, DYNAMICS does not attempt a restart. If the restart snapshot is greater than 1, when DYNAMICS executes it attempts to read a plot-data file from a previous execution (named either by default or in the file block—Section 4.2.11). If the file does not exist, an error results. If the plot-data file is available, DYNAMICS attempts to read the restart number of snapshots. If the file contains less than the restart number of snapshots, an error results. When DYNAMICS has read the specified number of snapshots, execution begins at the time snapshot in the boundary-condition block (Section 4.2.10) that corresponds to the restart-snapshot number.

The user is cautioned to check that the materials, geologic units, and mesh are the same in the old input-data file (the file used to produce the existing plot-data file) and the new input-data file. DYNAMICS does not check for consistency between the old results and the new calculation. The new input-data file should be identical to the old input-data file except for the following: in the constants block, the timestep factor, the implicitness factor, the GWIT positions, and (of course) the restart-snapshot number can be different; in the boundary-condition block, any snapshots with numbers greater than or equal to the restart number can be different; in the file block, everything can be different, except the plot-data-file name.

When a pond-drain boundary condition is used in DYNAMICS, additional time snapshots might have automatically been added to plot-data file. A new snapshot is inserted if and when a pond completely drains. The user is cautioned to check the output from the previous calculation carefully to note any added time snapshots, and to take them into account when determining the restart number, otherwise the restart time snapshot might not correspond to the expected time snapshot.

4.5 Contaminant-Transport Module (TRANS)

The TRANS module of TOSPAC is used to calculate contaminant transport. TRANS solves for the concentration of contaminants in groundwater at given problem times. TRANS presently can only accept the hydrology results from STEADY as input--not DYNAMICS. (This situation could change in future versions of TOSPAC.) The TRANS module uses a finite-difference method, differenced across three mesh points, to solve the coupled matrix-fracture transport equations (*Volume 1*).

This section contains a discussion about the structure of the TRANS module (Section 4.5.1), followed by a discussion of how to execute TRANS (Section 4.5.2).

4.5.1 TRANS Module Structure

Figure 4.19 contains a diagram of the top-level logical flow of the TRANS module. TRANS begins by reading the TRANS input-data file in subroutine 'TX'INPT, and the hydrologic plot-data file (created by STEADY), in subroutine 'TINPT'.

TRANS initializes parameters and variables in subroutine 'TINTLZ'. Included are the initial values for time, hydrologic velocities and moisture contents (calculated in VELCALC--note that STEADY only passes pressure-head data to TRANS, because passing all the data would make the plot file prohibitively long, plus TRANS uses a different definition of velocity and would have to recalculate it anyway), contaminant retardation factors (RTRD), contaminant dispersion coefficients (DSPRSN), decay rates for radionuclide contaminants, and matrix/fracture coupling rates (RATES).

The initial problem setup is written to the TRANS output-listing file and the TRANS plot-data file in subroutine 'TINTLZ'.

The main calculational section of TRANS consists of one major loop. The loop begins with the calculation of a timestep in subroutine 'TTMCNTL'. The timestep is added to the problem time. The new problem time is then checked to determine if a time snapshot has been met or if the maximum time has been exceeded; if yes, various flags are set to write results, change boundary conditions, or possibly, to halt the problem. After this bookkeeping, TRANS begins the solution.

The total contaminant inventory at the problem time is calculated in BTMN, immediately followed by a calculation of the amount of contaminant in the source region, in precipitate form, and outside the mesh boundaries, in subroutine BTMNSRC. The "BTMN" in the name of these subroutines refers to the Bateman equations used to evaluate exponential (radioactive) decay.

The difference equations (*Volume 1*) are implemented in subroutine 'TMXSET' to construct a pentadiagonal matrix **A** and an inhomogenous vector **b** (i.e., the linear system: $\mathbf{A} \cdot \mathbf{c} = \mathbf{b}$). The first time through the loop, the initial condition concentrations are used to construct **A** and **b**. Within 'TMXSET', the boundary conditions are set in subroutine BDRYMX, the contribution of the source is determined in either subroutine CONGLCH (congruent leach), or subroutine SRCE (solubility-limited leach), or subroutine USERSRC (to read a source file), and the linear system is solved in subroutine PENTAD. This solution procedure is performed for each contaminant species in each chain; the solution is the concentration of each species in each mesh cell at the problem time.

The new concentration values are checked in subroutine PRECIP to see if they exceed the solubility

Figure 4.19: TOSPAC TRANS module structure.

limits of the various contaminants. If yes, the excess is precipitated. The amount of contaminant that crosses the upper and lower boundaries (i.e., released from or entered the domain) is calculated in subroutine FLUXCALC.

At the end of the loop, the time is checked. If the time exceeds a snapshot time, the concentration solutions and the amounts released from or entered into the domain are written to the output-listing file and the plot-data file in subroutine TWRITE. Also, a mass-balance calculation is made in subroutine MSBAL to aid in determining the acceptability of the solution.

Finally, at the end of the loop, if the time is less than the maximum snapshot time, control returns to the next timestep calculation in subroutine TTMCNTL. If the final time has been reached, then the calculational loop halts, and the TRANS module terminates.

4.5.2 TRANS Execution

TRANS is executed by selecting choice number 4 when presented with the TOSPAC main menu:

```
TOSPAC VERSION 1.10 MAIN MENU
```

```
0. STOP
1. INDATA
2. STEADY
3. DYNAMICS
4. TRANS
5. OUTPLOT
```

```
ENTER CHOICE: 4
```

TOSPAC indicates that TRANS is executing with the following message:

```
TOSPAC MODULE TRANS
```

At this point, TRANS asks for the name of the input-data file:

```
ENTER TRANS INPUT-DATA FILE (DEFAULT=TRANS.DAT):
```

If the input-data file does not exist, an error message results and the prompt is repeated for a maximum of three times, after which control is returned to the TOSPAC SHELL and the TOSPAC main menu appears on the terminal screen.

If the input-data file exists, TOSPAC reads it, and informs the user:

```
READING INPUT-DATA FILE input-data_file_name.
```

Errors or inconsistencies in the input-data file are discussed below.

If the input-data file does not contain a file block (Section 4.2.11), TOSPAC prompts for the names of the input file and two output files:

```
ENTER STEADY PLOT-DATA FILE (DEFAULT=STEADY.PLT):
```

ENTER TRANS PLOT-DATA FILE (DEFAULT=TRANS.PLT):
 ENTER TRANS OUTPUT-LISTING FILE (DEFAULT=TRANS.LIS):

Default file names are handled similarly to the method used by STEADY. Section 4.2.2 contains a discussion of default file names. Section 4.2.2 also contains a discussion of creating multiple files with the same name.

If a file block is present in the input-data file, TRANS reads the hydrology plot-data file and creates the output files:

CREATING TRANS PLOT-DATA FILE *plot-data_file_name*.
 CREATING TRANS OUTPUT-LISTING FILE *output-listing_file_name*.
 READING STEADY PLOT-DATA FILE *hydrology_plot-data_file_name*.

If the initial condition is specified in the TRANS input-data file as a file, another status message indicates that the initial-condition file is being read:

READING TRANS INITIAL-CONDITION FILE *initial-condition_file_name*.

If the TRANS input-data file, the STEADY plot-data file, or the initial-condition file contain errors or inconsistencies, one or more error messages will appear on the terminal screen. Any error causes the interruption of TRANS; control is then returned to the TOSPAC SHELL and the TOSPAC main menu appears on the terminal screen.

After the input and output file names are defined and if no errors have been registered, TRANS enters the calculational loop with the following report:

INITIALIZING VARIABLES...

BEGINNING TRANSPORT CALCULATION...

SNAPSHOT 1... TIME(UNITS) = ????

ITERATION =	1	STEP(UNITS) =	????	TIME(UNITS) =	????
ITERATION =	10	STEP(UNITS) =	????	TIME(UNITS) =	????
ITERATION =	20	STEP(UNITS) =	????	TIME(UNITS) =	????

○
○
○

ITERATION =	??	STEP(UNITS) =	????	TIME(UNITS) =	????
-------------	----	---------------	------	---------------	------

SNAPSHOT 2... TIME(UNITS) = ????

ITERATION =	??	STEP(UNITS) =	????	TIME(UNITS) =	????
ITERATION =	??	STEP(UNITS) =	????	TIME(UNITS) =	????

○
○
○

where the question marks are replaced by appropriate numbers and the word UNITS is replaced by appropriate time units (deduced from the time-conversion menu). The iteration status report is written every ten iterations of the main calculational loop, or when a time snapshot has occurred. The status is reported at the end of the tenth time iteration; STEP is the amount of time that the tenth iteration stepped; TIME is the problem time at the end of that tenth iteration. The snapshot status message is written when the boundary conditions defined by the time snapshot take effect, or when the results are written to the output-listing and plot-data files.

Transport calculations begin at the time specified for the first time snapshot in the boundary-condition block of the TRANS input-data file, typically problem time 0. TRANS has an automatic timestep controller that adjusts the timestep for every iteration, including the first. The timestep controller uses the concentration divided by the temporal derivative of the concentration (the quantity C'/C) multiplied by a timestep factor. The timestep factor cannot be adjusted by the user.

When the problem time reaches the time of the final snapshot, the calculation ceases and the following message appears on the user's terminal:

NORMAL TRANS TERMINATION

Control is then returned to the TOSPAC SHELL and the TOSPAC main menu appears on the user's terminal.

In general, a transport calculation does not involve the highly nonlinear coefficients of a partially saturated flow calculation. Thus, TRANS can be expected to run more stably than STEADY or DYNAMICS. Numerical dispersion, a numerical problem that causes spreading of a concentration front, can occur, however. The user is advised to read about the mathematical model for TRANS in *Volume 1* for more information. The user should still carefully check the results for nonphysical behavior (e.g., negative concentrations, curious spikes in concentration). Also, the user is advised to consider whether the mass balance reported in the TRANS output-listing file is acceptable for the problem being solved.

4.6 Computer-Graphics Module (OUTPLOT)

TOSPAC incorporates two methods for presenting results from the calculational modules: output listings and computer graphics. Examples of the output listings are given in Figures 2.5, 2.6, 3.3, 3.22, and 3.23.

The amount of output for a given problem can be so large that it becomes difficult for the analyst to assess. TOSPAC circumvents this limitation by having extensive computer-graphics capabilities. The OUTPLOT module of TOSPAC is used to produce computer graphics, specifically two-dimensional and three-dimensional, preformatted plots. A typical OUTPLOT run proceeds as follows:

- 1) using OUTPLOT, the user constructs a *plot-definition file* (default name OUTPLOT.PDF);
- 2) after the user enters the plot definitions, OUTPLOT reads the plot-definition file it has just created and constructs the plots in a *graphics-driver file* (default name OUTPLOT.DRV);
- 3) after the TOSPAC session is terminated, the user submits the *graphics-driver file* to an output graphics device.

The purpose of the plot-definition file is to allow OUTPLOT to process the plots as efficiently as possible and to allow the user to easily reproduce plots. In this regard, plot-definition files can be configured to operate only on specific plot-data files, or they can be configured to operate on any plot-data file (from a given TOSPAC module). Plots for STEADY, DYNAMICS, and TRANS results can be defined in a single plot-definition file. As with an input-data file, a plot-definition file can be created and modified with a text editor (Section 4.7.12).

Definition of the plots in OUTPLOT is analogous to definition of input data in INDATA. OUTPLOT and INDATA both create data files organized according to data blocks. OUTPLOT and INDATA differ in two aspects. First, OUTPLOT has no capability to modify plot-definition files; it can only create a new plot-definition file, or append new plot definitions to an existing plot-definition file. Second, OUTPLOT handles default values for plot parameters differently than INDATA handles default values for input data. OUTPLOT has no provision for supplying file-specific default answers to the prompts used in the plot definitions. The default value for a plot parameter in the plot-definition file is the word DEFAULT. The actual value is calculated during construction of the graphics-driver file (Section 4.6.6). The user may not be certain of any particular default value at the time of plot definition: the advantage is that the plot-definition file can apply to a number of plot-data files; the disadvantage is that the plots may be a surprise to the user.

The graphics-driver file is in a format that can drive a graphics device (i.e., a plotter or a printer with graphics capability). The graphics-driver file *cannot* drive just *any* computer-graphics device, because device languages are not standardized. The graphics-driver file must be submitted to the graphics device that was indicated when TOSPAC was installed on the user's computer (Section 4.7.13).

Some implementations of TOSPAC may draw the plots on the user's terminal screen as OUTPLOT is executed. The implementations of TOSPAC that produce plots directly on the user's terminal screen do not produce a graphics-driver file. Some implementations of TOSPAC may produce an intermediate-output graphics file that can be postprocessed to either draw the plots on the user's terminal screen or be sent to any of a number of graphics devices. Alternate implementations are not discussed further in this Guide.

TOSPAC computer graphics are generated using the CA-DISSPLA graphics software package (CAL, 1989). Contact the Authors for information on what can be done if your computer system does not have DISSPLA.

This section contains a discussion of the structure of the OUTPLOT module (Section 4.6.1), followed by a discussion of how to execute OUTPLOT. The discussion of how to execute OUTPLOT begins with an overview (Section 4.6.2), and includes discussions of defining plots for results from STEADY (Section 4.6.3), DYNAMICS (Section 4.6.4), and TRANS (Section 4.6.5). A further description of the plot-definition and graphics-driver files is contained in Sections 4.7.12 and 4.7.13, respectively.

4.6.1 OUTPLOT Module Structure

A diagram of the top-level logical flow of the OUTPLOT module is presented in Figure 4.20.

Figure 4.20: TOSPAC OUTPLOT module structure.

OUTPLOT begins by asking the user for the name of the plot-definition file in subroutine NAMEPDF. If the file does not exist, OUTPLOT creates it. If it does exist, OUTPLOT proceeds to the end of the file to append new plot definitions.

The OUTPLOT main menu is presented next. OUTPLOT is designed to operate in the interactive mode. Its organization is based on the plotting options for each calculational module in TOSPAC. The top-level menu allows the user to choose which results are to be used to define plots (choices 1, 2, and 3 on the OUTPLOT main menu). Each TOSPAC calculational module—STEADY, DYNAMICS, and TRANS—then has its own specific plot options controlled by its own specific submodule.

The user can place definitions for STEADY, DYNAMICS, and TRANS results in a single plot-definition file. The user can also construct more than one graphics-driver file in a single session.

Within each OUTPLOT submodule, the plot-data files that contain the results to be plotted can be specified. Specifying a plot-data file is optional and the capability to do so is included to allow an audit trail. The time-dependent modules, DYNAMICS and TRANS, have plots showing different time lines to allow the user to follow the course of a calculation. Thus, OUTPLOT only allows one DYNAMICS or TRANS plot-data file to be specified at a time. For STEADY results, OUTPLOT allows plotting results for more than a single calculation on each plot. In this way the user can examine changes in variables at different steady-state conditions.

Figures 4.21, 4.22, and 4.23 show the logical flow of submodules within OUTPLOT that allow the user to create plot-definition files for STEADY results, DYNAMICS results, and TRANS results, respectively. For all three submodules, a menu is first presented. After the user makes a menu selection, control is passed to a subroutine that prompts for information specific to the requested plot. As the subroutine acquires the input data, it writes a block of data onto the plot-definition file. When no more plots are to be defined, the submodule terminates and control is returned to the OUTPLOT main menu.

When OUTPLOT actually constructs plots (choice 4 on the OUTPLOT main menu), it does so from information on the plot-definition file. Thus, the user can create a plot-definition file on a text editor and then tell OUTPLOT to construct plots based on this file. OUTPLOT constructs plots by making a graphics-driver file that is sent to a computer-graphics device to produce the hardcopy. Figure 4.24 presents the structure of the submodule within OUTPLOT that constructs the graphics-driver file.

Within the graphics-driver submodule, the current plot-definition file is read in subroutine GRAPHDRV. After GRAPHDRV has determined whether STEADY, DYNAMICS, or TRANS results are to be plotted, plot blocks are read from the plot-definition file, using subroutines SPLOT (for plots of STEADY results), DPLOT (for plots of DYNAMICS results), and TPLOT (for plots of TRANS results). Once a plot block is read, control is transferred to the appropriate subroutine to construct the plot in the graphics-driver file. At this time, if no plot-data file has been defined yet (that is, if *NONE* was entered for the plot-data file name when the plots were defined—see Section 4.6.3), then OUTPLOT prompts for the plot-data file(s) to work from. The plot subroutine reads the plot-data file to extract the data to be plotted. When the subroutine begins work on a particular plot, a status message is written to the user's terminal screen.

An error in the plot-definition file causes the plot block to be skipped; execution continues with the next plot block. An error in the plot-data file can have one of two results: If the error is minor—for example, if the file is incomplete because of premature termination of the flow or transport calculation—then the plot will be constructed with the information available. A message is printed to the user's terminal screen warning that the results may be in error. If the error is sufficiently severe, it may be impossible to construct a plot at all, in which case a message is written to the user and control is transferred back to GRAPHDRV.

After all the plot blocks for a particular calculation type are exhausted, or in the case of a severe error

Figure 4.21: Structure of submodule to define STEADY plots.

Figure 4.22: Structure of submodule to define DYNAMICS plots.

Figure 4.23: Structure of submodule to define TRANS plots.

Figure 4.24: Structure of submodule to construct the graphics-driver file.

as just described, control returns to GRAPHDRV to find another group of STEADY, DYNAMICS, or TRANS plot definitions. If no other group of plot definitions exists (i.e., the end of the plot-definition file has been reached), FINISH is called to complete the graphics-driver file, and control is returned to the OUTPLOT main menu.

4.6.2 OUTPLOT Execution (Top Level)

OUTPLOT is executed by selecting choice number 5 when presented with the TOSPAC main menu:

```
TOSPAC VERSION 1.10 MAIN MENU
0. STOP
1. INDATA
2. STEADY
3. DYNAMICS
4. TRANS
5. OUTPLOT
```

```
ENTER CHOICE: 5
```

TOSPAC indicates OUTPLOT is executing with the following message:

```
TOSPAC MODULE OUTPLOT
```

The first prompt issued by OUTPLOT is for the name of a plot-definition file:

```
ENTER OUTPLOT PLOT-DEFINITION FILE (DEFAULT=OUTPLOT.PDF):
```

Acceptable file names are discussed in Section 4.2.2. The user *must* enter an acceptable file name (or a <CR> for the default name), or after three invalid responses control is returned to the TOSPAC main menu.

If the user enters the name of a plot-definition file that does not exist, a new file is created. If the plot-definition file does exist, the user can append new plot definitions to it. No provision is made for modifying or deleting data already in a plot-definition file. *Modifications must be performed using a text editor.*

If the plot-definition file does not exist, OUTPLOT reports the following:

```
plot-definition_file_name DOES NOT EXIST...
CREATING plot-definition_file_name.
```

If the plot-definition file does exist, OUTPLOT reports the following:

```
plot-definition_file_name EXISTS...
```

Whether the plot-definition file exists or not, OUTPLOT now displays the OUTPLOT main menu:

OUTPLOT MAIN MENU

- 0. STOP
- 1. DEFINE STEADY PLOTS
- 2. DEFINE DYNAMICS PLOTS
- 3. DEFINE TRANS PLOTS
- 4. CONSTRUCT GRAPHICS-DRIVER FILE

ENTER CHOICE:

Entering a choice of 0 returns the user to the TOSPAC main menu. The following subsections contain a discussion of each of the other choices, in order.

4.6.3 Define STEADY Plots

Entering a choice of 1 in response to the OUTPLOT main menu allows the user to define plots for STEADY results. Plotting of STEADY results begins with identification of the STEADY plot-data file(s) that contain the results:

ENTER STEADY PLOT-DATA FILE (DEFAULT=NONE):

The default answer implies that the plot-definition file being created will work with a general plot-data file (any STEADY plot-data file). If the user wants to create an audit trail for a specific analysis, the user can enter the name of a STEADY plot-definition file and OUTPLOT will use this plot-definition file *only* with the given plot-data file, with the exception given below.

OUTPLOT allows more than one STEADY plot-data file to be specified. If the user enters the name of a STEADY plot-data file, the prompt is repeated, and the prompt continues to be repeated until the user finally answers *NONE*. Note that if the user answers *NONE* after having given one or more plot-data file names, the *NONE* no longer implies a general plot-definition file; the plot-definition file will *only* work with the given plot-data files. If more than one plot-data file is specified, the data from each file are included on any given plot (where feasible—some plots are not conducive to multiple sets of data). Hence, results of various problems can be directly compared and the number of plots reduced.

Thus OUTPLOT repeats the plot-data file query until the user runs out of responses:

```
ENTER STEADY PLOT-DATA FILE (DEFAULT=NONE):  file_name_1
ENTER STEADY PLOT-DATA FILE (DEFAULT=NONE):  file_name_2
ENTER STEADY PLOT-DATA-FILE (DEFAULT=NONE):  file_name_3
```

```
o
o
o
```

OUTPLOT can handle up to ten STEADY plot-data files at a time. The STEADY plot-data files that are combined in this manner should probably be based on the same stratigraphy and have the same calculational mesh, otherwise the plots might not make sense.

