

SAND81-1504

SWIFT/SSP Self-Teaching Curriculum

Margaret S. Chu
Nancy C. Finley
Mark Reeves*
Sandia National Laboratories
Albuquerque, New Mexico 87185

Manuscript Submitted: September 1981

Sandia National Laboratories
Albuquerque, New Mexico 87185
operated by
Sandia Corporation
for the
U.S. Department of Energy

Prepared for
Division of Waste Management
Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
Under Memorandum of Understanding DOE 40-550-75
NRC FIN No. A-1158

*INTERA Environmental Consultants

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights.

ABSTRACT

The purpose of this manual is to assist new users of SWIFT/SSP computer code. SWIFT/SSP is a specialization of SWIFT computer code which is a fully transient, three-dimensional model describing transport in geologic media. In the SWIFT/SSP version, only steady-state fluid flow and transient trace-species migration are considered in order to achieve computer efficiency for what has been found to be a relatively large class of applications. The teaching method in this manual is based on seven problems. All of these problems have been used in the SWIFT Self-Teaching Curriculum, and the numbering used there has been retained herein to facilitate cross comparison. The Office of Research at NRC is releasing for public use a copy of the more complex SWIFT code during late 1981. The SWIFT/SSP version most probably will not be released at the same time. This curriculum and the SWIFT/SSP User's Manual (SAND81-2047) will provide a record of this work under NRC FIN No. A-1158 until such time that a public version of this code is released.

CONTENTS

<u>Chapter</u>		<u>Page</u>
1	INTRODUCTION	1
	1.1 Brief Description of SWIFT	1
	1.2 Purpose of the Self-Teaching Curriculum	2
2	PHYSICAL SETTING	3
	2.1 The Reference Site	3
	2.2 Hydrology	4
	2.3 System Dimensions	12
3	SAMPLE PROBLEMS	16
	3.1 PROBLEM 1	16
	I-D Flow with Aquifer-Influence Boundary Conditions	
	3.2 PROBLEM 2	25
	I-D Flow with Pressure-Limited Well Boundary Conditions	
	3.3 PROBLEM 3	30
	I-D Transport of a Decaying Radionuclide	
	3.4 PROBLEM 4	38
	2-D Flow for a Reference Bedded-Salt Depository Site	
	3.5 PROBLEM 5	47
	2-D Near-Field Transport from a Bedded-Salt Reference Repository	
	3.6 PROBLEM 7	58
	I-D Transport of a 5-Member Radionuclide Chain	
	3.7 PROBLEM 10	70
	2-D Flow Including Brine for a Reference Bedded-Salt Depository Site	
	APPENDIX COMPLETED DATA SETS	78
	REFERENCES	93

FIGURES

<u>Figure</u>	<u>Page</u>
2-1 Physiographic Setting for Reference Site	5
2-2 Geologic Cross Section A-B Through Reference Site	5
2-3 Reference Site as Gridded for USGS-SWIFT Comparisons	7
2-4 Reference Site as Gridded for Transport Calculations in this Document	13
2-5 Near-Field System of the Reference Depository	15
3-1 One-Dimensional Representation of Middle Sandstone Aquifer	18
3-2 Partial Listing of SWIFT/SSP Input Data for Problem 1	21
3-3 Partial Listing of SWIFT/SSP Input Data for Problem 2	28
3-4 Partial Listing of SWIFT/SSP Input Data for Problem 3	35
3-5 Partial Listing of SWIFT/SSP Input Data for Problem 4	43
3-6 The U-Tube Breachment Scenario	50
3-7 Partial Listing of SWIFT/SSP Input Data for Problem 5	53
3-8 Partial Listing of SWIFT/SSP Input Data for Problem 7	66
3-9 Partial Listing of Swift/SSP Input Data for Problem 10	74

TABLES

<u>Table</u>	<u>Page</u>
2-1 Aquifer Properties	8
2-2 Fluid Properties	9
3-1 Hydrologic Properties for Problems 1, 2 and 3	19
3-2 Radionuclide Parameters for Problem 3	32
3-3 Numerical Criteria for Radionuclide Transport	36
3-4 Properties of a Hypothetical Radioactive-Waste Component	52
3-5 Geometric and Hydrological Parameters for Problem 7	61
3-6 Properties of the Radionuclide Chain Used in Problem 7	62
3-7 Migration Times and Time-Step Criteria	64
3-8 Brine Transport Data	72

SWIFT/SSP Self Teaching Curriculum

New Right Hand Page

Notebook Divider Should Read. INTRODUCTION

CHAPTER I

INTRODUCTION

I.1 BRIEF DESCRIPTION OF SWIFT

There are two computer codes SWIFT (Sandia Waste Isolation, Flow and Transport). One of the codes, denoted simply as SWIFT, is a fully transient, three-dimensional model which solves the coupled equations for transport in geologic media. The processes considered are:

- (1) fluid flow
- (2) heat transport
- (3) dominant-species miscible displacement (brine)
- (4) trace-species miscible displacement (radionuclide)

The first three processes are coupled via fluid density and viscosity. Together they provide the velocity field on which the fourth process depends.

The second computer model, SWIFT/SSP, is, for the most part, a specialization of the above. The processes considered in this case are:

- (1) steady-state fluid flow
- (2) transient trace-species migration

Like its counterpart, this model is three-dimensional and permits a transient solution of the radionuclide equation. However, in order to achieve computer efficiency for what has been found to be a relatively large class of applications, the SWIFT/SSP version is limited to steady-state fluid flow with no heat or brine transport.

1.2 PURPOSE OF THE SELF-TEACHING CURRICULUM

The purpose of this manual is to assist new users of the SSP version. The teaching method is based on seven problems. All of these problems have been used previously in the SWIFT Self-Teaching Curriculum (Finley and Reeves, 1981), and the numbering used there has been retained herein to facilitate cross comparison. Since the SWIFT/SSP version is limited to steady-state fluid flow with no heat transport, Problems 6, 8, 9 and 11 from SWIFT Self-Teaching Curriculum are omitted in this document. For this document, however, some of the input-data fields have been left blank. The reader is expected to fill in these blanks using the data provided and the User's Manual for SWIFT/SSP (Cranwell and Reeves, 1981). Correct data sets (with blanks filled) are given in the appendix (upside down, of course).

SWIFT/SSP STC

No. 2 Right Hand Page

Notebook Divider Should read.

PHYSICAL SETTING-
~~Physical Setting~~

CHAPTER 2

PHYSICAL SETTING

2.1 THE REFERENCE SITE

The illustrative problems used in this document are based on a bedded-salt reference site. In Problems 1, 2, 3 and 7, this system is simplified rather substantially in order to demonstrate the basic operation of the SWIFT code. In the others, i.e., Problems 4, 5 and 10, both regional and depository near-field representations are used. Hence, it is expedient to discuss the bedded-salt system.

The reference site is entirely hypothetical, yet its physiographic setting and geologic and hydrologic properties are analogous to several regions of the continental USA. The site is located in a symmetrical upland valley, half of which is shown schematically in Figure 2-1. The crest of the ridge surrounding the valley is at an elevation of 6000 feet; the crest is a surface and groundwater divide so that only water moving in the valley falls in the valley itself. The valley is drained by a major river, River L, which is at elevation 2500 feet opposite the surface structures of the repository. Stream valleys tributary to River L exist, such as River U, but these are normally dry. The valley receives a mean annual rainfall of 40 inches per year, of which 16 inches are lost by evapotranspiration and the remaining 24 inches recharge the groundwater system.

The geology of the area near the site is shown in cross section in Figure 2-2. The valley is underlain by crystalline bedrock which crops out only over a narrow strip lying at the ridge crest surrounding the valley. This bedrock is assumed impermeable to groundwater flow. Above the bedrock is the sequence of sedimentary rocks sketched in Figure 2-2.

2.2 HYDROLOGY

The location of the repository was chosen to be far enough from the head of the valley that groundwater flow around the depository would be perpendicular to River L and to the valley axis. Thus, the groundwater flow and radioactive waste transport models could be used in their one- and two-dimensional modes to simulate the conditions around the repository. They were used in their one- and two-dimensional modes in the sample problems for speed and ease of computation only. In a real situation the three-dimensional configuration of flow and transport around a repository should be considered.