OUTPLOT does not read the plot-data files at this time; they are only read during the construction of the graphics-driver file (Section 4.6.6). OUTPLOT has no provision for supplying file-specific default answers to the prompts used in the plot definitions. The default value for a plot parameter in the

plot-definition file is the word DEFAULT.

If more than one STEADY plot-data file was entered, OUTPLOT next prompts for an overall title to use on the plots:

DEFAULT TITLE: TOSPAC Steady-State Calculation
ENTER PLOT TITLE:

Normally, OUTPLOT uses the title given in the title block of the input-data file as the title for each plot. However, when several STEADY runs are to be combined on a single plot, rather than use one of the titles, the user is given the opportunity to specify an overall title to go on the plot. The titles from the individual STEADY files are not used.

OUTPLOT now displays the STEADY-results menu on the user's terminal screen:

```
OUTPLOT (STEADY RESULTS) MENU
0. STOP
1. PLOT MESH/STRATIGRAPHY
2. PLOT CHARACTERISTIC CURVES
3. PLOT COMPOSITE CONDUCTIVITY AND CAPACITANCE CURVES
4. PLOT PRESSURE HEAD VS ELEVATION
5. PLOT SATURATION VS ELEVATION
6. PLOT FLUX VS ELEVATION
7. PLOT VELOCITY VS ELEVATION
8. PLOT CONDUCTIVITY VS ELEVATION
9. PLOT CAPACITANCE VS ELEVATION
10. PLOT TRAVEL TIMES
```

ENTER CHOICE:

The choices are as follows:

- 0) Return to the OUTPLOT main menu.
- 1) Plot the mesh and stratigraphy for each plot-data file entered; examples of these plots are given in Figures 2.7, 3.4, and 3.24.
- 2) Plot the saturation and hydraulic-conductivity characteristic curves for each material specified; examples of these plots are given in Figures 3.5 and 3.25.
- 3) Plot composite hydraulic conductivity and capacitance versus pressure head for each geologic unit specified; examples of these plots are given in Figures 3.6 and 3.26 for the conductivity curves, and Figures 3.7 and 3.27 for the capacitance curves.
- 4) Plot STEADY-calculated pressure head versus elevation for each plot-data file entered; an example of this plot is given in Figure 3.28.
- 5) Plot STEADY-calculated saturation versus elevation for each plot-data file entered; an example of this plot is given in Figure 3.29.
- 6) Plot STEADY-calculated flux versus elevation for each plot-data file entered (this quantity is also called the Darcy velocity, the percolation rate, or the rate of infiltration); an example of this plot is given in Figure 3.30.

- 7) Plot STEADY-calculated average linear velocity versus elevation for each plot-data file entered; examples of these plots are given in Figures 2.8 and 3.31 (both matrix-water velocity) and 3.32 (fracture-water velocity).
- 8) Plot STEADY-calculated hydraulic conductivity versus elevation for each plot-data file entered; an example of this plot is given in Figure 3.33.
- 9) Plot STEADY-calculated capacitance versus elevation for each plot-data file entered; an example of this plot is given in Figure 3.34.
- 10) Plot, on a bar chart, the groundwater travel times (minimum, composite, matrix, and fracture) between any two specified points in the column; an example of this plot is given in Figure 3.35.

Depending on the plot choice, OUTPLOT will query for additional information. This additional information typically includes the following:

- 1) whether results for matrix flow, fracture flow, or composite flow (i.e., the area-weighted average of the matrix and the fractures) are to be plotted;
- 2) whether the plot should be oriented in portrait or landscape mode;
- 3) whether the axes are to have linear or logarithmic scaling;
- 4) whether the axis labels should be changed;
- 5) whether the units of the data should be changed (multiplying the data by a factor introduced by the user);
- 6) whether the user desires to override the automatic axis scaling; and,
- 7) whether a legend is to be placed on the plot, and if so, where it should be placed and what should be written in it.

Four basic types of plots are listed in the OUTPLOT (STEADY RESULTS) menu. The mesh/stratigraphy plot gives a visual check of the assignments for the mesh, geologic units, and material properties. The characteristic-curve plots are all graphed with respect to pressure head. Various hydrologic variables plotted against elevation all follow a similar two-dimensional format. The plot of travel time is a bar chart.

The remainder of this subsection contains a description of the definitions of these four plot types.

4.6.3.1 Mesh/Stratigraphy Plots (Choice 1)

To define a mesh/stratigraphy plot, the user enters choice 1 in response to the OUTPLOT (STEADY RESULTS) menu:

ENTER CHOICE: 1

OUTPLOT responds:

DEFINING MESH/STRATIGRAPHY PLOT...

A mesh/stratigraphy plot consists of an elevation axis alongside a representation of the mesh and a representation of the geologic units with the material-property assignments written inside. Seven parameters are available for the user to change: the axis type, the axis units and scaling of the data, the axis limits, the number of mesh points to be included in each box in the drawing of the mesh, and the step in the label of the mesh-point number written alongside the mesh drawing. OUTPLOT begins by asking about the axis type:

ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):

The default is the first item in the list, which indicates a linear axis.

OUTPLOT queries for the data-scaling parameters as follows:

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

A discussion of these prompts and possible responses is given in Section 4.6.3.2.

OUTPLOT continues with prompts allowing the user to set the elevation-axis bounds:

SET AXIS LIMITS...

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

The axis limits give the range of the elevation; they can be adjusted to illustrate any part of the mesh/stratigraphy. A discussion of the preceding axis prompts and the appropriate responses is contained in Section 4.6.3.2.

OUTPLOT prompts for the final two parameters as follows:

ENTER # OF MESH POINTS IN BOX:

ENTER STEP SIZE FOR MESH-POINT-NUMBER LABEL:

The defaults for these two parameters vary depending on the number of cells in a mesh. For example, if there are 200 cells in a mesh, then a box is drawn for every cell and every twentieth cell is labeled. If there are 2000 cells in a mesh, then a box is drawn for every 16 cells and every hundredth cell is labeled.

OUTPLOT signals that it has created a plot block for mesh/stratigraphy in the plot-definition file as follows:

PLOT DEFINITION COMPLETED.

Examples of the mesh/stratigraphy block in a plot-definition file are given in Figures 2.12, 3.16, and 3.46. Examples of mesh/stratigraphy plots are given in Figures 2.7, 3.4, and 3.24.

4.6.3.2 Plots of Composite Conductivity and Capacitance (Choice 3)

As used by TOSPAC, characteristic curves are hydrologic variables (either saturation, hydraulic conductivity, or capacitance coefficients) for a material defined as a function of pressure head. The composite conductivity and capacitance curves differ from simple characteristic curves because they

include both matrix and fracture materials. For characteristic-curve plots (choice 2), separate plots containing graphs of the saturation characteristic curve and the hydraulic-conductivity characteristic curve are made for each material specified. For plots of composite conductivity and composite capacitance (choice 3), separate plots are made for both the conductivity and the capacitance for each geologic unit specified.

Consider the definition of a characteristic curve for composite hydraulic conductivity. The user enters choice 3 in response to the OUTPLOT (STEADY RESULTS) menu:

ENTER CHOICE: 3

First, OUTPLOT works on the composite hydraulic conductivity:

DEFINING COMPOSITE-CONDUCTIVITY PLOT...

For this plot, the user is allowed to specify one or more geologic units, to change the type of axes, to change the axis labels and scaling of the data, to change the axis limits, and to specify the location of a legend if one is desired.

ENTER GEOLOGIC UNIT:

An allowable response is either an integer corresponding to a geologic unit in an input-data file, the character string corresponding to the name of a geologic unit, or the word *ALL*. The default is all the geologic units; in this case, characteristic-curve plots will be defined for all the geologic units, and all subsequent parameters will apply to all the plots.

The plot axes can be either linear (the default), logarithmic, or for negative data, negative logarithmic:

ENTER CONDUCTIVITY-AXIS TYPE (LIN, LOG, NEGLOG):

Now OUTPLOT seeks information about the units of the axis:

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

OUTPLOT assumes *SI* units (although the time can be changed from seconds to another unit using the time-conversion menu, Section 4.2.10). If English units had been used in the input-data file for the calculation, the axis labels could be changed. If *SI* units had been used, but elevation was wanted in centimeters, the axis labels could be changed and a scale factor could be entered to scale the data. If the user responds with a *YES* to this prompt, OUTPLOT issues several prompts allowing changes in the axis labels and data scaling, as follows:

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y): Y

ENTER NEW CONDUCTIVITY UNITS:

ENTER CONDUCTIVITY SCALE FACTOR:

Acceptable answers to the new-units prompts are any character strings up to 80 characters long. The defaults are the *SI* units: "m/s" for conductivity. The data scale factor can be any positive number (real or integer). Default scale factors are always 1.

As an example of a scale-factor change, consider that the data are in *SI* units, but conductivity units for the plot are to be in units of millimeters and years. The scale factor for the conductivity should be

3.16×10^{10} (a meter is 10^3 millimeters and a year is 3.16×10^7 seconds: therefore, m/s is $10^3 \times 3.16 \times 10^7$ mm/yr). For these changes, the prompts and the responses would be as follows:

```
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y): Y
ENTER NEW CONDUCTIVITY UNITS: mm/yr
ENTER CONDUCTIVITY SCALE FACTOR: 3.16E+10
```

A second example illustrates changing the axis labels without introducing a scale factor. If all data in the input-data file had been entered using length units of millimeters and time units of years, then the plot data would already have the desired units, but it is necessary to inform OUTPLOT that *SI* units are not being used:

```
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y): Y
ENTER NEW CONDUCTIVITY UNITS: mm/yr
ENTER CONDUCTIVITY SCALE FACTOR:
```

OUTPLOT allows changing the axis limits with the following prompts:

```
SET AXIS LIMITS...
ENTER CONDUCTIVITY-AXIS MINIMUM:
ENTER CONDUCTIVITY-AXIS MAXIMUM:
```

If the user enters a real number of the axis minimum, that number becomes the axis origin. If the user enters for the the axis minimum a real number which is greater than the value of the axis minimum, that number becomes the axis maximum. Both values must be within the range of the computer (between $\sim -10^{38}$ and $\sim 10^{38}$ for VAX FORTRAN compiled with the D-floating option). If the user enters only a <CR>, the default value is selected. The default (which ends up as the word *DEFAULT* in the plot-definition file) is to show the entire column. It is possible to choose the default minimum but specify the maximum, or to choose the default maximum but specify the minimum. An example of this sort follows:

```
SET AXIS LIMITS...
ENTER CONDUCTIVITY-AXIS MINIMUM:
ENTER CONDUCTIVITY-AXIS MAXIMUM: 1
```

In this example, the default minimum will be used for the axis, but the maximum will be set to 1 in whatever the plot units are. If the default units are being used, that means 1 m/s for the conductivity axis maximum. If the conductivity units have been changed to mm/yr, as in the examples above, then the maximum will be 1 mm/yr. Note that OUTPLOT may occasionally change your specified minimum or maximum value slightly to obtain more aesthetically pleasing axis limits.

Continuing with the composite-conductivity plot, the axis prompts are repeated for the pressure-head axis:

```
ENTER PRESSURE-HEAD-AXIS TYPE (LIN, LOG, NEGLOG):
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER PRESSURE-HEAD-AXIS MINIMUM:
ENTER PRESSURE-HEAD-AXIS MAXIMUM:
```

The possible responses are the same as already discussed for the conductivity axis.

On the composite-conductivity plot, there are three curves: the hydraulic conductivity of the fracture material (a dashed line), the hydraulic conductivity of the matrix material (a chain-dot line), and the hydraulic conductivity of the composite material (a solid line). If desired, a legend will be printed on the plot showing the line types and the labels COMPOSITE, MATRIX, and FRACTURE, respectively. The user is not allowed to change these labels, but the legend is optional and the legend location can be specified:

DO YOU WANT A LEGEND (Y OR N OR SAME):

If the user enters *NO*, OUTPLOT responds by skipping the legend-related prompts and no legend will appear on the plot. If the user enters *SAME*, OUTPLOT uses the same legend information from the previous plot of the session and OUTPLOT responds by skipping the legend-related prompts. Note that if the user enters *SAME* for the first plot of a session, *no legend is produced*. If the user enters *YES*, OUTPLOT prompts for the legend location:

ENTER LEGEND LOCATION:

The user is allowed to specify the location either by a descriptive pair (e.g., *LEFT, TOP*), or by a pair of numbers (e.g., 4,6). A descriptive pair indicates a place in the plot where the legend should be located. A descriptive pair must have a horizontal component (*LEFT* or *RIGHT* or *CENTER*), and a vertical component (*TOP* or *BOTTOM* or *CENTER*). Order is important. As with all TOSPAC data, the letter case is not significant. The descriptive pair must be separated by a blank or a comma. Based on the descriptive pair, OUTPLOT calculates the actual location values to fit the legend in the specified location.

The number pair must also be separated by a blank or a comma. The first number of the pair tells the distance, in the X-axis direction, in centimeters, from the origin to the lower-left corner of the legend. The second number of the pair tells the distance, in the Y-axis direction, in centimeters, from the origin to the lower-left corner of the legend.

Location defaults vary for the different plots; for the characteristic-curve plots the default is the upper-right corner (e.g., *RIGHT, TOP*).

For plots with landscape orientation (orientation will be discussed in Section 4.6.3.3, but note that composite-conductivity and capacitance plots are always plotted with landscape orientation), there is an additional option, *OUTSIDE*. If this option is chosen, the X-axis is shortened slightly and the legend is placed outside the plot, on the right-hand side. Such a choice is not particularly useful for the composite-conductivity plot, but for plots with many curves (for example, a release plot with 20 species—see Section 4.6.5.5) it can be helpful.

OUTPLOT signals that it is working on, and has created, a plot block for composite conductivity in the plot-definition file as follows:

PLOT DEFINITION COMPLETED.

At this point, the above sequence is repeated to define a plot for composite-capacitance coefficients.

Examples of the plot blocks for composite conductivity and composite capacitance in a plot-definition file are given in Figures 3.16 and 3.46. Examples of plots for composite conductivity and composite capacitance are given in Figures 3.6, 3.7, 3.26, and 3.27.

Definition of characteristic-curve plots (choice 2) is similar. Examples of plot blocks for characteristic curves in a plot-definition file are given in Figures 3.16 and 3.46. Examples of the characteristic-curve plots are given in Figures 3.5 and 3.25.

4.6.3.3 Plots of Velocity versus Elevation (Choice 7)

For a typical plot of a hydrologic variable versus elevation, consider the entry of choice number 7 in response to the OUTPLOT (STEADY RESULTS) menu.

ENTER CHOICE: 7

OUTPLOT responds:

DEFINING VELOCITY-VS-ELEVATION PLOT...

Velocity is the average linear velocity of a parcel of water, defined as the flux divided by the moisture content. Section 3.2 contains a discussion of the difference between how the average linear velocity is calculated in the hydrology and transport modules.

There is more than one type of plot for average linear velocity; OUTPLOT responds with the velocity-plot menu:

OUTPLOT (STEADY RESULTS) VELOCITY MENU

0. STOP

1. PLOT COMPOSITE-WATER VELOCITY

2. PLOT MATRIX-WATER VELOCITY

3. PLOT FRACTURE-WATER VELOCITY

4. PLOT ALL

ENTER CHOICE:

The choices correspond to plotting only the velocity of water in the composite material, only the velocity of water in the matrix material, only the velocity of water in the fracture material, or plotting the velocity of water in the composite, matrix, and fracture materials on a single plot. For the first three choices, one plot is defined containing one velocity curve from each of the identified plot-data files. For the *ALL* choice (choice 4), a plot is defined for each identified plot-data file, and each plot contains three velocity curves.

For plots of velocity versus elevation, the user is allowed to specify plot orientation, axis types, axis labels and data scale factors, axis limits, and a legend. OUTPLOT begins prompting as follows:

SET ORIENTATION (PORTRAIT OR LANDSCAPE):

The orientation is the way the plot is situated on the page: portrait orientation places the plot with the longer edges of the page vertical; landscape turns the page horizontal. The default is *PORTRAIT*. For landscape orientation, the user enters the word *LANDSCAPE*. For example, Figure 2.8 shows a velocity plot in portrait orientation and Figure 3.31 shows a velocity plot in landscape orientation.

OUTPLOT continues:

```
ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):  
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):  
SET AXIS LIMITS...  
ENTER ELEVATION-AXIS MINIMUM:  
ENTER ELEVATION-AXIS MAXIMUM:
```

```
ENTER VELOCITY-AXIS TYPE (LIN, LOG, NEGLOG):  
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):  
SET AXIS LIMITS...  
ENTER VELOCITY-AXIS MINIMUM:  
ENTER VELOCITY-AXIS MAXIMUM:
```

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

For portrait orientation, the elevation axis is nominally 20 cm long. Elevation default values are chosen so that the entire column fits in this area with approximately a one-cm blank area above and below. The velocity axis is nominally 15 cm long. Labels identifying the geologic units are placed in approximately three cm of the right-hand side of the graph.

OUTPLOT now attempts to define a legend and asks the user to identify the various velocity-data curves.

One curve is plotted for each plot-data file identified when a STEADY-results plot is requested. Five different line types are available: solid line, chain-dot line, dashed line, chain-dash line and dotted line. These line types are used in the above order; the first plot-data file is represented with the solid line, the second is represented with the chain-dot, etc. If more than five plot-data files are specified, the line types are repeated. The user is not given any choice in this matter.

An exception to this format is made when the *ALL* choice---choice 4---is selected in response to the OUTPLOT (STEADY RESULTS) velocity menu. Then a separate plot is made for each plot-data file. Each plot contains three curves, representing the velocity of water in the fractures, the matrix, and the composite material.

Legend-related prompts are as follows:

```
DO YOU WANT A LEGEND (Y OR N OR SAME):
```

Possible response to this prompt are described in Section 4.6.3.2. If the user enters *YES*, OUTPLOT continues with legend-related prompts. If the user selected COMPOSITE-WATER, MATRIX-WATER, or FRACUTURE-WATER VELOCITY (choices 1, 2, or 3 in response to the velocity menu), the legend prompts are as follows:

```
ENTER LABEL FOR CURVE # 1:  
ENTER LABEL FOR CURVE # 2:  
ENTER LABEL FOR CURVE # 3:
```

```
o  
o  
o
```

There are as many prompts as there are plot-data files. Allowable labels are any character strings up

to 80 characters long. For example, curve labels can be *Case 1* or $q=0.5 \text{ mm/yr}$. Default labels are the file names where the STEADY results are located.

If the user selected *ALL* (choice 4 in response to the velocity menu), then there is no choice; the labels used are the words COMPOSITE, MATRIX, and FRACTURE.

OUTPLOT now asks where to locate the legend:

ENTER LEGEND LOCATION:

Responses to this prompt are discussed in Section 4.6.3.2. Location default for the velocity plots is the upper-left corner: *LEFT, TOP*.

After the legend has been defined, OUTPLOT announces:

PLOT DEFINITION COMPLETED.

Examples of plot blocks for plots of hydrologic variables versus elevation in plot-definition files are given in Figures 2.12, 3.16, and 3.46. Examples of plots of hydrologic variables versus elevation are given in Figures 2.8 and 3.28 through 3.34.

4.6.3.4 Travel-Time Plot (Choice 10)

OUTPLOT displays travel-time results on a bar chart. The bar chart shows the travel time of water, across a user-specified range of elevation, for one or more different STEADY calculations.

In this discussion, the different calculations are referred to as files, because the results are taken from one or more STEADY plot-definition files (Section 4.6.3). Travel times are plotted for every STEADY plot-data file listed when the DEFINE STEADY PLOTS option is first selected. The bar charts have the different calculation names listed across the horizontal or X-axis, and time displayed on the vertical or Y-axis. If there are more than five plot-definition files, the results will be broken into two plots to avoid overcrowding.

For travel-time plots with multiple STEADY files, it is not necessary that the different files all have the same mesh and stratigraphy; however it is required that all files use the same time units. An error will result if one of the files has time units of seconds (choices 1-4 on the time conversion menu) and another one has time units of years (choices 5-8 on the time conversion menu). It is also preferable that all files have the same elevation units; otherwise the elevation specification may be incorrect. (If the default elevations are specified, there is no problem--the top and bottom of the column will be used.)

Consider the entry of choice number 10 in response to the OUTPLOT (STEADY RESULTS) menu.

ENTER CHOICE: 10

OUTPLOT responds:

DEFINING TRAVEL-TIME PLOT...

Travel time can be defined in a number of ways. *Volume 1* and Section 3.2 of this User's Guide contain

a discussion of how it is defined and calculated in STEADY. It will suffice here to say that four values are computed over a distance specified by the user:

- 1) a minimum travel time calculated for an "average fastest particle" that takes whichever is faster, the matrix path or the fracture path, as long as the path carries at least 1% of the total flux;
- 2) a composite travel time based on the composite velocity of water—i.e., the velocity calculated as the area-weighted average of the velocity in the matrix and in the fractures.
- 3) the travel time for an average water particle confined to the matrix; and,
- 4) the travel time for a particle confined to the fractures;

Four bars are produced for each file, one for each travel time. Above each bar is written the travel time and the percent of the user-specified distance across which the travel time is valid.

The user is only allowed to specify changes in a few parameters for travel-time bar charts. The axis type and axis label for the time axis can be changed, and the time data can be scaled. The elevation range across which travel time is to be calculated can be specified. OUTPLOT begins by prompting for axis-related information:

```
ENTER TIME-AXIS TYPE (LOG, LIN, NEGLOG):
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER TIME-AXIS MINIMUM:
ENTER TIME-AXIS MAXIMUM:
```

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

OUTPLOT continues by prompting for the range of elevation over which the travel time is to be calculated:

```
SET DISTANCE FOR CALCULATING TRAVEL TIME...
ENTER UPPER ELEVATION:
ENTER LOWER ELEVATION:
```

Allowable elevations are any real numbers, with the condition that the upper elevation must be above the lower elevation. If the specified upper elevation is above the uppermost mesh-point elevation in a STEADY plot-data file, OUTPLOT uses the uppermost mesh-point elevation. A similar correction is made for a specified lower elevation that is below the lowermost mesh-point elevation. If the user specifies elevations that do not include any part of an elevation range in a STEADY plot-data file, travel times are set to zero. The default values for elevation are set so that travel time is computed for the entire column in each file. If the two elevation values are specified by the user, those values are used in calculating travel times for all the STEADY plot-data files; i.e., different elevations cannot be specified for each file. However, if the default is specified (for upper or lower or both), then the default is calculated separately for each file, so that the range over which travel time is calculated may be different for each file. An example of this situation is shown in Figure 3.35—default lower and upper elevations were specified, and travel times were calculated over a range of 0 to 100 m for the mill-tailings problem and 0 to 530.4 m for the waste-repository problem.

Finally, OUTPLOT prompts for the names to be associated with the calculation (each STEADY

plot-data file). The labels appear on the horizontal or X-axis of the bar chart. The following prompts are given:

```
ENTER LABEL FOR CURVE # 1:
ENTER LABEL FOR CURVE # 2:
ENTER LABEL FOR CURVE # 3:
```

```
o
o
o
```

Allowable labels are any character strings up to 80 characters long. The default values are the names of the plot-data files. There are as many prompts as specified files.

OUTPLOT now indicates completion of the plot definition:

PLOT DEFINITION COMPLETED.

An example of a plot block for travel time in a plot-definition file is given in Figure 3.46. An example of a travel-time bar chart is given in Figure 3.35.

4.6.4 Define DYNAMICS Plots

Entering a choice of 2 in response to the OUTPLOT main menu allows the user to define plots for DYNAMICS results.

Plotting of DYNAMICS results begins with the identification of the plot-data file:

ENTER DYNAMICS PLOT-DATA FILE (DEFAULT=NONE):

The default answer implies that the plot-definition file being created will work with any DYNAMICS plot-data file. If the user wants to create an audit trail for a specific analysis, the user can enter the name of a DYNAMICS plot-definition file and OUTPLOT will use this plot-definition file only with the given plot-data file.

OUTPLOT allows *only one* DYNAMICS plot-data file to be specified. Data from multiple transient-flow calculations cannot be plotted on the same graph as they can with steady-state-flow calculations.

Even if a plot-data file is entered, OUTPLOT only reads it immediately before constructing the graphics-driver file (Section 4.6.6). OUTPLOT does not provide explicit default values for defining plots. The default value for a plot parameter in the plot-definition file is the word *DEFAULT*.

OUTPLOT now displays the DYNAMICS-results menu on the user's terminal screen:

OUTPLOT (DYNAMICS RESULTS) MENU

0. STOP
1. PLOT MESH/STRATIGRAPHY
2. PLOT CHARACTERISTIC CURVES
3. PLOT COMPOSITE CONDUCTIVITY AND CAPACITANCE CURVES
4. PLOT PRESSURE HEAD VS ELEVATION
5. PLOT SATURATION VS ELEVATION
6. PLOT FLUX VS ELEVATION
7. PLOT VELOCITY VS ELEVATION
8. PLOT CONDUCTIVITY VS ELEVATION
9. PLOT CAPACITANCE VS VELEVATION
10. PLOT SATURATION VS TIME
11. PLOT MASS VS TIME

ENTER CHOICE:

The choices are as follows:

- 0) Return to the OUTPLOT main menu.
- 1) Plot the mesh and stratigraphy for the plot-data file entered; an example of this plot is given in Figures 2.7, 3.4, and 3.24.
- 2) Plot the saturation and hydraulic-conductivity characteristic curves; an example of these plots is given in Figures 3.5 and 3.25.
- 3) Plot composite hydraulic conductivity and capacitance; examples of these plots are given in Figures 3.6 and 3.26 for the conductivity curves, and Figures 3.7 and 3.27 for the capacitance curves.
- 4) Plot DYNAMICS-calculated pressure head versus elevation for selected time snapshots; an example of this plot is given in Figure 3.8.
- 5) Plot DYNAMICS-calculated saturation versus elevation for selected time snapshots; an example of this plot is given in Figure 3.9.
- 6) Plot DYNAMICS-calculated flux versus elevation for selected time snapshots (this quantity is also called the Darcy velocity, the percolation rate, or the rate of infiltration); an example of this plot is given in Figure 3.10.
- 7) Plot DYNAMICS-calculated average linear velocity versus elevation for selected time snapshots; an example of this plot is given in Figure 3.11.
- 8) Plot DYNAMICS-calculated hydraulic conductivity versus elevation for selected time snapshots; an example of this plot is given in Figure 3.12.
- 9) Plot DYNAMICS-calculated capacitance versus elevation for selected time snapshots; an example of this plot is given in Figure 3.13.
- 10) Plot DYNAMICS-calculated average sample saturation over time; an example of this plot is given in Figure 3.14.
- 11) Plot DYNAMICS-calculated water mass over time; an example of this plot is given in Figure 3.15.

OUTPLOT does not presently plot groundwater-travel-time results from DYNAMICS.

Depending on the plot choice, OUTPLOT will query for additional information. The additional information is typically the same as that requested for STEADY-results plots; it is listed in Section 4.6.3.

The plots listed in the OUTPLOT (DYNAMICS RESULTS) menu are of four basic types. First, the mesh/stratigraphy plot gives a visual check of the assignments for the mesh, geologic units, and material properties. The mesh/stratigraphy plot is identical for STEADY and DYNAMICS results. The mesh/stratigraphy plot is selected by choice 1 from the OUTPLOT (DYNAMICS RESULTS) menu; it is discussed in Section 4.6.3.1. Second, the characteristic-curve plots show saturation, hydraulic conductivity, and capacitance coefficients graphed with respect to pressure head. The characteristic-curve plots are selected by choices 2 and 3 from the OUTPLOT (DYNAMICS RESULTS) menu; they are discussed in Section 4.6.3.2. Third, the various hydrologic variables plotted against elevation are the most useful plots of DYNAMICS results. Although these plots are similar to those discussed in Section 4.6.3.3, they differ enough to be reexamined in Section 4.6.4.1. Finally, the plots of average sample saturation and water mass show saturation and mass change over time for an entire column. These plots are discussed in Section 4.6.4.2.

4.6.4.1 Plots of Flux versus Elevation (Choice 6)

For a typical plot of a hydrologic variable versus elevation, consider the entry of choice number 6 in response to the OUTPLOT (DYNAMICS RESULTS) menu.

ENTER CHOICE: 6

OUTPLOT responds:

DEFINING FLUX-VS-ELEVATION PLOT...

Flux is defined as the volume of water passing through an area during a time. It has the dimensions of a velocity. In hydrology, flux is also known as Darcy velocity, or percolation rate, or rate of infiltration.

There is more than one type of flux plot; OUTPLOT responds with the flux-plot menu:

OUTPLOT (DYNAMICS RESULTS) FLUX MENU

- 0. STOP
- 1. PLOT NORMALIZED COMPOSITE FLUX
- 2. PLOT COMPOSITE FLUX
- 3. PLOT MATRIX FLUX
- 4. PLOT FRACTURE FLUX
- 5. PLOT MATRIX, FRACTURE, AND COMPOSITE FLUX TOGETHER

ENTER CHOICE:

The choices correspond to plotting only the flux of water in the composite material with the data normalized, only the flux in the composite material, only the flux in the matrix material, only the flux in the fracture material, or plotting the flux in the composite, matrix, and fracture materials on a single plot. For the first four choices, one plot is defined that contains flux curves from specified time

snapshots. For the multiple-flux choice (choice 5), a plot is defined for each specified time snapshot, and each plot contains three flux curves.

For the imbibition problem given in Section 3.1, the water flux through the matrix is plotted (Figure 3.10). The sample is unfractured, so a plot of flux through the fractures would not be useful. A plot of normalized flux is not shown because data are normalized with respect to the final flux at the lower boundary. For the imbibition problem, the final flux is virtually zero, and an error would result if we tried to produce a normalized flux plot. Normalized flux plots are used often in *Volume 1*.

Consider a plot of the water flux in the matrix:

ENTER CHOICE: 3

For plots of flux versus elevation, the user is allowed to specify plot orientation, axis types, axis labels and data scale factors, axis limits, and a legend. OUTPLOT begins prompting as follows:

SET ORIENTATION (PORTRAIT OR LANDSCAPE):

ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

ENTER FLUX-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER FLUX-AXIS MINIMUM:

ENTER FLUX-AXIS MAXIMUM:

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

Note that if a normalized-flux plot were being defined, the user should answer *NO* to the prompt for changing axis units, because OUTPLOT automatically normalizes the data. If units are changed *and* data are normalized, the scale factor has no effect.

If the user specifies flux-axis limits, the user should allow for labels identifying the geologic units that are placed in approximately three cm of the right-hand side of the graph (for portrait orientation).

OUTPLOT now asks the user to identify the time snapshots that define the flux-data curves. It is here that the elevation plots differ significantly from the corresponding STEADY-results plots.

ENTER TIME SNAPSHOTS TO BE PLOTTED:

Acceptable responses are one or more numbers or the word *ALL*. If more than one number is entered, the numbers must be separated by spaces or commas, and all numbers must be entered on one line before the user enters a <CR>. The numbers correspond to the numbers of the time snapshots in the DYNAMICS input-data file that lead to the results that are being plotted. If a pond-drain boundary condition was used in the calculation, extra time snapshots could be included in the DYNAMICS plot-data file, and these extra time snapshots must be taken into account when the time snapshots are enumerated (Sections 4.2.10 and 4.4.3). On the plot, a curve is drawn for each time snapshot that is

specified. The default choice is the word *ALL*: plot all the time snapshots.

Each time snapshot plotted has a different type of line and a legend of the line types can be created. Again, five different line types are available: solid line, chain-dot line, dashed line, chain-dash line, and dotted line. These line types are used in the above order; the first time snapshot specified is represented with the solid line, the second is represented with the chain-dot, etc. If more than five time snapshots are specified, the line types are repeated.

An exception is made when the multiple-flux choice—choice 5—is selected in response to the OUTPLOT (DYNAMICS RESULTS) flux menu. Then a separate plot is made for each time snapshot specified. Each plot contains three curves, representing the water flux in the fractures, the matrix, and the composite material.

OUTPLOT now attempts to define a legend and asks the user to identify the flux-data curves. Legend-related prompts are as follows:

DO YOU WANT A LEGEND (N OR Y OR SAME):

Possible responses to this prompt are discussed in Section 4.6.3.3.

If the user enters *YES*, OUTPLOT continues with legend-related prompts. If one of the first four choices was selected in response to the OUTPLOT (DYNAMICS RESULTS) flux menu (i.e., if the multiple-flux choice—choice 5—was *not* selected), then the following prompts are given:

```
ENTER LABEL FOR SNAPSHOT #  ? :
ENTER LABEL FOR SNAPSHOT #  ? :
ENTER LABEL FOR SNAPSHOT #  ? :

    o
    o
    o
```

The question marks are replaced by the numbers of the time snapshots selected. Allowable labels are any character strings up to 80 characters long. The default value is the snapshot time given in the time units specified in the time conversion menu of the DYNAMICS input-data file (Section 4.2.10). There are as many prompts as specified time snapshots.

However, if the multiple-flux choice was selected (choice 5), then the labels used are the words *COMPOSITE*, *MATRIX*, and *FRACTURE*, with no choice allowed.

OUTPLOT now asks where to locate the legend:

ENTER LEGEND LOCATION:

A discussion of how the legend is placed on the plot and possible responses to this prompt is given in Section 4.6.3.3. Location defaults vary for the different elevation plots; for the flux plots the default is the lower-left corner: *LEFT,BOTTOM*.

After the legend has been defined, OUTPLOT announces:

PLOT DEFINITION COMPLETED.

An example of a plot block for flux versus elevation in a plot-definition file is given in Figure 3.16. The resulting plot is given in Figure 3.10.

Additional examples of plots of hydrologic variables versus elevation for DYNAMICS results, also defined in Figure 3.16, are given in Figures 3.8 through 3.13.

4.6.4.2 Plots of Saturation versus Time (Choice 10)

To define the saturation-change plot, enter choice 10 in response to the OUTPLOT (DYNAMICS RESULTS) menu.

ENTER CHOICE: 10

OUTPLOT responds:

DEFINING SATURATION-VS-TIME PLOT...

Average sample saturation is calculated by summing the length-weighted saturations of every cell in an entire column (Section 3.1). The plot of average sample saturation is similar to the plot of water mass, which is plotted with choice 11.

The average sample saturation and mass are calculated at every time snapshot. The average sample saturation and water mass are plotted against time, to give the saturation- and mass-change plots. Unless there are many time snapshots, the curves do not look smooth.

The user is allowed to change only a few plot parameters: the axis types, the units, and the axis limits.

ENTER SATURATION-AXIS TYPE (LIN, LOG, NEGLOG):
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER SATURATION-AXIS MINIMUM:
ENTER SATURATION-AXIS MAXIMUM:

ENTER TIME-AXIS TYPE (LIN, LOG, NEGLOG):
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER FLUX-AXIS MINIMUM:
ENTER FLUX-AXIS MAXIMUM:

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

OUTPLOT signals that it has created a saturation-plot block in the plot-definition file as follows:

PLOT DEFINITION COMPLETED.

An example of a plot block for average sample saturation in a plot-definition file is given in Figure 3.16. Example plots of saturation and mass versus time are given in Figures 3.14 and 3.15, respectively.

4.6.5 Define TRANS Plots

Entering a choice of 3 in response to the OUTPLOT main menu allows the user to define plots for TRANS results. As with STEADY and DYNAMICS plot definitions, plotting of TRANS results begins with the identification of the plot-data file:

ENTER TRANS PLOT-DATA FILE (DEFAULT=NONE):

The default answer implies that the plot-definition file being created will work with any TRANS plot-data file. If the user wants to create an audit trail for a specific analysis, the user can enter the name of a TRANS plot-definition file and OUTPLOT will use the plot-definition file *only* with the given plot-data file.

OUTPLOT allows *only one* TRANS plot-data file to be specified. Data from multiple transport calculations cannot be plotted on the same graph.

Even if a plot-data file is entered, OUTPLOT only reads it immediately before constructing the graphics-driver file (Section 4.6.6). OUTPLOT does not provide explicit default values for defining plots. The default value for a plot parameter in the plot-definition file is the word *DEFAULT*.

OUTPLOT now displays the TRANS-results menu on the user's terminal screen:

```
OUTPLOT (TRANS RESULTS) MENU
0. STOP
1. PLOT MOISTURE CONTENT VS ELEVATION
2. PLOT VELOCITY VS ELEVATION
3. PLOT DISPERSION COEFF VS ELEVATION
4. PLOT RETARDATION VS ELEVATION
5. PLOT COUPLING CONSTANT VS ELEVATION
6. PLOT CONCENTRATION VS ELEVATION
7. PLOT CONCENTRATION VS ELEVATION VS TIME (3-D)
8. PLOT CONCENTRATION VS TIME
9. PLOT RELEASE VS TIME
```

ENTER CHOICE:

The choices are as follows:

- 0) Return to the OUTPLOT main menu.
- 1) Plot moisture content versus elevation in the matrix and the fractures (similar to the steady-state saturation plots described in Section 4.6.3; however, moisture content is the product of the saturation and the porosity); an example of this plot is given in Figure 3.37.
- 2) Plot average linear water velocity versus elevation in the matrix and the fractures (similar to the steady-state water velocity plots described in Section 4.6.3, however the average linear water velocity as used by TRANS does not omit the residual-saturation water from the computation); an example of this plot is given in Figure 3.36.
- 3) Plot dispersion coefficient versus elevation for one or more contaminants in the matrix and the fractures; an example of this plot is given in Figure 3.38.

- 4) Plot retardation factor versus elevation for one or more contaminants in the matrix and the fractures; an example of this plot is given in Figure 3.39.
- 5) Plot advective and diffusive coupling constants versus elevation for one or more contaminants; an example of this plot is given in Figure 3.40.
- 6) Plot concentration versus elevation for one or more contaminants in the matrix and the fractures at specified times; examples of these plots are given in Figures 2.11 and 3.41.
- 7) Plot in three dimensions the concentration versus elevation versus time for one or more contaminants in the matrix or the fractures; examples of these plots are given in Figures 2.10 and 3.42.
- 8) Plot concentration versus time for one or more contaminants in the matrix and the fractures at a given elevation; an example of this plot is given in Figure 3.43.
- 9) Plot release versus time for one or more contaminants; examples of these plots are given in Figures 2.9, 3.44, and 3.45.

The remainder of this subsection contains a discussion of how to obtain representative TRANS-results plots. This discussion includes the dispersion-coefficient plot (choice 3), the plot of concentration versus elevation (choice 6), the three-dimensional plot of concentration versus elevation versus time (choice 7), the plot of concentration versus time (choice 8), and the contaminant releases plot (choice 9). This discussion excludes the retardation factor (choice 4) and coupling-constant (choice 5) plots, which are very similar to the dispersion-coefficient plot (choice 3); and the moisture-content (choice 1) and water-velocity (choice 2) plots, which are very similar to the steady-state water-velocity and saturation plots described in Section 4.6.3.

4.6.5.1 Plots of Dispersion Coefficients versus Elevation (Choice 3)

To define a plot of the dispersion coefficients versus elevation, enter choice 3 in response to the OUTPLOT (TRANS RESULTS) menu.

ENTER CHOICE: 3

OUTPLOT responds:

DEFINING DISPERSION-COEFF-VS-ELEVATION PLOTS...

The dispersion coefficient is a measure of the amount of diffusion and hydrodynamic dispersion a contaminant undergoes as it is transported through a geologic unit (Section 3.2). Each contaminant has a dispersion coefficient for the matrix and the fractures at every mesh cell.

Because dispersion coefficients, as defined in TOSPAC, remain constant in time, this plot type does not have time lines and OUTPLOT does not query for time snapshot data.

To define this plot, OUTPLOT asks the user whether the dispersion coefficient for the matrix or the fractures or both should be plotted, then the plot orientation, the axis labels and data scaling, axis limits, the contaminant to be plotted, and information concerning a legend.

OUTPLOT begins with the menu for the dispersion coefficient plot:

OUTPLOT (TRANS RESULTS) DISPERSION-COEFF MENU

0. STOP

1. PLOT DISPERSION COEFF IN THE MATRIX

2. PLOT DISPERSION COEFF IN THE FRACTURES

3. PLOT DISPERSION COEFF IN THE MATRIX AND FRACTURES TOGETHER

ENTER CHOICE:

Choices 1 and 2—plot dispersion coefficient in the matrix and plot dispersion coefficient in the fractures—each result in a single plot with a curve for each contaminant species chosen. Choice 3—plot dispersion coefficient in the matrix and fractures together—results in a separate plot for each species, each plot containing two curves (one each for matrix and fracture dispersion coefficients).

OUTPLOT continues prompting as follows:

SET ORIENTATION (PORTRAIT OR LANDSCAPE):

ENTER DISPERSION-COEFF-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER DISPERSION-COEFF-AXIS MINIMUM:

ENTER DISPERSION-COEFF-AXIS MAXIMUM:

ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

OUTPLOT now asks for the contaminant that is the subject of this plot:

ENTER CONTAMINANT:

Allowable responses are one or more contaminant numbers, one or more contaminant names, or the word *ALL*. A contaminant number is an integer greater than zero. A contaminant name is a character string of up to 80 characters in length. The contaminant numbers and contaminant names must correspond to contaminants in the contaminant-property block of a TRANS input-data file. The user can enter more than one number or name, in which case each number or name must be separated by spaces or commas. If more than one contaminant number or contaminant name is entered, all must be entered before the user enters a <CR>. Contaminant numbers and contaminant names can be mixed in a response. Default response to this prompt is all the contaminants (the word *ALL*).

If more than a single contaminant is entered, all data entered for this plot type apply to all plots produced. That is, if two contaminant numbers are entered, then the specified time snapshots and legends apply to each contaminant plot. The exception to this rule is if the default axis limits are selected, then each plot could have different axis limits, chosen by the autoscaling routine in OUTPLOT.