The groundwater flow in the entire valley cross section shown in Figure 2-2 was simulated by the Albuquerque District Office of the U.S. Geological Survey, Water Resources Division, with the commonly used finite-difference model of Trescott. (See Trescott (1975) and Trescott and Larson (1976)). In the remainder of this section, this model is referred to as the USGS model. The finite-difference grid used to represent the entire cross section through the depository is shown in

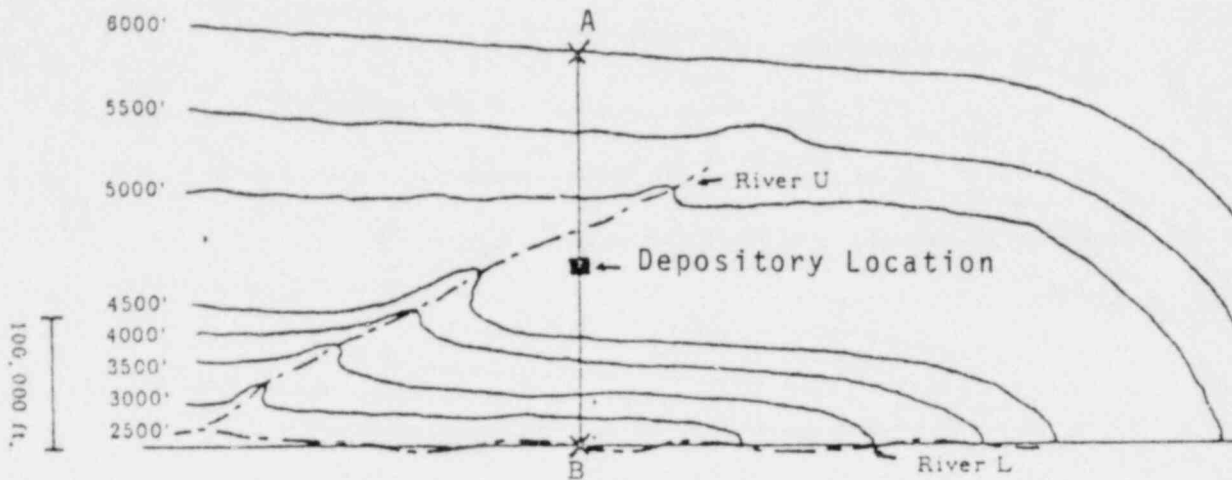


Figure 2-1. Physiographic Setting for Reference Site (One-Half of Parabolic Basin Shown).