If the user wants to plot different contaminants with different time snapshots or legends (or if the user wants to specify axis limits other than the default), the user can do so by entering each contaminant in a separate block, entering the data for that contaminant, returning to the OUTPLOT (TRANS RESULTS) menu, then repeating the process for the next contaminant. This procedure causes longer execution times when constructing the graphics-driver file (Section 4.6.6) because the plot-data file is reread for each plot block.

If only the dispersion coefficients in the matrix or the fractures are being plotted (choice 1 or 2 in response to the dispersion-coefficient-plot menu), then one plot is constructed containing the dispersion coefficients for all the contaminants specified. In this case, a different line type identifies each contaminant on the plot, and the legend associates the contaminants with the line types. If the dispersion coefficients in the matrix and fractures are to be plotted together (choice 3 in response to the dispersion-coefficient-plot menu), then one plot is constructed for each contaminant specified. In this case, the different line types identify the matrix and fracture dispersion coefficients on the plot, and the legend associates the matrix and fracture dispersion coefficients with the line types.

TOSPAC now prompts for a legend as follows:

DO YOU WANT A LEGEND (N OR Y OR SAME):

Responses to this prompt, plus a general description of the legend-related commands, are offered in Section 4.6.3.3.

For dispersion-coefficient plots (and retardation plots and coupling-constant plots), the legend labels are not optional; therefore, no label prompts are presented. If the user asks for the dispersion coefficients for either the matrix or the fractures (menu choices 1 or 2), the labels used are the contaminant names, as given in the contaminant-property block of a TRANS input-data file. If the user asks for plots of the matrix and fracture dispersion coefficients together (menu choice 3), then the labels are simply the words MATRIX and FRACTURE.

OUTPLOT now asks where to locate the legend:

ENTER LEGEND LOCATION:

A discussion of how the legend is placed on the plot and possible responses to this prompt is given in Section 4.6.3.3. For a dispersion-coefficient plot, the default legend location is *LEFT, TOP*.

OUTPLOT now indicates that it has all the information to define the plot block for concentration versus elevation, and that it is writing it in the plot-definition file:

PLOT DEFINITION COMPLETED.

An example of a plot block for dispersion versus elevation in a plot-definition file is given in Figure 3.46. The resulting plot is given in Figure 3.38.

Example retardation versus elevation and coupling constant versus elevation plots are also defined in Figure 3.46, and the resulting plots are given in Figures 3.39 and 3.40, respectively.

4.6.5.2 Plots of Concentration versus Elevation (Choice 6)

To define a plot of concentration versus elevation, enter choice 6 in response to the OUTPLOT (TRANS RESULTS) menu.

ENTER CHOICE: 6

OUTPLOT responds:

DEFINING CONC-VS-ELEVATION PLOT...

A plot of concentration versus elevation shows the concentration, in either the matrix, the fractures, or both, of one or more contaminants at one or more time snapshots specified by the user. This plot has much the same information as the three-dimensional plot of concentration versus elevation versus time (choice 7) but allows the user to analyze concentration values more easily.

To define this plot, OUTPLOT asks the user whether concentration in the matrix or the fractures should be plotted, then the plot orientation, axis labels and data scaling, axis limits, the contaminant to be plotted, the time snapshots to be plotted, and information concerning a legend.

OUTPLOT begins with the concentration-plot menu:

```
OUTPLOT (TRANS RESULTS) CONCENTRATION MENU
0. STOP
1. PLOT CONC IN THE MATRIX
2. PLOT CONC IN THE FRACTURES
3. PLOT CONC IN BOTH MATRIX AND FRACTURES TOGETHER
```

ENTER CHOICE:

For choices 1 or 2, a plot is made for each contaminant selected, with curves for each time snapshot selected. For choice 3, a plot is made for each contaminant selected at each time snapshot selected, and each plot has just two curves, representing matrix and fracture concentrations.

OUTPLOT continues prompting as follows:

SET ORIENTATION (PORTRAIT OR LANDSCAPE):

ENTER CONCENTRATION-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER CONCENTRATION-AXIS MINIMUM:

ENTER CONCENTRATION-AXIS MAXIMUM:

ENTER ELEVATION-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

OUTPLOT now asks for the contaminant that is the subject of this plot:

ENTER CONTAMINANT:

Allowable responses to this prompt were discussed in Section 4.6.5.1. If the user enters the number of more than a single contaminant, one plot for each specified contaminant is produced. If the word *ALL* is entered, one plot for every contaminant is produced. If the concentrations in the matrix and the fractures are to be plotted together (choice 3 on the concentration-plot menu), then the number of plots will equal the number of contaminants times the number of time snapshots specified.

TOSPAC now asks for the times of the concentration results to be plotted:

ENTER TIME SNAPSHOTS TO BE PLOTTED:

A discussion of possible responses to this prompt is contained in Section 4.6.4.1.

Each time snapshot plotted has a different type of line and a legend of the line types is created if desired. TOSPAC prompts for the legend as follows:

DO YOU WANT A LEGEND (N OR Y OR SAME):

Responses to this prompt, plus a general description of the legend-related commands, are offered in Section 4.6.3.3.

If the user enters *YES*, OUTPLOT continues with legend-related prompts. If one of the first two choices was selected in response to the concentration-plot menu then the following prompts are given:

ENTER LABEL FOR SNAPSHOT # ?:

ENTER LABEL FOR SNAPSHOT # ?:

ENTER LABEL FOR SNAPSHOT # ?:

o
o
o

The question marks are replaced by the numbers of the time snapshots selected. Allowable labels are any character strings up to 80 characters long. The default value is the snapshot time given in the time units specified in the DYNAMICS input-data file. There are as many prompts as specified time snapshots.

However, if choice 3 was selected on the concentration-plot menu (plot matrix and fracture concentrations together), then the labels used are the words *MATRIX* and *FRACTURE*, with no choice allowed.

OUTPLOT now asks where to locate the legend:

ENTER LEGEND LOCATION:

A discussion of how the legend is placed on the plot and possible responses to this prompt is given in

Section 4.6.3.3. For concentration-versus-elevation plots, the default legend location is *LEFT, TOP*.

OUTPLOT now indicates that it has all the information to define the plot block of concentration versus elevation, and that it is writing it in the plot-definition file:

PLOT DEFINITION COMPLETED.

Examples of plot blocks for concentration versus elevation are given in Figures 2.12 and 3.46. The concentration versus elevation plots are shown in Figures 2.11 and 3.41, respectively.

4.6.5.3 Plots of Concentration versus Elevation versus Time (Choice 7)

To define a three-dimensional plot of the concentration versus elevation versus time, enter choice 7 in response to the OUTPLOT (TRANS RESULTS) menu.

ENTER CHOICE: 7

OUTPLOT responds:

DEFINING CONC-VS-ELEVATION-VS-TIME PLOTS...

Three-dimensional plots of concentration versus elevation versus time show the concentration of one or more contaminants, in either the matrix or the fractures, as a function of elevation and time.

To define this plot, OUTPLOT asks the user whether concentration in the matrix, the fractures, or both should be plotted, then the view coordinates, axis labels and data scaling, axis limits, the contaminant to be plotted, and the number of elevation and time lines.

OUTPLOT begins with the three-dimensional-plot menu:

OUTPLOT (TRANS RESULTS) CONCENTRATION MENU
0. STOP
1. PLOT CONC IN THE MATRIX
2. PLOT CONC IN THE FRACTURES
3. PLOT CONC IN BOTH MATRIX AND FRACTURES

ENTER CHOICE:

If choice 1 or choice 2 is selected, a three-dimensional plot is defined for each contaminant specified (see below). If choice 3 is selected, then two separate plots are defined, one for the concentration in the matrix and one for the concentration in the fractures, for each contaminant specified.

OUTPLOT continues prompting as follows:

ENTER VIEW RADIUS (DEFAULT=125.):
ENTER VIEW POLAR ANGLE (DEFAULT=75.):
ENTER VIEW AZIMUTHAL ANGLE (DEFAULT=340.):

The view coordinates define the place in space that the viewer is located with respect to the

three-dimensional plot. The view coordinates are specified using spherical coordinates, with the radius in centimeters and the angles in degrees. The radius can be any nonnegative number, the polar angle must be between 0 and 180 degrees, and the azimuthal angle must be between 0 and 360 degrees.

Only linear axes are allowed for three-dimensional plots; therefore, no prompts are issued for axis types. OUTPLOT continues prompting:

CONCENTRATION AXIS...

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER CONCENTRATION-AXIS MINIMUM:

ENTER CONCENTRATION-AXIS MAXIMUM:

ELEVATION AXIS...

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER ELEVATION-AXIS MINIMUM:

ENTER ELEVATION-AXIS MAXIMUM:

TIME AXIS...

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER TIME-AXIS MINIMUM:

ENTER TIME-AXIS MAXIMUM:

A discussion of these prompts and the possible responses is contained in Section 4.6.3.2.

OUTPLOT now asks for the contaminant that is the subject of this plot:

ENTER CONTAMINANT:

A discussion of contaminant names and numbers is contained in Section 4.6.5.1.

If the user enters the number of more than a single contaminant, at least one plot for each specified contaminant is produced. If more than a single contaminant is specified, all data entered for this plot type apply to all plots produced. That is, if two contaminant numbers are entered, then the specified view coordinates, etc., apply to each contaminant plot. The exception to this rule is if the default axis limits are selected, then each plot could have different auto-scaled axis limits.

TOS PAC now asks for the number of the elevation lines and time lines to make up the fabric of the three-dimensional surface:

ENTER # OF ELEVATION LINES:

ENTER # OF TIME LINES:

An acceptable entry is an integer or the word *ALL*, implying that the plot should have all available data on it. The default number of elevation lines is either 100 or the number of mesh points, whichever is smaller. If the number of elevation lines entered is greater than the number of mesh points, the number of mesh points is used. The default number of time lines is the number of time snapshots. If

the number of time lines entered is greater than the number of time snapshots, the number of time snapshots is used.

The number of elevation lines actually drawn in the plots will generally be somewhat higher than the number specified, because of the following requirements. The elevation lines corresponding to the top and bottom of the column are always drawn. The elevation lines in the source region are always drawn. Beyond that, elevation lines are drawn for every multiple of some number. For example, consider the plot in Figure 3.42. That calculation had 2302 cells, and so 2302 potential elevation lines. The default number of elevation lines is 100, and $2302/100 \approx 23$. Thus, all cells that are multiples of 23 are drawn (cells 23, 46, ..., 2300); the top and bottom cells are drawn (cells 1 and 2302); and source-region cells are drawn (cells 1006, 1007, ..., 1025). This makes a total of 122 elevation lines for Figure 3.42 even though 100 were specified.

OUTPLOT now indicates that it has the information needed to define the plot block for concentration versus elevation versus time, and that it is writing it in the plot-definition file:

PLOT DEFINITION COMPLETED.

Examples of plot blocks for concentration versus elevation versus time are given in Figures 2.12 and 3.46. The resulting plots are shown in Figures 2.10 and 3.42, respectively.

4.6.5.4 Plots of Concentration versus Time (Choice 8)

Plots of concentration versus time are selected when the user responds to the OUTPLOT (TRANS RESULTS) menu with choice 8:

ENTER CHOICE: 8

OUTPLOT responds with the following message:

DEFINING CONC-VS-TIME PLOTS...

Plots of concentration versus time show the concentration of one or more contaminants, in either the matrix, the fractures, or both, at one or more elevations, as a function of time. These plots are similar to plots of concentration versus elevation (choice 6), except that they have elevation lines over a time axis rather than time lines over an elevation axis. This plot has much of the same information as the three-dimensional plot of concentration versus elevation versus time (choice 7) but allows the user to more easily analyze concentration values.

To define this plot, OUTPLOT asks the user if concentration in the matrix, the fractures, or both should be plotted, then asks for the axis labels and data scaling, axis limits, the contaminant to be plotted, the elevations to be plotted, and information concerning a legend.

OUTPLOT begins with the concentration-plot menu:

OUTPLOT (TRANS RESULTS) CONCENTRATION MENU

- 0. STOP
- 1. PLOT CONC IN THE MATRIX
- 2. PLOT CONC IN THE FRACTURES
- 3. PLOT CONC IN BOTH MATRIX AND FRACTURES TOGETHER

ENTER CHOICE:

For choices 1 or 2, a plot is made for each contaminant selected (below), with lines for each elevation selected (below). For choice 3, a plot is made for each contaminant selected at each elevation selected, and each plot has just two lines, representing matrix and fracture concentrations.

OUTPLOT continues prompting as follows:

ENTER CONCENTRATION-AXIS TYPE (LIN, LOG, NEGLOG):
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER CONCENTRATION-AXIS MINIMUM:
ENTER CONCENTRATION-AXIS MAXIMUM:

ENTER TIME-AXIS TYPE (LIN, LOG, NEGLOG):
DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):
SET AXIS LIMITS...
ENTER TIME-AXIS MINIMUM:
ENTER TIME-AXIS MAXIMUM:

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

OUTPLOT now asks for the contaminant that is the subject of this plot:

ENTER CONTAMINANT:

A discussion of contaminant names and numbers is contained in Section 4.6.5.1.

As previously mentioned, if more than a single contaminant number is entered, all data entered for this plot type apply to all plots produced. That is, if two contaminant numbers are entered, then the specified orientations, elevations, and legends apply to each contaminant plot. The exception to this rule is if the default axis limits are selected, then each plot could have different axis limits.

If the user wants to plot different contaminants with different elevations or legends (or if the user wants to specify axis limits other than the default), the user can do so by entering a plot block for each contaminant separately, entering the data for that contaminant, returning to the OUTPLOT (TRANS RESULTS) menu, then repeating the process for the next contaminant. It is generally more efficient to specify several contaminants in one plot definition, rather than in several plot definitions; however, the user then loses the freedom to specify individual axis limits.

TOSPAC now asks for the elevations at which concentrations are to be plotted:

ENTER ELEVATIONS TO BE PLOTTED:

An acceptable elevation is a real number or one of the following words: *SOURCE* (corresponding to the center of the source region), and *MAX* or *MAXIMUM* (plot the maximum concentration as a function of time, at whichever elevation it occurs). Elevations should be between the minimum and maximum elevations for a TRANS calculation; if an elevation lies beyond these boundaries, it is reset to the nearest boundary during construction of the graphics-driver file. If more than one number is entered, they must be separated by spaces or commas. All the numbers and words must be entered on one line before the user enters a <CR>. TRANS calculates concentrations at the midpoint of a cell; i.e., halfway between mesh points. OUTPLOT allows entry of any elevation. If the entered elevation does not correspond to the midpoint of a cell, the concentration value is linearly interpolated between the two closest cell midpoints. The default is the elevation of the center of the source (*SOURCE*).

Each elevation plotted has a different type of line and a legend of the line types is created. TOSPAC now prompts for a legend as follows:

DO YOU WANT A LEGEND (N OR Y OR SAME):

Responses to this prompt, plus a general description of the legend-related commands, are offered in Section 4.6.3.3.

If the user enters *YES*, OUTPLOT continues with legend-related prompts. If one of the first two choices was selected in response to the concentration-plot menu then the following prompts are given:

SPECIFY LABELS...

ENTER LABEL FOR ELEVATION CURVE # 1:

ENTER LABEL FOR ELEVATION CURVE # 2:

ENTER LABEL FOR ELEVATION CURVE # 3:

- o
- o
- o

Allowable labels are any character strings up to 80 characters long. The default is the elevation value. There are as many prompts as specified elevations.

However, if choice 3 was selected on the concentration-plot menu (plot matrix and fracture concentrations together), then the labels used are the words *MATRIX* and *FRACTURE*, with no choice allowed.

OUTPLOT now asks where to locate the legend:

ENTER LEGEND LOCATION:

A discussion of how the legend is placed on the plot and possible responses to this prompt is given in Section 4.6.3.3. For concentration versus time plots, the default legend location is *LEFT, TOP*.

OUTPLOT now indicates that it has all the information to define the plot block for concentration versus elevation, and that it is writing it in the plot-definition file:

PLOT DEFINITION COMPLETED.

An example of a plot block for concentration versus time in a plot-definition file is given in Figure 3.46.

The resulting plot is given in Figure 3.43.

4.6.5.5 Plots of Release versus Time (Choice 9)

Plots of release versus time are selected when the user responds to the OUTPLOT (TRANS RESULTS) menu with choice 9:

ENTER CHOICE: 9

OUTPLOT responds with the following message:

DEFINING RELEASE-VS-TIME PLOTS...

A plot of release versus time shows the amount of a given contaminant that crosses a specified problem boundary (either upper or lower boundary) during the problem time. There are three ways of defining this release, as follows:

- 1) actual amount outside boundary: a running total of the contaminant *accounting for* radionuclide decay; and
- 2) cumulative amount reaching the boundary: a running total of the contaminant *without* considering radioactive decay;
- 3) rate of release across the boundary.

If the contaminant does not decay, the first two ways are equivalent. The cumulative amount reaching the boundary is the time integral of the rate of release across the boundary.

The release can be presented in terms of mass, radioactivity, or EPA ratio. The EPA-ratio release type is a special plot of release versus time. If a plot of the EPA ratio is chosen, the releases for each contaminant are divided by the EPA release limit for that contaminant. To get the quantity specified in the EPA regulations, cumulative releases should be chosen (from the menu for this plot type presented below). The regulatory EPA sum is the sum of all the individual ratios. Note, however, that the EPA sum is not correct unless *all* significant contaminants--radionuclides and daughter products--expected at the repository are included in the input to TOSPAC (the contaminant-property block of the TRANS input-data file). The EPA limit for a contaminant is specified in the input-data file (Section 4.2.16).

To define a plot of release versus time, OUTPLOT asks the user whether the cumulative release, actual quantity present, or release rate should be plotted, then asks for the release type, the boundary to consider, axis information, the contaminant to be plotted, and a legend.

OUTPLOT begins with the release-plot menu:

OUTPLOT (TRANS RESULTS) RELEASE MENU

- 0. STOP
- 1. PLOT BOTH ACTUAL AND CUMULATIVE AMOUNTS TOGETHER
- 2. PLOT ACTUAL AMOUNT PRESENT
- 3. PLOT CUMULATIVE RELEASE
- 4. PLOT RATE OF RELEASE

ENTER CHOICE:

For choice 1, a separate plot is produced for each contaminant (below), with each plot having two curves, representing actual and cumulative releases. For choices 2, 3, and 4, one plot is defined with curves for each contaminant selected (below).

And OUTPLOT continues prompting as follows:

ENTER RELEASE TYPE (MASS, RADIOACTIVITY, OR EPA RATIO):

The release type determines the axis label and the type of data used. Acceptable answers are the words *MASS*, *RADIOACTIVITY* (or *RAD*), *EPA RATIO* (or *EPA*). The default is *MASS*. The radioactivity and EPA-ratio responses only apply to radioactive contaminants.

OUTPLOT now asks for the boundary across which the releases are to be considered:

ENTER RELEASE BOUNDARY (BOTTOM, TOP, OR BOTH):

An acceptable response is one of the following words: *BOTTOM* (corresponding to releases across the lower boundary), *TOP* (corresponding to releases across the upper boundary), or *BOTH* (corresponding to the sum of the releases across both boundaries). The default is the same as the word *BOTTOM*.

Continuing, OUTPLOT asks for information about the axes:

ENTER RELEASE-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER RELEASE-AXIS MINIMUM:

ENTER RELEASE-AXIS MAXIMUM:

ENTER TIME-AXIS TYPE (LIN, LOG, NEGLOG):

DO YOU WANT TO CHANGE AXIS UNITS OR SCALE DATA (N OR Y):

SET AXIS LIMITS...

ENTER TIME-AXIS MINIMUM:

ENTER TIME-AXIS MAXIMUM:

A discussion of these prompts and possible responses is contained in Section 4.6.3.2.

OUTPLOT now asks for the contaminant that is the subject of this plot:

ENTER CONTAMINANT:

A discussion of contaminant names and numbers is contained in Section 4.6.5.1.

If the user enters the names or numbers of more than a single contaminant, all contaminants are plotted together, along with a curve for their sum. An exception is made, however, when the actual and cumulative releases are plotted together (choice 4 in response to the release-plot menu); in this case, a separate plot is produced for each contaminant that is specified. For an EPA-ratio plot, the cumulative releases of all individual contaminants are plotted with various line types, and the sum is plotted as a solid line.

For each contaminant plotted or, in the case of the actual/cumulative-release plot (choice 4), for each release type, a different type of line is used and a legend of the line types is created if desired. TOSPAC now prompts for a legend as follows:

DO YOU WANT A LEGEND (N OR Y OR SAME):

Responses to this prompt, plus a general description of the legend-related commands, are offered in Section 4.6.3.3.

Release plots are like dispersion-coefficient plots (Section 4.6.5.1) in that there is no choice about the legend labels and thus no prompts. If the user asks for one of the first three choices in response to the release-plot menu, the labels will be the contaminant names, as given in the contaminant-property block of the TRANS input-data file. If all contaminants are being plotted, a curve for the sum is drawn. It is labeled by the word TOTAL. If the user asks for plots of the actual and cumulative releases together (choice 4 in response to the release-plot menu), then the legend labels are the words ACTUAL and CUMULATIVE.

OUTPLOT now asks where to locate the legend:

ENTER LEGEND LOCATION:

A discussion of how the legend is placed on the plot and possible responses to this prompt is given in Section 4.6.3.3. For release plots, the default legend location is *LEFT, TOP*.

OUTPLOT now indicates that it has all the information to define the plot block for release versus time, and that it is writing it in the plot-definition file:

PLOT DEFINITION COMPLETED.

Examples of plot blocks for release versus time are given in Figures 2.12 and 3.46. Release versus time plots are shown in Figures 2.9, 3.44, and 3.45.

4.6.6 Construct Graphics-Driver File

Entering a choice of 4 in response to the OUTPLOT main menu allows the user to construct plots in a form that can be read by a graphics output device. Two files are manipulated: for input, an existing plot-definition file is required; for output, a graphics-driver file is created. (see the beginning of Section 4.6 and Sections 4.7.12 and 4.7.13). The plot-definition file is specified upon initial entry into the OUTPLOT module, before the OUTPLOT main menu is presented (Section 4.6.2).

OUTPLOT prompts for the name for the graphics-driver file immediately after selecting choice 4 from the OUTPLOT main menu:

ENTER OUTPLOT GRAPHICS-DRIVER FILE (DEFAULT=OUTPLOT.DRV):

Acceptable file names are discussed in Section 4.2.2.

If all plot-data file names have been specified in the plot-definition file, OUTPLOT proceeds to construct the graphics-driver file (below). If any plot-data file names are missing (see Sections 4.6.3, 4.6.4, and 4.6.5), OUTPLOT prompts for the names. If the missing files are for STEADY plots, the following prompt is issued:

ENTER STEADY PLOT-DATA FILE (DEFAULT=STEADY.PLT):

The default file name could be different if a STEADY plot-data file had been defined earlier in the session. After the user enters a STEADY plot-data file name, the prompt is repeated, and repeated until no more file names are entered:

ENTER STEADY PLOT-DATA FILE (DEFAULT=NONE):

Up to ten STEADY plot-data files can be specified.

If plots for DYNAMICS results are defined, but a DYNAMICS plot-data file is not specified in the plot-definition file, the following prompt is issued (again the default file name could be different):

ENTER DYNAMICS PLOT-DATA FILE (DEFAULT=DYNAMICS.PLT):

If plots for TRANS results are defined, but a TRANS plot-data file is not specified in the plot-definition file, the following prompt is issued (the default file name could be different):

ENTER TRANS PLOT-DATA FILE (DEFAULT=TRANS.PLT):

OUTPLOT now reads the individual plot blocks from the plot-definition file, and constructs the graphics-driver file, writing a status message to the screen telling each plot that it is working on. (At this point, for some installations of TOSPAR, the actual plots will appear on the user's terminal screen. In these cases, after a plot is drawn, it will remain on the screen until the user enters a <CR>. The next plot will then be drawn.) The following is an example of the status messages written to the terminal screen.

STEADY PLOT SECTION
CREATING MESH PLOTS.
CREATING VELOCITY VS. ELEVATION PLOTS.

DYNAMICS PLOT SECTION
CREATING CHARACTERISTIC CURVE PLOTS.
CREATING WATER MASS PLOTS.

TRANS PLOT SECTION
CREATING RELEASE PLOTS.
CREATING CONCENTRATION VS. ELEVATION PLOTS.

When the end of the plot-definition file is reached and all plots have been constructed on the graphics-driver file, the following message appears:

NORMAL OUTPLOT TERMINATION. ?? PLOTS PRODUCED.

where the question marks are replaced by the appropriate number. Then the OUTPLOT main menu reappears on the user's terminal screen.

The graphics-driver file contains the plots in a graphics language, either in the final driver language of the graphics device, or some intermediate language that must be postprocessed before submittal to a graphics device. In either case the file will probably be an unformatted file (binary), and the user would not be able to examine or edit it. To actually create the plots, the user must send the graphics-driver file to the appropriate graphics device with a command to execute it. This process is system-dependent. It is recommended that the user contact the manager or consultant for the computer system that is being used to determine the necessary commands (or procedures).

4.7 TOSPAC Files

The TOSPAC modules communicate with each other through data files. These files are named by the user during execution of TOSPAC, and remain available to the user at the completion of a TOSPAC run. However, the TOSPAC file system has been designed to be opaque to the user. Typically, the user would only need to know of the input-data files and the graphics-driver file (which, after a TOSPAC run, the user would submit to the graphics device available on his computer system).

TOSPAC uses both formatted (text) and unformatted (binary) files. Text files are used where it is important for the user to be able to read or create them (e.g., input-data files, initial-condition files, plot-definition files, etc.). The binary files cannot be examined or modified by the user. Binary files are used to minimize space (e.g., plot-data files) or where required by external devices (e.g., graphics-driver files). Binary files contain data as it is stored in the computer, and therefore, are machine-dependent. Binary files from one type of computer may not be readable by another type.

TOSPAC also uses several "scratch" files to temporarily store data. These files are automatically deleted by TOSPAC and are not mentioned in this section.

A discussion of each TOSPAC file follows. The discussion includes the formal name of the file, and its typical default name in various TOSPAC prompts. The initial default answers to these queries are typically as shown (e.g., STEADY.DAT, STEADY.PSI, STEADY.LIS, etc.). However, if an input-data file had been created previously in a TOSPAC session, then that name is the default. This scheme presents no problem on computers that allow multiple files with the same name. If, for example, an output-listing file already exists with the name OUT.LIS, and this name is the default that the user selects, then a new version or cycle of OUT.LIS is created by TOSPAC and the user has two files. If the user enters the name of an existing file on a computer system that does not allow multiple files with the same name, TOSPAC returns an error message and asks for another file name.

Also discussed in the following subsections is the purpose of each file, how it is used by TOSPAC, the subroutines within TOSPAC that read and write the file, and a description of the file contents and format. Examples or references to examples are given where appropriate. Examples of binary files are not given because the contents cannot be printed; for these files, the FORTRAN statements that write the files are given, and the user can surmise the contents based on these statements. The discussion of the graphics-driver file contains no example or FORTRAN statements; the structure of this file is controlled by the proprietary CA-DISSPLA software.

Figure 4.25 shows which TOSPAC modules use the various TOSPAC files.

4.7.1 STEADY, DYNAMICS, and TRANS Input-Data Files

Default Name: Initial default names for STEADY, DYNAMICS, and TRANS input-data files are STEADY.DAT, DYNAMICS.DAT, and TRANS.DAT, respectively. These defaults can change as a TOSPAC session progresses.

Purpose: The TOSPAC input-data files define the input data necessary for steady-state-flow and transient-flow calculations (geologic parameters, material properties, calculational mesh for the finite-difference scheme, boundary conditions, etc.), and contaminant-transport calculations (source parameters, contaminant properties, boundary conditions, etc.).

Figure 4.25: Interrelationship of TOSPAC files.

Use: Use of the STEADY input-data file by the STEADY module is discussed in Sections 2.6, 3.2, and 4.3. Use of the DYNAMICS input-data file by the DYNAMICS module is discussed in Sections 3.1 and 4.4. Use of the TRANS input-data file by the TRANS module is discussed in Sections 2.7, 3.2, and 4.5.

Type: Input to the calculational modules (STEADY, DYNAMICS, and TRANS); output from INDATA.

Read Subroutine: Subroutine SINPUT reads STEADY and DYNAMICS input-data files; subroutine TXTINPT reads TRANS input-data files.

Create Subroutine: Various subroutines in INDATA.

Format: Text File.

Description: Section 4.2 contains a complete description of the data that TOSPAC input-data files hold. What follows here is a description of the structure of these files and the rules for placement of data.

All TOSPAC input-data files are sequences of *data blocks* consisting of various character and numeric data and comments. Data blocks can be in any order.

TOSPAC recognizes the beginning of a data block by a line containing the keyword BLOCK and another keyword. Input-data files use the following keywords:

TITLE
CONST
GEOLO
SATUR
MATER
MESH
BOUND
INITI
SOURC
CONTA
FILE

Keywords recognized in STEADY input-data files are as follows: TITLE, CONST, GEOLO, MATER, MESH, BOUND, and FILE. Keywords recognized in DYNAMICS input-data files are as follows: TITLE, CONST, GEOLO, MATER, MESH, BOUND, INITI, and FILE. Keywords recognized in TRANS input-data files are as follows: TITLE, SOURC, GEOLO, SATUR, CONTA, BOUND, INITI, and FILE. Keywords MESH and FILE must be followed by a space (five characters total); other keywords can be embedded in text. Keywords can be written in any combination of upper or lower

case and can be parts of longer words; e.g., "Constants Block" is an acceptable block designator. The user *must not* combine BLOCK with another reserved word anywhere *except* in the first line of a data block.

Input data are of two types: character and numeric. Character data are the problem title, notes, names of geologic units, materials, and contaminants, and names of files. Character data can be arbitrary strings of characters up to 80 characters long, except for names of files which cannot include spaces or tabs within the name. If the character data begins with spaces or tabs, these characters are stripped off before TOSPAC uses the data. The vertical-bar character (|) is a special character in titles and names: it can be inserted within the titles and names to force OUTPLOT to make a line break at that position when computer graphics are produced. The vertical bar is removed when the character string is used.

Numeric data are formatted as follows:

- 1) zero or more spaces or tabs,
- 2) a number (integer or real, in any FORTRAN-recognizable format),
- 3) one space or one tab,
- 4) a character string containing the units comment (optional),
- 5) one or more spaces or tabs,
- 6) a character string containing a comment (optional).

The number *must* be in the first 20 characters of the line. The units and the comment are optional. If a units comment is included, the number and the units should be in the first 20 characters of the line. If a units comment is not included, a minimum of two spaces or tabs must be present between the number and any other comment.

TOSPAC allows the user to place the units after an input value in the input-data file. But TOSPAC does *not* read and understand the units—they are only a note to the user. TOSPAC considers the units to be a special type of comment. During modification of an input-data file, the units remain attached to a value, but other comments do not. To retain this feature, there must be a single space or a single tab between the input value and the corresponding unit.

When INDATA creates a STEADY, DYNAMICS, or TRANS input-data file, INDATA includes comments that describe the various data elements, and the user is allowed to enter units. It is perfectly acceptable for the user to circumvent INDATA and create or modify input-data files with his or her computer system's text editor. The user can then create or modify input-data files without the comments, or with the user's own comments. However, although the numbers and titles can be entered almost in free format, three rules must be followed:

- 1) all required block designators (see above) must be present;
- 2) each line in a block must contain at most one datum; and
- 3) all data must be in the proper order, as given in Section 4.2 (if a datum is unknown, type the word *unknown*—the file will not be satisfactory for a calculation, but at least proper order is maintained).

A block terminator (a blank line, another data-block designator, or an end-of-file) is necessary, but is fulfilled by the first rule.

Figure 4.26 shows an example of the STEADY input-data file used in Chapter 2 in a minimized form, created on a text editor. Compare this figure with Figure 2.3. Note the absence of comments and how difficult it would be to know if a mistake were made.

Example: Examples of STEADY input-data files are given in Figures 2.3, 3.20, and 4.26. An example of a DYNAMICS input-data file is given in Figure 3.2. Examples of TRANS input-data files are given in Figures 2.4 and 3.21.

4.7.2 STEADY Solution File

Default Name: STEADY.PSI (this default could change as a TOSPAC session progresses).

Purpose: The STEADY solution file defines the pressure-head values for a given calculational mesh, as constructed by the steady-state solver (STEADY). The STEADY solution file is only used by TOSPAC as an initial pressure-head condition for a dynamic-flow (DYNAMICS) calculation. The STEADY solution file is also called the initial-condition file when used as such by DYNAMICS. DYNAMICS can use a facsimile of a STEADY solution file as an initial-condition file (discussed below).

Use: Creation of the STEADY solution file is discussed in Section 4.2.11; its use by the DYNAMICS module is discussed in Section 4.4.

Type: Output from STEADY (can be used as input to DYNAMICS).

Read Subroutine: SINPUT (if specified by name in a file block in a DYNAMICS input-data file) or DINTLZ (if specified by default).

Create Subroutine: SITWRITE.

Format: Text File.

Description: The STEADY solution file is written with the following FORTRAN statement:

```
WRITE(ICFL,*) (PH(J),J=JMIN,JMAX)
```

To elaborate, it is written as a simple free-formatted list of the pressure-head values at every mesh point. In DYNAMICS, the initial-condition file is read the same way. Thus, DYNAMICS can read any list of numbers as an initial condition.

The user can construct an initial-condition file by making a list of real numbers: the first number in the list is the pressure head that is to be assigned to mesh-point number 1; the second number in the list is the pressure head that is to be assigned to mesh-point number 2; the third number... etc.

This feature is useful for simulating a column that is initially dry (or at least near residual saturation). For instance, the user creates a list of numbers as follows:

```
-1.E+5
```

```

title block
Simplified Mill-Tailings Problem

constants block
1000.
4.3E-6
1.E+6
0.1
0.5
top
bottom
0

geologic-unit block
1
unit 1
Sandstone
0.
100.
1
1
0.
0.
0.

material-property block
1
material 1
Sandstone (van Genuchten, 1980)
0.25
1
1.
0.612
0.79
10.4
1.25E-5

mesh block
500
1
submesh 1
0.
100.
500

boundary-condition block
1
1
snapshot 1
0.
12
0.
-1.585E-10
0.

file block
STEADY.PSI
STEADY.PLT
STEADY.LIS
1

```

Figure 4.26: STEADY input-data file created by a text editor, containing the same data as the input-data file shown in Figure 2.3.

```

-1.E+5
-1.E+5
  0
  0
  0
-1.E+5

```

More than one number can be on a line; numbers must be separated by spaces, tabs, commas, or carriage returns. If this list is entered as an initial-condition file for DYNAMICS, DYNAMICS sets every mesh point to an initial pressure head of -10^5 , which in the case of most characteristic curves is very near residual saturation. (Note that van Genuchten-defined characteristic curves approach a pressure head of negative infinity at residual saturation, and therefore, residual saturation can never be reached. Note also that the above initial condition can be entered without using a file, by choosing an initial-condition flag 3 in the initial-condition block; Section 4.2.12.)

Because DYNAMICS is not particular about the file it reads for an initial condition, the user can inadvertently enter the wrong data. DYNAMICS will only issue an error if the file is too short (i.e., does not contain a number for every mesh point); if the file is long enough, DYNAMICS will accept any list of numbers.

Example: None.

4.7.3 STEADY Output-Listing File

Default Name: STEADY.LIS (this default could change as a TOSPAC session progresses).

Purpose: The STEADY output-listing file contains the results of a steady-state calculation in tabular form. It is used primarily to check the detailed behavior of one or more variables.

Use: The STEADY output-listing file is mentioned in Sections 2.6 and 3.2. Section 4.2.11 contains a discussion of how to control the amount of data written to the output-listing file.

Type: Output from STEADY.

Read Subroutine: None.

Create Subroutine: SINWRITE and SITWRITE.

Format: Text file.

Description: The STEADY output-listing file repeats the STEADY input-data file that was used to create it; this repetition is to create an audit trail.

After the replicated input-data file, the STEADY output-listing file contains the results of the STEADY run. First, a list of mesh points where the solution may be unacceptable is given. Here, if the calculated flux exceeds the imposed flux (this value is known as the flux deviation) by more than 10% anywhere in the solution, then a message is written for each mesh point where this condition occurs, reporting the flux deviation, the mesh-point number where it occurs, and the corresponding

elevation. If the calculated flux does not exceed the imposed flux by more than 10% anywhere, then only a single message is given, reporting the greatest flux deviation, the mesh-point number where it occurs, and the corresponding elevation.

Next, information concerning the condition of the entire column is presented.

- 1) The average saturation of the entire column.
- 2) The total void volume of the column (the sum of the volume occupied by air and by water).
- 3) The volume of the column occupied by water.
- 4) The volume of the column occupied by air.
- 5) The mass of water in the column.

The boundary conditions that were used in the calculation are stated next.

Then, in tabular form, the final conditions at each mesh point are given. The number of mesh points for which values are written can be controlled in the file block of the STEADY input-data file. The table columns are defined as follows.

- 1) The mesh-point number (J).
- 2) The corresponding geologic-unit number (UNIT).
- 3) The matrix-material number for the unit (MAT).
- 4) The fracture-material number for the unit (FRK).
- 5) The corresponding elevation (Z).
- 6) The computed pressure head (PRES HEAD)—the variable for which STEADY actually solves.
- 7) The ratio of how much the calculated flux in the composite material (i.e., both matrix and fractures) deviates from the imposed flux (QDEVIATION)—multiply this value by 100 to make it a percentage.
- 8) The calculated flux in the composite material (FLUX).
- 9) The calculated flux in the matrix (FLXMAT).
- 10) The calculated flux in the fractures (FLXFRK).
- 11) The calculated hydraulic conductivity in the composite material (HK).

Following this group of results is another section of columns, as follows:

- 1) The mesh-point number (J).
- 2) The corresponding unit number (UNIT).
- 3) The matrix-material number for the unit (MAT).

- 4) The fracture-material number for the unit (FRK).
- 5) The calculated saturation in the composite material (SAT).
- 6) The calculated derivative of the saturation with respect to pressure head in the composite material (DSAT).
- 7) The calculated saturation of the matrix (SATMAT).
- 8) The calculated saturation of the fractures (SATFRK).
- 9) The calculated average linear velocity of water in the composite material (VEL).
- 10) The calculated average linear velocity of water in the matrix (VELMAT).
- 11) The calculated average linear velocity of water in the fractures (VELFRK).

The final part of the STEADY output-listing file gives GWTT information for the distance between the start and end positions specified in the constants block of the STEADY input-data file. Four travel-time values are specified: the minimum, or average-fastest-particle travel time, the composite-velocity travel time, the travel time of water in the matrix, and the travel time of water in the fractures (Section 3.2). In the travel-time calculations the part of the distance not carrying at least 1% of the flow is omitted, because often the travel time is extremely long in these areas (when the velocity is zero, the travel time is infinite) and would thus not be useful information. This 1% cutoff is presented as a reminder in the last line of the STEADY output-listing file.

Example: Figures 2.5 and 3.22.

4.7.4 STEADY and DYNAMICS Plot-Data Files

Default Name: Initial default name for the STEADY plot-data file is STEADY.PLT; default name for the DYNAMICS plot-data file is DYNAMICS.PLT. These defaults could change as a TOSPAC session progresses.

Purpose: The STEADY plot-data file stores input data and calculation results for steady-state flow. It is used by TRANS to provide the hydrologic background for a transport calculation. It is used by OUTPLOT for plotting steady-state results. The DYNAMICS plot-data file stores transient-flow input data and calculation results. It is used by OUTPLOT for plotting transient-flow results.

Use: Creation of the STEADY plot-data file is discussed in Sections 2.6, 3.2, and 4.2.11; its use by the TRANS module is discussed in Sections 2.7, 3.2, and 4.5; its use by the OUTPLOT module is discussed in Sections 2.8, 3.2, and 4.6. Creation of the DYNAMICS plot-data file is discussed in Sections 3.1 and 4.2.11; its use by the OUTPLOT module is discussed in Sections 3.1 and 4.6.

Type: The STEADY plot-data file is output from STEADY; input to TRANS and OUTPLOT. The DYNAMICS plot-data file is output from DYNAMICS; input to OUTPLOT.

Read Subroutine: TINPT, HINIT, and HDATA.

Create Subroutine: SINWRITE and SITWRITE create the STEADY plot-data file; DINWRITE and DITWRITE create the DYNAMICS plot-data file.

Format: Binary file.

Description: Because the plot-data files are written in binary format (the format that is used inside the computer), they cannot be examined or modified by the user. Binary format is used for these files because it typically requires less space and is more quickly read by the computer, but also because the user should not be examining or modifying these files.

To describe these files, the FORTRAN statements used to create them are presented below. In the following listings, HPLTFL is the variable that contains the FORTRAN logical-unit number for the STEADY and DYNAMICS plot-data files.

Notice that many of the variables concern time; these variables are not used by STEADY, but are included for compatibility with the DYNAMICS plot-data file. The STEADY plot-data file is almost identical to a DYNAMICS plot-data file; the only difference is that in STEADY, one section of setup data and one section of results are written; in DYNAMICS after the setup-data section is written, multiple copies of the results are written—one copy for each time snapshot.

The format for the setup-data section follows. First, title data are written:

```

WRITE(HPLTFL) 1+NUNITS+NMAT
WRITE(HPLTFL) PTITLE
DO 34 I=1,NUNITS
WRITE(HPLTFL) GTITLE(I)
34  CONTINUE
DO 36 I=1,NMAT
WRITE(HPLTFL) MTITLE(I)
36  CONTINUE

```

where 1+NUNITS+NMAT is the number of titles, PTITLE is the problem title, GTITLE contains the names of the geologic units, and MTITLE contains the names of the materials.