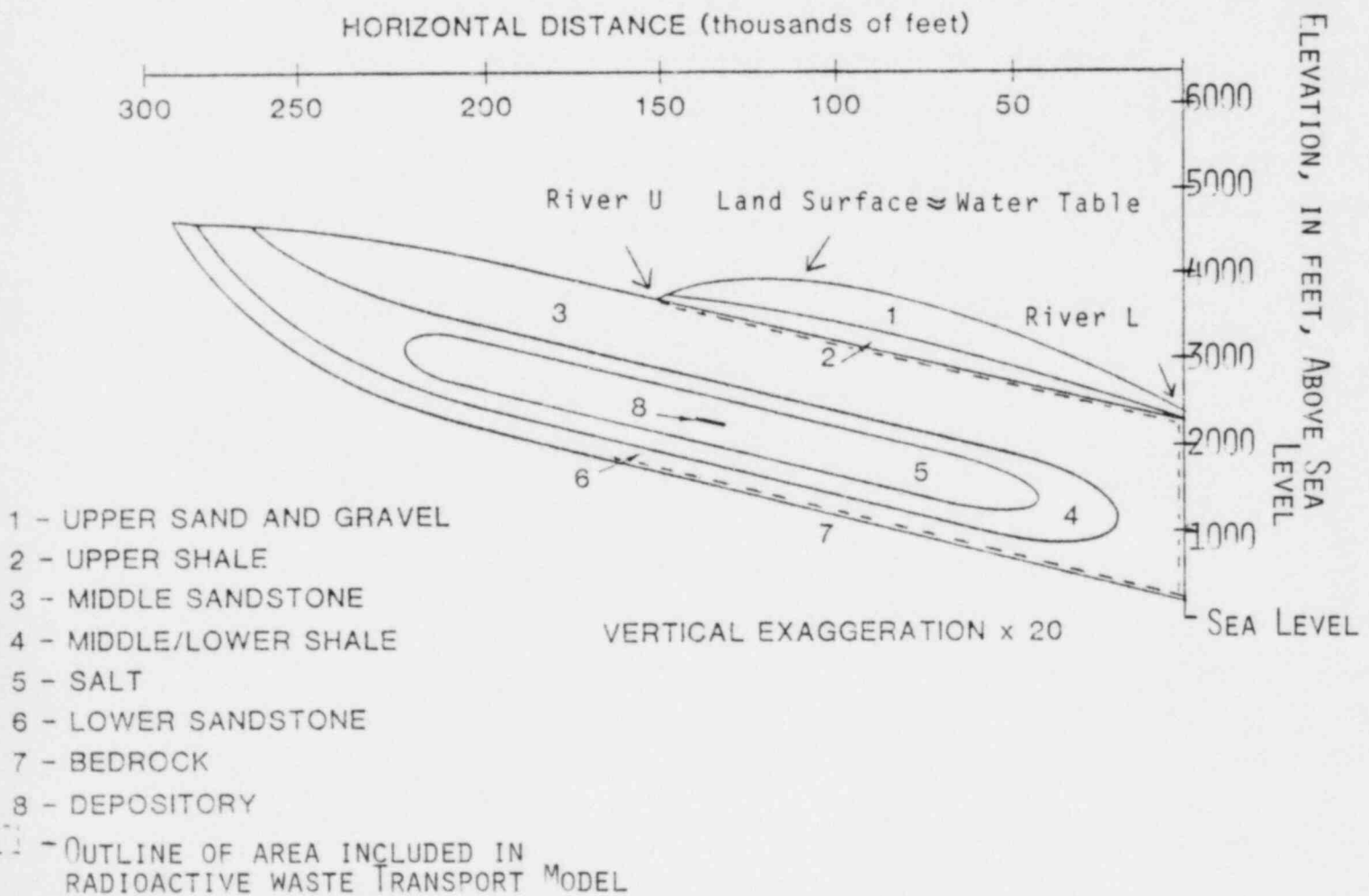


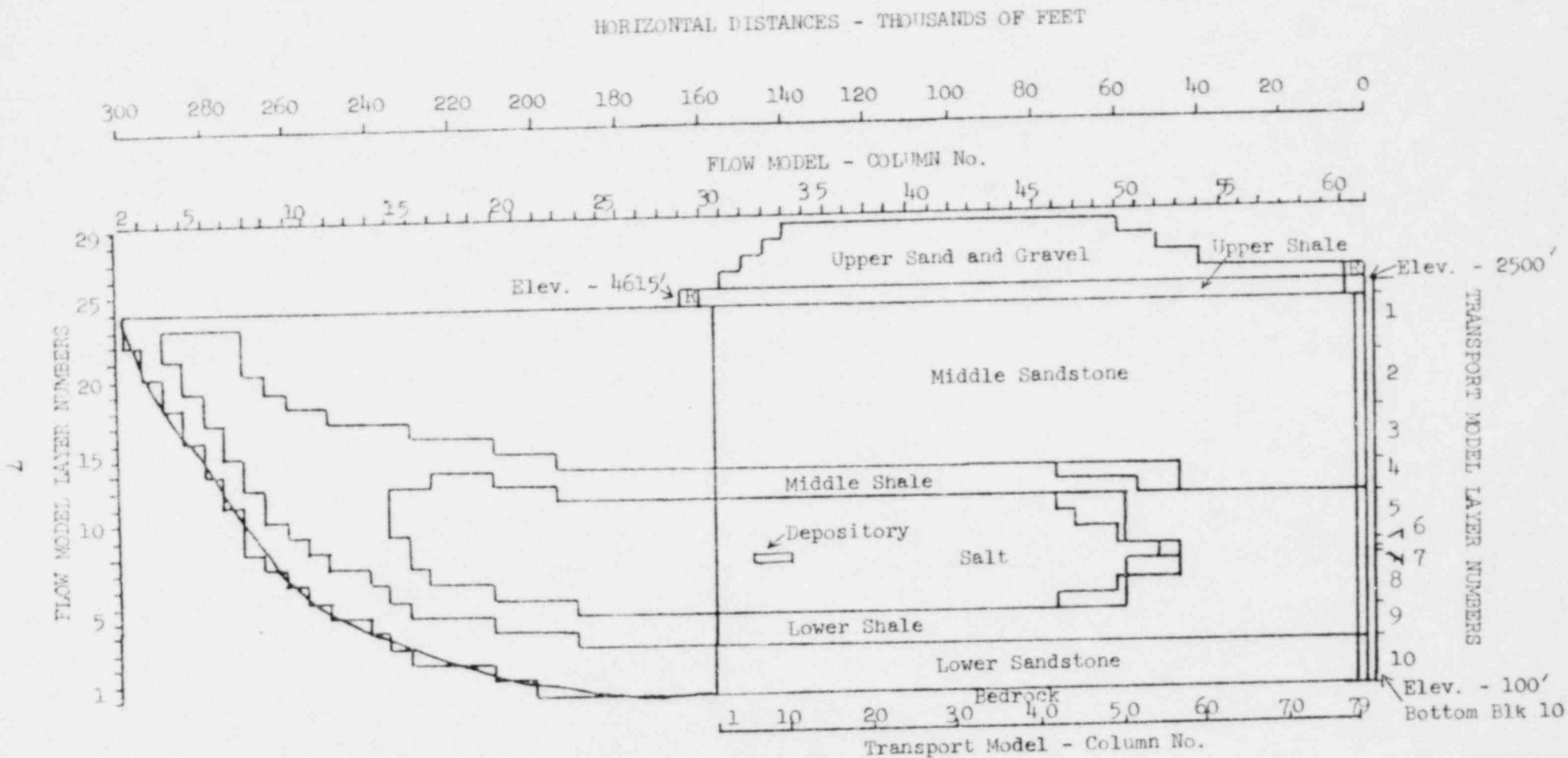
Figure 2-2. Geologic Cross Section A-B Through Reference Site.

Figure 2-3. In Problems 4 and 10 of this document, the SWIFT model is also used to simulate the entire valley cross section. However, subsets of the entire region may be used if the boundaries are specified appropriately. Figure 2-3 shows the "half-system" model which has been used in some previous simulations. In this document two other specializations are used, namely, a one-dimensional treatment of the middle sandstone and a two-dimensional depository near-field representation.

The hydraulic properties of the rock units used in the USGS flow model and in the Groundwater Transport Model are given in Table 2-1. They are the properties of real rocks of the type assumed to make up the reference site, as given by Franke and Cohen (1972). The site described in Franke and Cohen does not contain salt. Therefore, the hydraulic conductivity and porosity of salt were arbitrarily assumed to be 10^3 and 10 times lower, respectively, than those of the lower shale bed. The effects of variations in the hydraulic properties of the rocks and salt on flow and transport in the system have been investigated. The values given in Table 2-1 are merely starting points for the purpose of testing the flow and transport models. The fluid properties required for the Groundwater Transport Model are given in Table 2-2.

The following assumptions are made for flow modeling:

1. The bedrock underlying the sediments in the valley is impermeable and thus is a no-flow boundary.



Right Edge of Transport Col. 1 - Center of Flow Col. 30 - 157,000 ft.

Center of Transport Col. 79 - Center of Flow Col. 61 - 2,500 ft.

R - RIVER

Figure 2-3. Reference Site as Gridded for USGS-SWIFT Comparisons.