Next, the numerical variables are written:

```

WRITE(HPLTFL) TCONVERT, ICONVERT, TMSG
WRITE(HPLTFL)
*   IT, TIME, DT, ASAT, AWT, TOTVOL, WATVOL, AIRVOL, JMIN, JMAX
WRITE(HPLTFL) TIME, DT, RHOWAT, ACOL, STDY, FUDGE1, OMEGA, VAXMIN,
*   VAXMAX, PI, JMAX, JMIN, IT, NDUMP, NUNITS, NMAT, MAXIT, NPRINT, NPLOT
WRITE(HPLTFL) (NOUNIT(J), J=JMIN, JMAX)
WRITE(HPLTFL) (MAT(J), J=JMIN, JMAX)
WRITE(HPLTFL) (MATFRK(J), J=JMIN, JMAX)

DO 38 I=1, NMAT
WRITE(HPLTFL) (SATD(J, I), J=1, 8)
WRITE(HPLTFL) (HKD(J, I), J=1, 8)
WRITE(HPLTFL) SATRES(I), BETAC, G, IFLAG(I)
WRITE(HPLTFL) MAXTAB(I),
*   (PHTAB(J, I), J=1, MAXTAB(I)),
*   (SATTAB(J, I), J=1, MAXTAB(I)),
*   (DSATAB(J, I), J=1, MAXTAB(I)),

```

```

*      (DS2TAB(J,I),J=1,MAXTAB(I)),
*      (HKTAB(J,I),J=1,MAXTAB(I)),
*      (DHKTAB(J,I),J=1,MAXTAB(I))
38  CONTINUE

      NDUMP=1
      WRITE(HPLTFL) NDUMP,
*      (TDUMP(J),J=1,NDUMP),
*      (IBTOP(J),J=1,NDUMP),(IBBOT(J),J=1,NDUMP),
*      (FLXTOP(J),J=1,NDUMP),(FLXBOT(J),J=1,NDUMP),
*      (PHTOP(J),J=1,NDUMP),(PHBOT(J),J=1,NDUMP),
*      (PONDMPX(J),J=1,NDUMP)

      WRITE(HPLTFL) (Z(J),J=JMIN,JMAX)
      WRITE(HPLTFL) (PH(J),J=JMIN,JMAX)
      WRITE(HPLTFL) (AF(J),J=JMIN,JMAX)
      WRITE(HPLTFL) (ACOMP(J),J=JMIN,JMAX)
      WRITE(HPLTFL) (FCOMP(J),J=JMIN,JMAX)
      WRITE(HPLTFL) (PORM(J),J=JMIN,JMAX)
      WRITE(HPLTFL) (PORF(J),J=JMIN,JMAX)

      WRITE(HPLTFL)
*      TOPMASSIN,BOTMASSIN,CALCMASS,
*      ORIGINALMASS,WATERBALANCE
      WRITE(HPLTFL)
*      PPSTART,PPEND,
*      PPAFP(KOUNT),PPCOMP(KOUNT),
*      TIMEIN(KOUNT),TIMEAFP(KOUNT),TIMECOMP(KOUNT),
*      ITAFP(KOUNT),ITCOMP(KOUNT),TFLAG

```

where KOUNT is the number of time snapshots reached (KOUNT = 1 for the setup-data section), and the other variables and the quantities they represent are as follows:

- 1) TCONVERT (double precision) is the time conversion factor;
- 2) ICONVERT (integer) is the time conversion number from the input-data file;
- 3) TMSG (character*8) is the time units;
- 4) IT (integer) is the number of iterations;
- 5) TIME (double precision) is the problem time;
- 6) DT (double precision) is the timestep;
- 7) TOTVOL (double precision) is the volume of the voids in the entire column;
- 8) WATVOL (double precision) is the volume of the water in the column;
- 9) AIRVOL (double precision) is the volume of the air in the column;
- 10) RHOWAT (double precision) is the density of water;
- 11) ASAT (double precision) is the average saturation of the column;

- 12) AWT (double precision) is the mass of water in the column;
- 13) JMIN (integer) is the mesh-point number of the lower boundary;
- 14) JMAX (integer) is the mesh-point number of the upper boundary;
- 15) ACOL (double precision) is the cross-sectional area of the column;
- 16) STDY (double precision) is the steady-state convergence-tolerance value;
- 17) FUDGE1 (double precision) is the timestep factor; OMEGA is the implicitness factor;
- 18) VAXMIN (double precision) is 10^{-38} ;
- 19) VAXMAX (double precision) is 10^{+38} ;
- 20) PI (double precision) is the circumference of the unit circle (not used);
- 21) NDUMP (integer) is the number of time snapshots;
- 22) NUNITS (integer) is the number of geologic units;
- 23) NMAT (integer) is the number of materials;
- 24) MAXIT (integer) is the maximum number of iterations allowed;
- 25) NPRINT (integer) is the flag that tells whether to write the output-listing file, and if so, number of mesh points to skip when writing the file;
- 26) NPLOT (integer) is the flag that tells whether to write the plot-data file;
- 27) NOUNIT (integer) is the array assigning geologic units to mesh points;
- 28) MAT (integer) is the array assigning matrix materials to mesh points;
- 29) MATFRK (integer) is the array assigning fracture materials to mesh points;
- 30) SATD and HKD (double precision) are arrays holding characteristic-curve information;
- 31) SATRES (double precision) is the array assigning residual saturations to each mesh point;
- 32) BETAC (double precision) is the compressibility of water;
- 33) G (double precision) is gravity (not used);
- 34) IFLAG (integer) is the array assigning characteristic-curve flags to materials;
- 35) MAXTAB (integer) is the array containing the maximum size of the characteristic-curve data table for each material;
- 36) PHTAB (double precision) is the data table for pressure head;
- 37) SATTAB (double precision) is the data table for saturation;
- 38) DSATAB (double precision) is the data table for the first derivative of the saturation;
- 39) DS2TAB (double precision) is the data table for the second derivative of the saturation;
- 40) HKTAB (double precision) is the data table for the hydraulic conductivity;
- 41) DHKTAB (double precision) is the data table for the first derivative of the conductivity;

- 42) TDUMP (double precision) is the array of time-snapshot times;
- 43) IBTOP (integer) is the array of upper boundary-condition flags;
- 44) IBBOT (integer) is the array of lower boundary-condition flags;
- 45) FLXTOP (double precision) is the array of upper-boundary flux boundary conditions;
- 46) FLXBOT (double precision) is the array of lower-boundary flux boundary conditions;
- 47) PHTOP (double precision) is the array of upper-boundary pressure-head boundary conditions;
- 48) PHBOT (double precision) is the array of lower-boundary pressure-head boundary conditions;
- 49) PONDMX (double precision) is the array of maximum-pond-height boundary conditions;
- 50) Z (double precision) is the elevation at each mesh point;
- 51) PH (double precision) is the pressure head at each mesh point;
- 52) AF (double precision) is the fracture porosity at each mesh point;
- 53) ACOMP (double precision) is the bulk-rock compressibility at each mesh point;
- 54) FCOMP (double precision) is the fracture compressibility at each mesh point;
- 55) PORM (double precision) and PORF (double precision) are the porosities of the matrix material and the fracture material, respectively, at each mesh point;
- 56) TOPMASSIN (double precision) is the cumulative mass of water entering (leaving) the top of the column;
- 57) BOTMASSIN (double precision) is the cumulative mass of water entering (leaving) the top of the column;
- 58) CALCMASS (double precision) is the mass of water that should be in the column (the sum of TOPMASSIN, BOTMASSIN, and ORIGINALMASS);
- 59) ORIGINALMASS (double precision) is the mass of water originally calculated to be the column;
- 60) WATERBALANCE (double precision) is the mass balance—the difference between the mass that should be in the column (CALCMASS) and the mass calculated to be in the column (AWT), divided by the the calculated mass (AWT), and expressed as a percentage;
- 61) PPSTART (double precision) is the start position where particles are released for the GWTT calculation;
- 62) PPEND (double precision) is the end position where particles are removed for the GWTT calculation;
- 63) 1 PAFP (double precision) is the array that keeps track of the present positions of the average fastest particles;
- 64) PPCOMP (double precision) is the array that keeps track of the present positions of the particles traveling at the composite velocity;
- 65) TIMEIN (double precision) is the array that keeps track of the time that particles were released;
- 66) TIMEAFP (double precision) is the array that keeps track of the present time for average fastest particles—if the particle is removed from the column, the time the particle leaves is saved;

- 67) TIMECOMP (double precision) is the array that keeps track of the present time for composite-velocity particles—if the particle is removed from the column, the time the particle leaves is saved;
- 68) ITAFP (integer) is the array that indicates whether an error has occurred in tracking average fastest particles;
- 69) ITCOMP (integer) is the array that indicates whether an error has occurred in tracking composite-velocity particles; and
- 70) TTFLAG (logical) is the flag that indicates whether travel times are to be calculated.

Finally, the following results section is written, once for a STEADY calculation, and once for every time snapshot for a DYNAMICS calculation:

```

WRITE(HPLTFL)
*   IT, TIME, DT, ASAT, AWT, TOTVOL, WATVOL, AIRVOL, JMIN, JMAX
WRITE(HPLTFL) (PH(J), J=JMIN, JMAX)

WRITE(HPLTFL)
*   TOPMASSIN, BOTMASSIN, CALCMASS,
*   ORIGINALMASS, WATERBALANCE
WRITE(HPLTFL)
*   (PPAFP(I), PPCOMP(I),
*   TIMEIN(I), TIMEAFP(I), TIMECOMP(I),
*   ITAFP(I), ITCOMP(I), I=1, KOUNT)

```

Example: None.

4.7.5 STEADY And DYNAMICS Saturation-Curve File

Default Name: SAT.CRV.

Purpose: The saturation-curve file defines the data for a saturation characteristic curve for a material in the material-property block of a STEADY or DYNAMICS input-data file. The data are read directly into pressure-head and saturation data tables.

Use: Use of this file is discussed in Section 4.2.8.

Type: Input to STEADY and DYNAMICS.

Read Subroutine: SINPUT.

Create Subroutine: None.

Format: Text file.

Description: The saturation-curve file must be in the following format. The first number must be an integer that indicates how many data pairs are in the data table (to a maximum of 1000). The remainder of the numbers must consist of order pairs of numbers: a pressure-head value (should be a nonpositive real number), immediately followed by a saturation value (should be a real number between 0 and 1, inclusive). The first ordered pair *must* be the pressure head and the saturation (S_s) corresponding to the air-entry pressure head. The last ordered pair *must* be the pressure head and the saturation at the residual saturation (S_r). The ordered pairs between these extremes must be decreasing in pressure head (i.e., the pressure head values must progress to increasing negative values). Figure 4.27 presents the format of a saturation data table.

Example: Figure 4.27.

4.7.6 STEADY And DYNAMICS Hydraulic-Conductivity-Curve File

Default Name: HK.CRV.

Purpose: The hydraulic-conductivity-curve file defines the data for a hydraulic-conductivity characteristic curve for a material in the material-property block of a STEADY or DYNAMICS input-data file. The data are read directly into pressure-head and hydraulic-conductivity data tables.

Use: Use of this file is discussed in Section 4.2.8.

Type: Input to STEADY and DYNAMICS.

Read Subroutine: SINPUT.

Create Subroutine: None.

Format: Text file.

Description: The hydraulic-conductivity-curve file is identical in form to a saturation-curve file. This file must be paired with a saturation-curve file. This file must have the same number of points as the saturation-curve file; furthermore, all ordered pairs must be at the same pressure-head values as the corresponding points in the saturation data table. Hydraulic-conductivity values should be positive real numbers. Figure 4.28 presents an example hydraulic-conductivity-curve file.

Example: Figure 4.28.

4.7.7 DYNAMICS Output-Listing File

Default Name: DYNAMICS.LIS (this default could change as a TOSPAC session progresses).

Purpose: The DYNAMICS output-listing file defines the results of a transient-flow calculation in tabular form. It is used primarily to check the detailed behavior of one or more variables.

Use: The DYNAMICS output-listing file is mentioned in Section 3.1. A discussion of how to control the amount of data written to the output-listing file is given in Section 4.2.11.

NUMBER OF DATA PAIRS
 PRESSURE HEAD ($\psi \leq 0$)
 SATURATION ($0 \leq S \leq 1$)

281
 -1 1.000000
 -2 0.9999997
 -3 0.9999985
 -4 0.9999950
 -5 0.9999872
 -6 0.9999723
 -7 0.9999468
 -8 0.9999065
 -9 0.9998461
 -10 0.9997597
 -11 0.9996405
 -12 0.9994806
 -13 0.9992716
 -14 0.9990037
 -15 0.9986665
 -16 0.9982488
 -17 0.9977380
 -18 0.9971213
 -19 0.9963844
 -20 0.9955124
 -21 0.9944898
 -22 0.9933001
 -23 0.9919260
 -24 0.9903497
 -25 0.9885529
 0
 0
 0

FIRST PAIR MUST BE AT THE AIR-ENTRY PRESSURE

PAIRS MUST BE AT THE SAME PRESSURE HEADS AS GIVEN IN THE SATURATION MATERIAL-PROPERTY FILE

-850 6.0525328E-02
 -860 6.0524106E-02
 -870 6.0522955E-02
 -880 6.0521871E-02
 -890 6.0520850E-02
 -900 6.0519889E-02
 -910 6.0518980E-02
 -920 6.0518123E-02
 -930 6.0517311E-02
 -940 6.0516544E-02
 -950 6.0515821E-02
 -960 6.0515139E-02
 -970 6.0514487E-02
 -980 6.0513873E-02
 -990 6.0513288E-02
 -1000 6.0512736E-02

LAST PAIR MUST CORRESPOND TO THE RESIDUAL SATURATION

Figure 4.27: Format of the saturation-curve file.

NUMBER OF DATA PAIRS
 PRESSURE HEAD ($\psi \leq 0$)
 HYDRAULIC CONDUCTIVITY ($K \geq 0$)

281
 -1 3.1481482E-09
 -2 3.1481482E-09
 -3 3.1481482E-09
 -4 3.1481482E-09
 -5 3.1481482E-09
 -6 3.1481482E-09
 -7 3.1481482E-09
 -8 3.1481482E-09
 -9 3.1481482E-09
 -10 3.1481480E-09
 -11 3.1481476E-09
 -12 3.1481462E-09
 -13 3.1481442E-09
 -14 3.1481402E-09
 -15 3.1481320E-09
 -16 3.1481180E-09
 -17 3.1480940E-09
 -18 3.1480643E-09
 -19 3.1479899E-09
 -20 3.1478888E-09
 -21 3.1477332E-09
 -22 3.1474987E-09
 -23 3.1471619E-09
 -24 3.1466469E-09
 -25 3.1459244E-09
 o
 o
 o
 -850 7.9530629E-21
 -860 7.1058918E-21
 -870 6.3572352E-21
 -880 5.6946963E-21
 -890 5.1075535E-21
 -900 4.5865202E-21
 -910 4.1235335E-21
 -920 3.7116063E-21
 -930 3.3446286E-21
 -940 3.0172925E-21
 -950 2.7249611E-21
 -960 2.4635801E-21
 -970 2.2295997E-21
 -980 2.0199078E-21
 -990 1.8317733E-21
 -1000 1.6527950E-21

FIRST PAIR MUST BE AT THE A/R-ENTRY PRESSURE
 PAIRS MUST BE ORDERED MONOTONICALLY DECREASING
 LAST PAIR MUST BE AT RESIDUAL SATURATION

Figure 4.28: Format of the hydraulic-conductivity-curve file.

Type: Output from DYNAMICS.

Read Subroutine: None.

Create Subroutine: DINWRITE and DITWRITE.

Format: Text file.

Description: The contents of the DYNAMICS output-listing file are as follows.

First, the DYNAMICS output-listing file repeats the DYNAMICS input-data file that was used to create it; this repetition is to create an audit trail.

Next, the initial conditions of the problem are presented in three parts. The information concerning the entire column is as follows.

- 1) The average saturation of the entire column.
- 2) The total void volume of the column (the sum of the volume occupied by air and by water)
- 3) The volume of the column occupied by water.
- 4) The volume of the column occupied by air.
- 5) The mass of water in the column.

Second, the boundary conditions that were used at the initial time are given.

Third, in tabular form, the initial conditions at each mesh point are given. The number of mesh points for which values are written can be controlled in the file block of the DYNAMICS input-data file. The table columns are defined as follows:

- 1) The mesh-point number (J).
- 2) The corresponding geologic-unit number (UNIT).
- 3) The matrix-material number for the unit (MAT).
- 4) The fracture-material number for the unit (FRK).
- 5) The corresponding elevation (Z).
- 6) The computed pressure head (PRES HEAD)-- the variable for which DYNAMICS actually solves.
- 7) The calculated saturation in the composite material (SAT).
- 8) The calculated flux in the composite material (FLUX).
- 9) The calculated average linear velocity of water in the composite material (VEL).
- 10) The calculated hydraulic conductivity in the composite material (HK).
- 11) The calculated capacitance (storage capacity) of the composite material (CAP).

- 12) The calculated derivative of the saturation with respect to pressure head in the composite material (DSAT).

Following the initial conditions, the information concerning the state of the problem at each time snapshot is presented in four parts. First, a summary of the problem is presented, including the state of the entire column and the results of a mass-balance calculation.

- 1) the iteration number;
- 2) the snapshot number;
- 3) the problem time;
- 4) the length of the previous timestep;
- 5) the average saturation of the entire column;
- 6) the total void volume of the column (the sum of the volume occupied by air and by water);
- 7) the volume of the column occupied by water;
- 8) the volume of the column occupied by air;
- 9) the total mass of water in the column;
- 10) the cumulative mass of water that has entered through the top of the column;
- 11) the cumulative mass of water that has entered through the bottom of the column;
- 12) the mass of water that should be in the column (the sum of the mass that crossed the boundaries and the mass that was originally in the column);
- 13) the difference between the total mass of water in the column and the mass that should be in the column; and,
- 14) the difference expressed as a percentage of the total mass in the column (the mass balance).

Second, the boundary conditions that were used at the time snapshot are given.

Third, in tabular form, the (intermediate) results at each mesh point are given. The table form is the same as that described for the initial conditions.

Fourth, GWTT results are presented (if the GWTT calculation was specified in the input-data file). GWTT is calculated by tracking the position of water particles. The start and end positions for the calculation are given, followed by two tables. One table presents the results for the average-fastest-particle method; the other for the composite-velocity method. Both table contain the following information.

- 1) the particle number (corresponds to the snapshot number);
- 2) the time the particle was released (corresponds to the snapshot time);
- 3) the current position of the particle--or if the particle has exited the GWTT range, either by the start position or the end position, then either the start position or the end position is given;

- 4) the current time—or if the particle has exited the GWTT range, the time of exit;
- 5) the travel time—or if the particle is still in the range, a note stating STILL IN RANGE; and,
- 6) in the event of an error in the particle tracking, the word WARNING.

The travel-time tables only list released particles; i.e., particles to be released at future time snapshots are not listed.

A particle flagged with the word WARNING has an inaccurate travel time. Typically, a reverse flow has occurred, and the particle has exited the GWTT range via the start position.

Example: Figure 3.3.

4.7.8 TRANS Source File

Default Name: TRANS.SRC.

Purpose: The TRANS source file contains the data necessary to define a source term for a transport calculation. It specifies contaminant releases from the source region at given times. This file is useful for transferring data from an independent source-term computer program into TOSPAC.

Use: Use of the TRANS source file is invoked by source-term flag 3 in the source block of a TRANS input-data file, as discussed in Section 4.2.13.

Type: Input to TRANS.

Read Subroutine: READSRC.

Create Subroutine: None.

Format: Text file.

Description: The source file consists of a list of real numbers. The first number represents a time. Then, a release rate is given for each contaminant listed in the contaminant-property block. The rate is the amount of contaminant released into the source region per unit time. After the release rates, a new time and new release rates can be given. The values for time and release rate can be formatted in any fashion, but each new time must start on a new line. Any number is accepted for time; the release rates must be nonnegative real numbers.

TOSPAC linearly interpolates the release rate from one time to the next. For instance, consider that contaminant 1 has a release rate of 10 at time 0 that increases to 20 at time 2: if TRANS takes a timestep from $t = 0$ to $t = 1$, it uses a rate of 12.5 (corresponding to the middle of the timestep, $t = 0.5$).

It is recommended that the last time in the source file coincide with the final problem time. If the times given in the source file exceed the problem time, the extra data are ignored when TRANS is executed (except for the next time after the final problem time, which may be used for the linear interpolation). If the problem time is longer than the last time given in the source file, it is assumed that the last rates given are constant until the end of the problem.

The source-file format is summarized in Figure 4.29.

Example: Figure 4.29.

4.7.9 TRANS Initial-Condition File

Default Name: TRANS.CON.

Purpose: The TRANS initial-condition file defines the initial concentration data for a TRANS calculation. It is useful in solving relaxation problems; i.e., problems examining the spread of a dissolved contaminant already present in the media at the start of the problem.

Use: Use of an initial-condition file is specified through an initial-condition flag 2 in the initial-condition block of a TRANS input-data file, as discussed in Section 4.2.18.

Type: Input to TRANS.

Read Subroutine: TINTLZ.

Create Subroutine: None.

Format: Text file.

Description: The initial-condition file is formatted as a sequence of groups. Each group contains a mesh-point number and the concentrations in the matrix and in the fractures for all the species. That is, a group is of the form: $j, C_{m,j}^1, C_{f,j}^1, C_{m,j}^2, C_{f,j}^2, \dots, C_{m,j}^I, C_{f,j}^I$, where $C_{m,j}^i$ indicates the matrix concentration at mesh point j for contaminant number i , and I is the number of contaminant species for the problem. Within a group, the numbers can be formatted on lines in any fashion, but each group must start on a new line. Concentrations of contaminants at any mesh points that do not appear in the initial-condition file are assumed to be zero. Every concentration value must be nonnegative. Figure 4.30 presents an annotated example of an initial-condition file.

Example: Figure 4.30.

4.7.10 TRANS Output-Listing File

Default Name: TRANS.LIS (this default could change as a TOSPAC session progresses).

Purpose: The TRANS output-listing file defines the results of a contaminant-transport calculation in tabular form. It is used primarily to check the detailed behavior of one or more variables.

Use: The TRANS output-listing file is mentioned in Sections 2.7 and 3.2. A discussion of how to control the amount of data written to the output-listing file is given in Section 4.2.11.

Type: Output from TRANS.

Read Subroutine: None.

1060	1	18080E-07	3	68806E-01	7	62414E-04
1100	1	74400E-07	3	26308E-01	7	62319E-04
1160	2	33280E-07	4	38110E-01	1	00323E-03
1200	2	64320E-07	4	68011E-01	1	06933E-03
1260	3	66200E-07	8	66716E-01	1	70284E-03
1300	6	43200E-07	1	86903E+00	3	76208E-03
1360	7	80800E-07	1	87204E+00	3	86109E-03
1400	9	21600E-07	2	17104E+00	4	62011E-03
1460	1	02400E-06	2	11904E+00	4	62011E-03
1600	1	17120E-06	7	32706E+00	6	01613E-03
1660	1	32160E-06	2	21006E+00	4	98314E-03
1600	1	72160E-06	3	19808E+00	6	66620E-03
1660	2	08320E-06	3	43209E+00	7	26023E-03
1700	1	66760E-06	1	69007E+00	3	66318E-03
1760	1	86660E-06	2	16808E+00	4	42221E-03
1800	1	47206E-06	6	67761E-01	1	37296E-03
1860	1	26120E-06	3	76762E-01	7	47634E-04
1900	1	27660E-06	3	66263E-01	7	66834E-04
1960	1	19360E-06	1	11198E-01	2	86233E-04
2000	1	06480E-06	1	77241E-02	6	68622E-06
C						
C						
C						
40000	6	30400E-07	2	99910E-06	9	62380E-08
41000	6	27200E-07	2	93280E-06	9	33900E-08
42000	6	24000E-07	2	88470E-06	9	17400E-08
43000	6	20800E-07	2	86480E-06	9	07600E-08
44000	6	20800E-07	2	82100E-06	8	96280E-08
45000	6	17600E-07	2	77420E-06	8	86060E-08
46000	6	14400E-07	2	74040E-06	8	77140E-08
47000	6	11200E-07	2	70660E-06	8	66920E-08
48000	6	11200E-07	2	67280E-06	8	64700E-08
49000	6	08000E-07	2	63900E-06	8	43480E-08
50000	6	04800E-07	2	60620E-06	8	36660E-08
60000	6	88800E-07	2	32830E-05	7	60000E-08
70000	6	76000E-07	2	14370E-06	7	17090E-08
80000	6	69600E-07	2	00850E-05	6	84760E-08
90000	6	63200E-07	1	89020E-05	6	64960E-08
100000	6	60000E-07	1	79630E-05	6	48810E-08
200000	6	40800E-07	1	19288E-06	6	78688E-08
300000	6	37600E-07	6	46280E-06	6	60835E-08
400000	6	37600E-07	6	06426E-06	6	63113E-08
600000	6	37600E-07	4	40219E-06	6	47371E-08
600000	6	37600E-07	3	17786E-06	6	46863E-08
700000	6	37600E-07	2	29883E-06	6	41696E-08
800000	6	37600E-07	1	67041E-06	6	37696E-08
900000	6	37600E-07	1	20609E-06	6	33798E-08
1000000	6	37600E-07	8	72092E-07	6	33419E-08

Figure 4.29: Format of the TRANS source file.

Figure 4.30: Format of the 'TRANS initial-condition file.

Create Subroutine: TXFINPT, TINTLZ, TWRITE, and MSBAL.

Format: Text file.

Description: The contents of the TRANS output-listing file are as follows.

The TRANS output-listing file first repeats the TRANS input-data file that was used to create it; this repetition is to create an audit trail.

Next, the initial conditions are written. For the hydrologic quantities, the water velocities for both the matrix and the fractures, the moisture contents for both the matrix and the fractures, and the coupling factors are given at each mesh point. For the transport quantities, the matrix and fracture retardation coefficients, the matrix and fracture dispersion coefficients, and the coupling factors are given at each mesh point, for each contaminant.

The results of the TRANS run are presented next. First, the time-snapshot time is given, along with how many iterations were taken to reach the snapshot, and the timestep. Also, the boundary conditions that were defined at that snapshot are stated.

Next on the output-listing file are matrix and fracture concentration results for each contaminant. The concentration values are specified at the midpoint between selected mesh points. (Mesh points are

selected with the output-listing control number given in the file block of a TRANS input-data file, Section 4.2.11) The results are given in columns, as follows:

- 1) The cell number (CELL).
- 2) The corresponding unit number (UNIT #).
- 3) The corresponding elevation at the center of the cell (ELEV).
- 4) The concentration of the contaminant in the matrix (MATRIX CONC).
- 5) The concentration of the contaminant in the fractures (FRACTURE CONC).

Following the concentration information are data concerning the mass conservation in the computation. The number of iterations and the time are repeated, then a table of mass-related values is given, structured in columns as follows:

- 1) The number of the chain (CHAIN).
- 2) The number of the contaminant in the chain (SPECIES).
- 3) The name of the contaminant (NAME).
- 4) The mass of the contaminant in solution in the matrix (MATRIX MASS).
- 5) The mass of the contaminant in solution in the fractures (FRACTURE MASS).
- 6) The mass of the contaminant adsorbed onto the matrix (ADSORBED MASS).
- 7) The mass of the contaminant precipitated out of solution (PRECIP MASS).
- 8) The mass of the contaminant in the source (SOURCE MASS).
- 9) The mass of contaminant entering through the top boundary (T BDRY MASS).
- 10) The mass of contaminant entering through the bottom boundary (B BDRY MASS).
- 11) The total mass of contaminant in the mesh, plus the amount that has passed out through the boundaries, calculated by summing the values in columns 4 through 7, plus the values in columns 9 and 10 *if they are negative* (MASS IN MESH + MASS RELEASED).
- 12) The total mass that has been injected into the mesh, adjusted by exponential (Bateman) decay, if applicable. This amount includes any initial-condition mass, the mass that has been removed from the source inventory, and any injection through the boundaries—columns 9 and 10 *if positive*—(MASS INJECTED INTO MESH).
- 13) The percent difference between the values in columns 11 and 12; i.e., the mass balance (PERCENT DIFF).

The final group of results is the amount of mass released at each time snapshot. Results are given for each contaminant with the information organized in columns, as follows:

- 1) The number of the chain (CHAIN).

- 2) The number of the contaminant in the chain (SPECIES).
- 3) The name the contaminant (NAME).
- 4) The actual mass of the contaminant outside the top boundary, with exponential (Bateman) decay taken into account, if applicable (TOP TOTAL).
- 5) The cumulative mass of the contaminant that passed out the top boundary; i.e., no decay (TOP CUMULATIVE).
- 6) The actual mass of the contaminant outside the bottom boundary, with exponential (Bateman) decay taken into account, if applicable (BOTTOM TOTAL).
- 7) The cumulative mass of the contaminant that passed out the bottom boundary; i.e., no decay (BOTTOM CUMULATIVE).

Example: Figures 2.6 and 3.23.

4.7.11 TRANS Plot-Data File

Default Name: TRANS.PLT (this default could change as a TOSPAC session progresses).

Purpose: The TRANS plot-data file stores the input data for, and the results from, a transport calculation. It is used by OUTPLOT for plotting contaminant-transport results.

Use: Creation of the TRANS plot-data file is mentioned in Sections 2.7, 3.2, and 4.2.11; its use by the OUTPLOT module is discussed in Sections 2.8, 3.2, and 4.6.

Type: Output file in TRANS; input file for OUTPLOT.

Read Subroutine: TINIT and TDATA.

Create Subroutine: TXTINPT, TINTLZ, and TWRITE.

Format: Binary file.

Description: To describe this file, the FORTRAN statements used to create it are presented below. In the following listings, TPLTFL is the variable that contains the FORTRAN logical-unit number for the TRANS plot-data file.

First, in subroutine TXTINPT, title data and other input data are written:

```
WRITE(TPLTFL) NTITLE
WRITE(TPLTFL) (TITLE(N),N=1,NTITLE)
WRITE(TPLTFL) NUMSPC
WRITE(TPLTFL) (NCHN(I),NSPEC(I),
*   ACTIVITY(I),ELIMIT(I),I=1,NUMSPC)
```

where the variables and the quantities they represent are as follows:

- 1) NHTITLE (integer) is the number of titles that are in the TRANS input-data file;
- 2) HTITLE (character*80) is an array that holds the titles from the TRANS input-data file (the problem title, the names of the geologic units, and the names of the contaminants);
- 3) NUMSPC (integer) is the number of contaminants;
- 4) NCHN (integer) is an array that tells in which chain each contaminant belongs;
- 5) NSPEC (integer) is an array that tells the ordinal position in its chain of each contaminant;
- 6) ACTIVITY (double precision) is an array containing the activity for each contaminant; and
- 7) ELIMIT (double precision) is an array containing the EPA limit for each contaminant.

Next, in subroutine TINTLZ, data concerning the initial state of the problem are written:

```

WRITE(TPLTFL) NHTITLE
WRITE(TPLTFL) (HTITLE(I), I=1, NHTITLE)
WRITE(TPLTFL) TCONVERT, ICONVERT, TMSG
WRITE(TPLTFL) JMIN, JMAX, NUNITS, NMAT, JMINs, JMAXs, NDUMP, AREP
WRITE(TPLTFL) (TDUMP(K), K=1, NDUMP)
WRITE(TPLTFL) (THM(J), THF(J), J=JMIN+1, JMAX),
*   (VELM(J), VELF(J), J=JMIN+1, JMAX),
*   (RATE1(J), J=JMIN+1, JMAX)
WRITE(TPLTFL) ((RATE2(J, I), J=JMIN+1, JMAX), I=1, NUMSPC),
*   ((RETARDM(J, I), RETARDF(J, I), J=JMIN+1, JMAX), I=1, NUMSPC),
*   ((DISPM(J, I), DISPF(J, I), J=JMIN+1, JMAX), I=1, NUMSPC)
WRITE(TPLTFL) (NOUNIT(J), J=JMIN, JMAX), (Z(J), J=JMIN, JMAX)

```

where the variables are as follows:

- 1) TCONVERT, ICONVERT, TMSG, JMIN, JMAX, NUNITS, NMAT, NDUMP, TDUMP, NOUNIT, and Z have the same meaning as in the STEADY and DYNAMICS plot-data files (Section 4.7.4);
- 2) NHTITLE (integer) is the number of titles that are in the STEADY plot-data file that TRANS has read;
- 3) HTITLE (character*80) is an array that holds the titles from the STEADY plot-data file (the problem title, the names of the geologic units, and the names of the materials);
- 4) JMINs (integer) is the mesh-point number for the lower boundary of an internal source region;
- 5) JMAXs (integer) is the mesh-point number for the upper boundary of an internal source region (note that for an external source, JMINs = JMAXs = JMAX);
- 6) AREP (double precision) is the area of the repository;
- 7) THM (double precision) is an array containing the moisture content in the matrix at every mesh point;
- 8) THF (double precision) is an array containing the moisture content in the fractures at every mesh point;

- 9) VELM (double precision) is an array containing the average linear velocity of water in the matrix at every mesh point;
- 10) VELF (double precision) is an array containing the average linear velocity of water in the fractures at every mesh point;
- 11) RATE1 (double precision) is the advective coupling coefficient at every mesh point;
- 12) RATE2 (double precision) is the diffusive coupling coefficient for each contaminant at every mesh point;
- 13) RETARDM (double precision) is the retardation factor of the matrix for each contaminant at every mesh point;
- 14) RETARDF (double precision) is the retardation factor of the fractures for each contaminant at every mesh point;
- 15) DISPM (double precision) is the dispersion coefficient of the matrix for each contaminant at every mesh point; and
- 16) DISPF (double precision) is the dispersion coefficient of the fractures for each contaminant at every mesh point.

And finally, for every time snapshot listed in the TRANS input-data file that was used to solve the problem, subroutine TWRITE writes iteration, time, concentration, release, and boundary-condition data:

```

WRITE(TPLTFL) IT,TIME,DT
DO 570 I=1,NUMSPC
  WRITE(TPLTFL) (CONCM(J,I),CONCF(J,I),J=JMIN+1,JMAX)
  WRITE(TPLTFL) RTAM(I),RTAF(I),RBAM(I),RBAF(I),
*   RTCM(I),RTCF(I),RBCM(I),RBCF(I),
*   FLUXTM(I),FLUXTF(I),FLUXBM(I),FLUXBF(I)
570 CONTINUE

```

where the variables are as follows:

- 1) IT, TIME, and DT are the same as in the STEADY and DYNAMICS plot-data files (Section 4.7.4);
- 2) CONCM (double precision) is the two-dimensional array containing the concentration in the matrix of each contaminant at every mesh point;
- 3) CONCF (double precision) is the two-dimensional array containing the concentration in the fractures;
- 4) RTAM (double precision) is the actual release through the matrix at the top boundary for each contaminant;
- 5) RTAF (double precision) is the actual release through the fractures at the top boundary for each contaminant;

- 6) RBAM (double precision) is the actual release through the matrix at the bottom boundary for each contaminant;
- 7) RBAF (double precision) is the actual release through the fractures at the bottom boundary for each contaminant;
- 8) RTCM (double precision) is the cumulative release through the matrix at the top boundary for each contaminant;
- 9) RTCF (double precision) is the cumulative release through the fractures at the top boundary for each contaminant;
- 10) RBCM (double precision) is the cumulative release through the matrix at the bottom boundary for each contaminant;
- 11) RBCF (double precision) is the cumulative release through the fractures at the bottom boundary for each contaminant;
- 12) FLUXTM (double precision) is the calculated contaminant flux through the matrix at the top boundary for each contaminant;
- 13) FLUXTF (double precision) is the contaminant flux through the fractures at the top boundary for each contaminant;
- 14) FLUXBM (double precision) is the contaminant flux through the matrix at the bottom boundary for each contaminant; and
- 15) FLUXBF (double precision) is the contaminant flux through the fractures at the bottom boundary for each contaminant.

Example: None.

4.7.12 OUTPLOT Plot-Definition File

Default Name: OUTPLOT.PDF (this default could change as a TOSPAC session progresses).

Purpose: The OUTPLOT plot-definition file contains the definitions of the plots for production of computer-graphics output for TOSPAC results. The plot-definition file allows plots to be re-created. It also allows development of a generic package of plot definitions that can be used simply and quickly to get a set of plots for any TOSPAC results.

Use: The plot-definition file is mentioned in Sections 2.8, 3.1, 3.2, and 4.6.

Type: Input to and output by OUTPLOT.

Read Subroutine: Various subroutines in OUTPLOT.

Create Subroutine: Various subroutines in OUTPLOT.

Format: Text file.

Description: OUTPLOT plot-definition files are organized in three levels:

PLOT SECTION,
PLOT BLOCK, and
DATA LINE.

Plot sections are an upper-level division of plot-definition files. There are three types of plot sections, corresponding to the three calculational modules of TOSPAC: STEADY, DYNAMICS, and TRANS. The GRAPHDRV subroutine reads the plot-definition file until it comes to a section designator and then transfers control to subroutine SPLOT, DPLOT, or TPLOT, depending on the type of section encountered. TOSPAC recognizes the beginning of a plot section by a line containing one of the following sets of keywords:

STEADY PLOT SECTION,
DYNAMICS PLOT SECTION, or
TRANS PLOT SECTION.

As with input-data files, all keywords words in plot-definition files can be written in any combination of upper or lower case.

Once OUTPLOT has determined a section, it looks for a plot-block designator. Control is then passed to one of several subroutines, where the block is read and the appropriate plot(s) produced. A plot block contains detailed instructions that specify the desired plot (e.g., log or linear axes, limits on the axes, which species to plot, various labels to use, etc.).

Every time a plot-block designator appears in a plot-definition file, at least one plot will be made (except for the plot-file block and the problem-title block). If only the plot-block designator appears, i.e., no data lines following it, default values are assumed for all parameters.

A list of acceptable plot blocks follows. Plot-block designators are shown in upper case. When plot-block designators are used in a plot definition file, they must be used exactly as shown (although they can be in combination of upper or lower case characters, and of course the colon can be omitted).

PLOT FILE BLOCK: to name one or more plot-data files for a STEADY section, or a single plot-data file for DYNAMICS or TRANS sections;

PROBLEM-TITLE BLOCK: to set a new problem title for a plot, if a title other than the default title is desired. The new title remains in effect until another problem-title block is encountered or a new plot section starts. A blank title line has the effect of reinstating the default title.

MESH PLOT BLOCK: to plot mesh and stratigraphy setups (applies to STEADY and DYNAMICS sections);

CHARACTERISTIC-CURVE PLOT BLOCK: to plot saturation versus pressure head and hydraulic conductivity versus pressure head for material(s) assigned to the problem (applies to STEADY and DYNAMICS sections);

COMPOSITE-CONDUCTIVITY PLOT BLOCK: to plot composite hydraulic conductivity versus pressure head for geologic unit(s) in the problem (applies to STEADY and DYNAMICS sections);

COMPOSITE-CAPACITANCE PLOT BLOCK: to plot composite capacitance versus pressure head for geologic unit(s) in the problem (applies to STEADY and DYNAMICS sections);

PRESSURE-HEAD PLOT BLOCK: to plot pressure head versus elevation (applies to STEADY and DYNAMICS sections);

SATURATION PLOT BLOCK: to plot saturation versus elevation (applies to STEADY and DYNAMICS sections);

VELOCITY PLOT BLOCK: to plot water velocity versus elevation (applies to STEADY, DYNAMICS, and TRANS sections);

FLUX PLOT BLOCK: to plot water flux versus elevation (applies to STEADY and DYNAMICS sections);

NORMALIZED-FLUX PLOT BLOCK: to plot normalized composite flux versus elevation. (applies to STEADY and DYNAMICS sections);

CONDUCTIVITY PLOT BLOCK: to plot hydraulic conductivity versus elevation, (applies to STEADY and DYNAMICS sections);

CAPACITANCE PLOT BLOCK: to plot capacitance versus elevation (applies to STEADY and DYNAMICS sections);

TRAVEL-TIME PLOT BLOCK: to plot water travel times between two specified points (applies to STEADY sections only);

AVERAGE-SATURATION PLOT BLOCK: to plot saturation versus time (applies to DYNAMICS sections only);

WATER-MASS PLOT BLOCK: to plot mass versus time (applies to DYNAMICS sections only);

MOISTURE PLOT BLOCK: to plot moisture content versus elevation (applies to TRANS sections only);

RETARDATION PLOT BLOCK: to plot retardation factors versus elevation (applies to TRANS sections only);

DISPERSION PLOT BLOCK: to plot dispersion coefficients versus elevation (applies to TRANS sections only);

COUPLING PLOT BLOCK: to plot matrix/fracture coupling versus elevation (applies to TRANS sections only);

CVST PLOT BLOCK: to plot concentration versus time (applies to TRANS sections only);

CVSE PLOT BLOCK: to plot concentration versus elevation (applies to TRANS sections only);

3-D PLOT BLOCK: to plot concentration versus time and elevation (applies to TRANS sections only); and

RELEASE PLOT BLOCK: to plot release versus time (applies to TRANS sections only).

Data lines are lines of data within a plot-data block. Data lines have the following format:

- 1) zero or more spaces or tabs,

- 2) a data-line keyword (see below),
- 3) a delimiter,
- 4) one or more arguments (depending on the keyword, discussed below) each separated by a delimiter,
- 5) and, optionally, another delimiter followed by a comment string.

Acceptable delimiters are spaces, tabs, or commas.