Table 2-1
Aquifer Properties

PROPERTY		UPPER SAND AND GRAVEL	UPPER SHALE	MIDDLE SANDSTONE	LOWER SHALE	SALT REPOSITORY	LOWER SANDSTONE	BE/DROCK	ENTERED ON CARD*
<u>Symbol used on Fig. 2-2</u>	ft/da	1	2	3	4	5	6	7	
<u>Hydraulic Conductivity</u>									
Horizontal	ft/da	270	10 ⁻²	50	10 ⁻²	10 ⁻⁵	40	N/A	R1-20,R1-21
Vertical	ft/da	27	10 ⁻⁵	1.4	10 ⁻³	10 ⁻⁶	7	N/A	R1-20,R1-21
<u>Porosity</u>	fractional	0.3	0.3	0.3	0.3	0.03	0.3	N/A	R1-20,R1-21
<u>Dispersivity</u>									
Longitudinal	ft	_____			500	_____		N/A	R1-2
Transverse	ft	_____			50	_____		N/A	R1-2
<u>Density - of solid rock</u>	lb/ft ³ 1/	_____			170	_____		N/A	R1-3
<u>Thermal Conductivity of fluid solid medium</u>	Btu ft-da-°F								
Horizontal	Btu ft-da-°F 1/	_____			58.05	_____		N/A	R1-2
Vertical	Btu ft-da-°F 1/	_____			49.34	_____		40.6	R1-2,R1-13
<u>Heat Capacity-of solid rock</u>	Btu ft ³ -°F	_____			28.0	_____		28.7	R1-1,R1-13
<u>Molecular Diffusivity</u>	ft ² /da	_____			1.0 x 10 ⁻³	_____		N/A	R1-2
<u>Compressibility of matrix</u>	(psi) ⁻¹	_____			3.0 x 10 ⁻⁶	_____		N/A	R1-1

1/ Thickness weighted averages of properties of individual layers as specified for thermal conduction model.

Table 2-
Fluid Properties

PROPERTY	TEMPERATURE		CONCENTRATION				Relative	UNITS		VALUE		Reference	Input on Card
	°C	°F	Wt. % NaCl	gmNaCl / 100 gm sol'n	lbNaCl / 100 lb sol'n	CgS		English	CgS	English			
Density - at 1 bar	25	77	0	0	0	0	gm/cm ³	lb/ft ³	0.9971	62.25	(1)	R1-3	
Compressibility 1 to 100 bars	0-100	68-212	0	0	0	0	bar ⁻¹	psi ⁻¹	4.7x10 ⁻⁵	3.2x10 ⁻⁶	Calc from (1)	R1-1	
Thermal Expansion 1 to 100 bars	20-100	68-212	0	0	0	0	°C ⁻¹	°F ⁻¹	5.3x10 ⁻⁴	2.9x10 ⁻⁴	Calc from (1)	R1-1	
Heat Capacity	20-100	68-212	0	0	0	0	Cal / gm-°C	Btu / lb-°F	1.00	1.00	(2)	R1-1	
Density - at 1 bar	25	77	25	296		1.0	gm/cm ³	lb/ft ³	1.1851	73.98	(3)	R1-3	
Viscosity:	of pure water	15	59	0	0	0		cp		1.138	(4)	R1-7	
	with temp.	40	104	0	0	0		cp		0.6531	(4)	R1-9	
		65	149	0	0	0		cp		0.4342	(4)	R1-9	
		90	194	0	0	0		cp		0.3156	(4)	R1-9	
	of brine	15	59	5	51.7	3.23	0.2	cp		1.209	Calc from (3) & (4)	R1-8	
	with conc.	15	59	12.5	136	8.49	0.5	cp		1.320	Calc from (3) & (4)	R1-8	
		15	59	20	229	14.3	0.8	cp		1.444	Calc from (3) & (4)	R1-8	
		15	59	25	296	18.5	1.0	cp		1.532	Calc from (3) & (4)	R1-7	
	of brine	25	77	25	296	18.5	1.0			1.260	Calc from (3) & (4)	R1-1	
	with temp.	25	77	25	296	18.5	1.0			1.055	Calc from (3) & (4)	R1-1	
	42.5	108.5	25	296	18.5	1.0			1.004	Calc from (3) & (4)	R1-1		

- References: (1) Clark, S.P., Jr., ed, 1966, Handbook of Physical Constants.
(2) Weast, Robert C., ed, CRC Handbook of Chemistry and Physics, 59th edition, 1978-79.
(3) Potter, R.W., II and Brown, David L., 1977, The Volumetric Properties of Aqueous Sodium Chloride Solutions ... U.S. Geol. Survey Bull. 1421-C.
(4) Robinson, R.A. and Stokes, R.H., 1959, Electrolyte Solutions: Butterworths, London, Appendix 1.1 and 11.3.