The following is a description of the data-line keywords used within the blocks. When keywords are used, they must be spelled exactly as presented (although, any combination of upper and lower case is acceptable, and the colon must *not* be present). Not all keywords are valid in every plot block

XLIMITS: sets limits on X-axis; should be followed by two numbers, the minimum and maximum. If the word **DEFAULT** is used in place of one of the numbers, that means to autoscale (i.e., use the minimum or maximum of the plotted data). In the plot blocks, the X-axis always refers to the *independent variable*—either elevation, time, or pressure head, depending on the plot type.

YLIMITS: same as **XLIMITS**, but for Y-axis.

ZLIMITS: same as **XLIMITS**, but for Z axis.

XAXIS: sets type of axis. Should be followed by **LIN** or **LINEAR** for a linear X-axis, **LOG** or **LOGARITHMIC** for a log X-axis, **NEGLOG** for a log plot of negative data.

YAXIS: same as **XAXIS**, but for Y-axis.

XUNITS: sets the units on the X-axis; could be used if *SI* units are not used for the input data. For example, if data are entered in ft-lb-s units, to get an elevation axis labeled in ft instead of the default m, use **XUNITS ft**.

YUNITS: same as **XUNITS**, but for Y-axis.

ZUNITS: same as **XUNITS**, but for Z axis.

XFACTOR: sets conversion factor for X-axis; could be used if it were desired to plot data using different units than the input units. For example, if mks units were used for input but elevations in cm were desired on a plot, the following commands would be given: **XUNITS cm**, **XFACTOR 100**. Note that this procedure is not necessary for time axes if a time-conversion was specified in the input file. That is, if mks units are used for input, but a time-conversion factor is specified so that snapshot times are entered in years, then the default for time axes will be years. Then, it would be necessary to specify **XUNITS** and **XFACTOR** if units other than years were desired.

YFACTOR: same as **XFACTOR**, but for Y-axis.

ZFACTOR: same as **XFACTOR**, but for Z axis.

LEGEND: sets position of legend in two-dimensional plot. Followed by: **NONE** for no legend; **OUT** or **OUTSIDE** to put the legend to the right of the plot (only valid in landscape orientation); or two numbers, giving the X and Y coordinates of the bottom left corner of the legend, in centimeters. X entry may also be **LEFT**, **CENTER**, or **RIGHT**; Y entry may also be **TOP**, **CENTER**, or **BOTTOM**.

LABEL: specify a legend entry. Whatever follows is used in the legend, if one is specified. Labels can only be entered after **SNAPSHOT**, **ELEVATION**, or **FILE** commands.

ORIENT or **ORIENTATION:** sets plot orientation; followed by **LANDSCAPE** (longer direction horizontal) or **PORTRAIT** (longer direction vertical). Plot orientation can only be specified when some quantity is being plotted against elevation.

MODE: sets plotting mode. Followed by **MULTI** or **MULTIPLE** if several curves (could be several species or several snapshots or several different **STEADY** runs, depending on the type of plot) are to be drawn on the same plot; **SINGLE** for the opposite—one species or one snapshot or one **STEADY** run per plot.

PLOTTYPE: chooses among different quantities that can be plotted. The choices that can follow **PLOTTYPE** depend on the type of plot. The following appear in various places: **MATRIX** to plot matrix quantities, **FRACTURE** to plot fracture quantities, **COMPOSITE** to plot composite quantities, **ADVECTIVE** to plot advective coupling rates, **DISPERSIVE** to plot dispersive coupling rates, **ACTUAL** to plot the amount of contaminant actually outside the computational mesh in a release plot, **CUMULATIVE** to plot the sum of the amounts crossing the boundary of the computational mesh in a release plot, **RATE** to plot the rate at which waste reaches the boundary in a release plot. **ALL** (and in some cases **BOTH**) is used to plot all quantities (e.g., **MATRIX** and **FRACTURE**, if those are the possibilities for a particular type of plot).

FILE: specifies which **STEADY** file to plot. Followed by a number identifying the file. For example, if the plot-file block lists the files **FILE1.DAT**, **FILE2.DAT**, and **FILE3.DAT**, in that order, then **FILE 2** would specify that plot data be taken from **FILE2.DAT**. **ALL** can be written instead of a number, to specify that all listed files should be used.

SNAPSHOT: specifies a snapshot to be plotted. Followed by the snapshot number. **ALL** can be written instead of a number, to specify that all snapshots should be plotted.

SPECIES: specifies a species to be plotted. Can be followed by either the species name (e.g., *SPECIES U-236*) or the species number (e.g., *SPECIES 3*). **ALL** can also be used, to specify that all species should be plotted.

ELEV or **ELEVATION:** specifies an elevation at which to plot concentration versus time. Followed by the elevation, in whatever units were used when specifying the calculational mesh. There are two special designations: **SOURCE** to plot concentration at a point in the middle of the source region, **MAX** or **MAXIMUM** to plot the maximum concentration in the entire mesh as a function of time.

BOUNDARY: for a release plot, specifies at which boundary releases are to be plotted. Followed by **TOP** to plot releases from top boundary, **BOTTOM** to plot releases from bottom boundary, **BOTH** or **ALL** to plot the sum of the releases from both boundaries.

RELEASE: for a release plot, specifies the type of release—**MASS** to plot release in terms of mass, **RADIOACTIVITY** or **RAD** to plot release in terms of radioactivity, **EPA RATIO** or **EPA** to plot release in terms of EPA ratio.

VIEW: for a three-dimensional plot, specifies the viewpoint. Followed by three numbers: the polar coordinates of the viewpoint—distance (in centimeters), polar angle, and azimuthal angle. If the word **DEFAULT** is used in place of one of the numbers, that means to use the default value for that number. The defaults are 125,75,340.

NUMX: for a three-dimensional plot, specifies the approximate number of time lines to draw. Followed by a number or the word **ALL** or the word **DEFAULT**. **DEFAULT** is equivalent to **ALL**.

NUMY: for a three-dimensional plot, specifies the approximate number of elevation lines to draw. Followed by a number or the word ALL or the word DEFAULT. DEFAULT is equivalent to the number 100.

BOX: for a mesh/stratigraphy plot, specifies the number of mesh points included in a "box" in the mesh-point column. Followed by a number or the word DEFAULT. DEFAULT is variable, depending on the total number of mesh points.

NUMBER: for a mesh/stratigraphy plot, specifies the size of the increment between the numeric mesh-point indicators in the mesh-point column. Followed by a number or the word DEFAULT. DEFAULT is variable, depending on the total number of mesh points.

MATERIAL: specifies the material for which a characteristic-curve plot is to be made. Can be followed by either the material name (e.g., *MATERIAL SANDSTONE*) or the material number (e.g., *MATERIAL 1*). ALL or DEFAULT can also be used, to specify that all materials should be plotted.

UNIT: for a plot of composite hydraulic conductivity or composite capacitance, specifies the geologic unit for which these variables are to be plotted. Can be followed by either the geologic-unit name (e.g., *UNIT TSw2*) or the geologic-unit number (e.g., *UNIT 2*). ALL or DEFAULT can also be used, to specify that the conductivity and capacitance curves for all units should be plotted.

Arguments for the above keywords are of two types: numeric and character. Numeric arguments are numbers (integer or real) in any FORTRAN-recognizable format. Character arguments are titles, names, units, labels, names of files, and special words, such as ALL, DEFAULT, NONE, etc. Character arguments are arbitrary strings of characters up to 80 characters long which do not include delimiters. If the character data begins with a space or tab, this character is stripped off before TOSPAC uses the data. The vertical-bar character (|) is a special character in titles and names: it can be inserted within the titles and names to force OUTPLOT to make a line break at that position when computer graphics are produced. The vertical bar is removed when the character string is used.

When OUTPLOT creates a plot-definition file, OUTPLOT includes comments that describe the various data elements. Unlike an input-data file, the plot-definition file does not accept units after data values, unless they occur in the comment section of a data line, or unless the datum expressly calls for units.

It is acceptable for the user to circumvent OUTPLOT and create or modify plot-definition files with his or her computer system's text editor. The user can then create or modify plot-definition files without the comments, or with the user's own comments. Although the data can be entered almost in free format, four rules must be followed:

- 1) at least one section designator (see above) must be present;
- 2) at least one plot-block designator (see above) must be present;
- 3) each plot block can contain zero or more data lines; and
- 4) a data line can contain at most one keyword, followed by the appropriate number of arguments (with delimiters), followed by a comment if desired.

A block terminator (a blank line) *must* follow each plot block.

Figure 4.31 shows an example of the OUTPLOT plot-definition file used in Chapter 2 in a minimized form, created on a text editor. Compare this figure with Figure 2.12.

Example: Figures 2.12, 3.16, 3.46, and 4.31.

4.7.13 OUTPLOT Graphics-Driver File

Default Name: OUTPLOT.DRV (this default could change as a TOSPAC session progresses).

Purpose: The OUTPLOT graphics-driver file contains intermediate-stage computer graphics information in unformatted (binary) form, created by the DISSPLA graphics package. This file must be submitted to a graphics device for hardcopy (or film or fiche) output of TOSPAC plots.

Use: The graphics-driver file is created when choice 4 from the OUTPLOT main menu is selected, as discussed in Section 4.6.

Type: Output from OUTPLOT.

Read Subroutine: None.

Create Subroutine: Various subroutines in OUTPLOT.

Format: Binary file.

Description: The graphics-driver file varies in format and contents from one graphics device to another. It should not be inspected or modified by the user.

Example: None.

```
steady plot section

mesh plot block
xaxis lin
xlimits default,default
box default
number default

velocity plot block
plottype matrix
mode single
orient portrait
xaxis lin
yaxis neglog
xlimits default,default
ylimits default,default
legend none

trans plot section

release plot block
plottype both
mode single
release mass
boundary bottom
xaxis lin
yaxis log
xlimits default,default
ylimits default,default
species all
legend default

3-d plot block
plottype matrix
view default,default,default
xlimits default,default
ylimits default,default
zlimits default,default
species all
numy default
numx default

cvse plot block
plottype matrix
mode multi
orient portrait
xaxis lin
yaxis lin
xlimits default,default
ylimits default,default
species all
snapshot 1
snapshot 2
snapshot 4
snapshot 7
snapshot 12
snapshot 17
snapshot 18
snapshot 20
snapshot 23
snapshot 28
snapshot 33
legend right,bottom
```

Figure 4.31: OUTPLOT plot-definition file created by a text editor, containing the same data as the plot-definition file shown in Figure 2.12.

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Appendix A

BATCH EXECUTION

TOSPAC can be executed in the batch mode on most computer systems. The user is required to create a command file (also known as a procedure file) that tells the computer system the information it needs during TOSPAC execution. This information is the same as the information needed during TOSPAC execution in the interactive mode. The command file is then submitted to the computer's batch-job queue.

Batch execution of TOSPAC modules STEADY, DYNAMICS, and TRANS can be helpful. These calculational modules can take a long time to run—especially DYNAMICS—and they require little user interaction. The data-entry modules, INDATA and OUTPLOT, typically require a great deal of user interaction, and therefore would require complex command files for batch execution. Command files for INDATA or OUTPLOT data entry could take longer to create than the amount of time needed for an interactive session. The OUTPLOT graphics-driver submodule, however, can be run in batch mode if a pre-existing plot-definition file is used.

The remainder of this appendix gives listings of command files that can be used to run TOSPAC on the three example problems contained in this User's Guide. These command files are created for execution on a DEC VAX computer system using the VAX/VMS operating system (DEC, 1988). The files would have to be modified for execution on other computer systems. It is assumed that the input files have been created and are named as follows:

STEADY.DAT: the STEADY input-data file for the simplified mill-tailings problem from Chapter 2, shown in Figure 2.3;

TRANS.DAT: the TRANS input-data file for the simplified mill-tailings problem from Chapter 2, shown in Figure 2.4;

OUTPLOT.PDF: the OUTPLOT plot-definition file for the simplified mill-tailings problem from Chapter 2, shown in Figure 2.12;

DYNAMICS.DAT: the DYNAMICS input-data file for the simulation of the laboratory imbibition experiment from Section 3.1, shown in Figure 3.2;

EX2OUTPLOT.PDF: the OUTPLOT plot-definition file for the simulation of the laboratory imbibition experiment from Section 3.1, shown in Figure 3.16;

EX3STEADY.DAT: the STEADY input-data file for the simulation of a high-level-radioactive-waste repository in tuff from Section 3.2, shown in Figure 3.20; and

EX3TRANS.DAT: the TRANS input-data file for the simulation of a high-level-radioactive-waste repository in tuff from Section 3.2, shown in Figure 3.21.

EX3OUTPLOT.PDF: the OUTPLOT plot-definition file for the simulation of a high-level-radioactive-waste repository in tuff from Section 3.2, shown in Figure 3.46.

Note that names for the output files can be given in the command procedure if the input-data file has no file block. However, all three examples shown here assume that the input-data file contains a file block with the appropriate file names. In the first example, the plot-data file names are entered in the OUTPLOT part of the command procedure because the plot-definition file in Figure 2.12 does not have a plot-file block.

The command file for the simplified mill-tailings problem from Chapter 2 follows. The comments are marked with an exclamation point (!). Comments are optional. The exclamation point is required by VAX VMS as a comment delimiter; it is not required on the lines that are read by TOSPAC.

```
!
! A command file to execute the simplified mill-tailings problem.
! (Everything on a line after an exclamation point is a comment.)
!
$ RUN TOSPAC      ! execute TOSPAC
2                ! choice 2 from the TOSPAC main menu -- execute STEADY
STEADY.DAT       ! the name of the STEADY input-data file
4                ! choice 4 from the TOSPAC main menu -- execute TRANS
TRANS.DAT        ! the name of the TRANS input-data file
5                ! choice 5 from the TOSPAC main menu -- execute OUTPLOT
OUTPLOT.PDF      ! the name of the OUTPLOT plot-definition file
4                ! choice 4 from the OUTPLOT main menu -- create plots
OUTPLOT.DRV      ! the name of the OUTPLOT graphics-driver file
STEADY.PLT       ! the name of the STEADY plot-data file
NONE             ! there is only one STEADY plot-data file
TRANS.PLT        ! the name of the TRANS plot-data file
0                ! choice 0 from the OUTPLOT main menu -- return to main menu
0                ! choice 0 from the TOSPAC main menu -- STOP
$ IMPRINT/IMPRESS OUTPLOT.DRV ! submit the graphics file to the printer
```

On a DEC VAX computer system, a command file is submitted to the batch job queue using the SUBMIT command. For example, if the command file were named EX1.COM, a submit command could be as follows:

```
$ SUBMIT/NOPRINT EX1.COM
```

where the NOPRINT qualifier specifies that the log file should be placed in the user's file space and not printed. After the batch job is completed, the output files will reside in the user's file space.

The last command in the command file—the one to submit the graphics-driver file to the printer—may vary from installation to installation. With the above command file, the problem could be submitted to run overnight and the plots would be waiting in the morning.

The command file for the laboratory imbibition experiment problem from Section 3.1 is as follows:

```
!
! A command file to execute the simulation of the laboratory
! imbibition experiment.
!
$ RUN TOSPAC      ! execute TOSPAC
3                ! choice 3 from the TOSPAC main menu -- execute DYNAMICS
DYNAMICS.DAT     ! the name of the DYNAMICS input-data file
5                ! choice 5 from the TOSPAC main menu -- execute OUTPLOT
EX2OUTPLOT.PDF   ! the name of the OUTPLOT plot-definition file
4                ! choice 4 from the OUTPLOT main menu -- create plots
EX2OUTPLOT.DRV   ! the name of the OUTPLOT graphics-driver file
0                ! choice 0 from the OUTPLOT main menu -- return to main menu
0                ! choice 0 from the TOSPAC main menu -- STOP
$ IMPRINT/IMPRESS EX2OUTPLOT.DRV ! submit the graphics file to the printer
```

The command file for the potential waste repository problem from Section 3.2 is as follows:

```
!
! A command file to execute the simulation of a potential
! waste repository in stratified tuff.
!
$ RUN TOSPAC      ! execute TOSPAC
2                ! choice 2 from the TOSPAC main menu -- execute STEADY
EX3STEADY.DAT    ! the name of the STEADY input-data file
4                ! choice 4 from the TOSPAC main menu -- execute TRANS
EX3TRANS.DAT     ! the name of the TRANS input-data file
5                ! choice 5 from the TOSPAC main menu -- execute OUTPLOT
EX3OUTPLOT.PDF   ! the name of the OUTPLOT plot-definition file
4                ! choice 4 from the OUTPLOT main menu -- create plots
EX3OUTPLOT.DRV   ! the name of the OUTPLOT graphics-driver file
0                ! choice 0 from the OUTPLOT main menu -- return to main menu
0                ! choice 0 from the TOSPAC main menu -- STOP
$ IMPRINT/IMPRESS EX3OUTPLOT.DRV ! submit the graphics file to the printer
```


Appendix B

DATA RELEVANT TO THE REFERENCE INFORMATION BASE

B.1 Information from the Reference Information Base Used in this Report:

This report contains no information from the Reference Information Base.

B.2 Candidate Information for the Reference Information Base:

This report contains no candidate information for the Reference Information Base.

B.3 Candidate Information for the Site and Engineering Properties Data Base:

This report contains no candidate information for the Site and Engineering Properties Data Base.

Appendix C

REQUIREMENTS FOR SOFTWARE DOCUMENTATION

At the time this User's Guide is written, acceptable software documentation to meet anticipated quality-assurance requirements must include the following (Sandia National Laboratories, Yucca Mountain Site Characterization Project, Quality Assurance Implementing Procedure QAIP 3-2, Rev. 01, 17 October 1991):

- software requirements specification,
- software design documentation,
- description of mathematical models and numerical methods used,
- user's manual,
- program listing,
- verification and validation documentation, and
- program modification and change records.

The requirements that TOSPAC was designed to meet, and the top-level-design decisions to address those requirements, are given in Chapter 1 of this User's Guide. TOSPAC was intended to be an analysis tool, and analysis software is unlike industrial software—spreadsheet, payroll, inventory, machine operation, etc. In industrial software, the tasks are well-defined and the algorithms for performing the tasks are known. TOSPAC was intended to investigate a physical regime that is not completely understood. As TOSPAC was being developed, the calculational difficulties associated with the physical regime were unknown. Therefore, design decisions and requirements evolved together.

Requirements consist of defining the function and scope of a computer program, as well as environmental concerns, such as how users will operate the program and on what computer systems it will execute. Section 1.3, Background, contains a discussion of the performance requirements and the performance attributes, including portability, calculational speed and correctness, and the facility of

use and the response time of the user interface. Section 1.5, Capabilities, and Section 1.6, Limitations and Assumptions, contain discussions of the functional requirements.

Top-level design consists of decisions that restrict how a computer program meets the requirements. For TOSPAC, top-level-design decisions include the use of modules, including the three basic calculational modules; the implementation of Darcy's Law, Richards' Equation, and the general advection-dispersion equation; and the restriction to one dimension. Section 1.3, Background, contains a discussion of the decision to use a high-level computer language. Section 1.4, Technical Overview, contains a discussion of the major physical and mathematical models used in TOSPAC and how the program structure follows these choices. Various simplifications in the models used in TOSPAC are discussed in Section 1.5, Capabilities, and Section 1.6, Limitations and Assumptions.

This User's Guide was written in parallel with the development of TOSPAC. Chapter 4 of this User's Guide, General Reference, represents the user-interface design specification for TOSPAC Version 1. That is, TOSPAC Version 1 shall operate as described in Chapter 4.

Both the mathematical models and the numerical methods used in TOSPAC Version 1 are discussed in *Volume 1*. Included are discussions of the purpose, the assumptions and limitations, and the derivation. Chapter 2 of *Volume 1* contains a description of the groundwater-flow model and the composite-porosity model of the flow media. Chapter 3 of *Volume 1* is devoted to describing the contaminant-transport model, including the submodels for source term, matrix diffusion, dispersion, radioactive decay, etc. Both chapters offer example problems that show the overall performance of the models and methods. The example problems in Chapters 2 and 3 of this User's Guide, *Volume 2*, supplement that discussion.

This User's Guide is both the user's manual and the reference manual for TOSPAC Version 1. Chapter 4, General Reference, contains top-level flow diagrams, descriptions of the input data (Sections 4.2 and 4.6) and the format of the input data (Section 4.7), and descriptions of the output data (Sections 4.6 and 4.7). Chapters 2 and 3 offer sample problems. System requirements are discussed in Chapter 1 and Section 4.6.

A listing of the source code for TOSPAC Version 1 is contained in the Sandia National Laboratories (SNL), Yucca Mountain Site Characterization Project (YMP), Software Configuration Management System.

Verification and validation documentation, other than that mentioned in Section 1.8, Applications, is incomplete. Either another volume will be added to the TOSPAC documentation, or verification and validation will be addressed by each analysis that uses TOSPAC as a tool.

TOSPAC Version 1 has been admitted to the SNL YMP Software Configuration Management System and Records Management System. A complete record of all documentation, versions, and modifications is maintained by this system.

A version number is shown in the TOSPAC main menu. This number is assigned by the SNL YMP Software Configuration Management System. This User Guide should, for the most part, apply to all TOSPAC versions 1.

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