2. The valley is symmetrical about its central axis, the line of River L. Thus, all discharge from the section modeled is to River L, and the vertical plane at River L is also treated as a no-flow boundary (plane of symmetry).
3. The elevation of River L, equivalent to the hydraulic head at the discharge point, is 2500 feet above sea level.
4. The surface of the entire region is recharged by infiltration at the constant rate of 24 inches per year.

In designing the ground-surface inclination of the reference site, the model was run to steady-state conditions with several different ground-surface slopes by varying the elevation of River U. It was desired that all the regional recharge should discharge to River L; i.e., River U should have as little flow as possible. A too steep slope would give heads that lay below the elevation of River U so that it would lose water to the groundwater system. A too shallow slope would give heads above the elevation of River U so that groundwater would discharge to and flow in River U. By trial and error, an elevation of 4615 feet for River U was chosen which gave essentially no recharge from or discharge to River U. The elevations of the water table elsewhere along the section are those calculated by the model at steady state. These elevations are those shown in the ground surface on Figure 2-2.

There are really two groundwater flow systems in the cross section. The upper system is restricted to the upper sand and gravel unit and upper clay unit. In the upper system, recharge between River U and River L flows and discharges to River L. The lower flow system is confined beneath the upper clay and is the system that influences the repository. The lower flow system receives all the recharge above River U which also discharges into River L.

In order to distinguish between these systems, the USGS flow model was gridded so that the discharge from each to River L was calculated separately. The results of the steady-state simulation can be summarized as follows:

Discharge to River L from upper flow system:	$8.2 \times 10^2 \text{ft}^3/\text{da.ft}$
Discharge to River L from lower flow system:	$7.5 \times 10^2 \text{ft}^3/\text{da.ft}$
Total discharge per 1 ft. length River L:	$15.7 \times 10^2 \text{ft}^3/\text{da.}$

To compare the flow simulations by the USGS model and SWIFT, SWIFT was run to steady-state flow conditions. The SWIFT comparison calculation covered the "half-system" shown in Figure 2-3. This system covers only the lower flow region and only that portion of the lower flow region extending from River L to a distance of 157,500 feet up-dip from River L. Constant boundary pressures were used along the left edge, taken from the USGS model results, and a well discharging at a head of 2500 feet in the upper right block was used to simulate the discharge to River L from the lower flow system. At steady state, the discharge from

that well was $7.3 \times 10^2 \text{ ft}^3/\text{da.ft}$, in agreement with the $7.5 \times 10^2 \text{ ft}^3/\text{da.ft}$ discharge from the lower flow system in the USGS model. Likewise, the heads in the lower right blocks of both models are in good agreement: 4093 feet in the SWIFT versus 4053 in the USGS model. Although a 40-foot difference in head may seem large, it is the hydraulic gradient which drives the flow. The vertical gradients (head/vertical distance) between the lower right block and the discharge point, River L, are

$$\text{USGS model: } (4053-2500)/2150 = 0.72$$

$$\text{SWIFT: } 4093-2500/2150 = 0.74$$

2.3 SYSTEM DIMENSIONS

Figure 2-4 is a general dimensional layout used by the sample problems. The middle sandstone layer is approximately 1000 feet thick divided into three sections of 333.3 ft, 333.4 ft, and 333.3 ft and approximately 300,000 feet long.

The lower shale layer is approximately 200 feet thick on each side of the salt layer and 260,000 feet long. The salt layer is approximately 700 feet thick divided into six sections of 200 ft, 100 ft, 50 ft, 50 ft, 100 ft and 200 ft and approximately 180,000 feet long. The lower sandstone layer is approximately 300 feet thick and 240,000 feet long. The dip angle of the system is 0.0129 radians and the overall length of the system is 305,000 feet. Thus, the vertical rise for the system is 3946 feet. The River L is

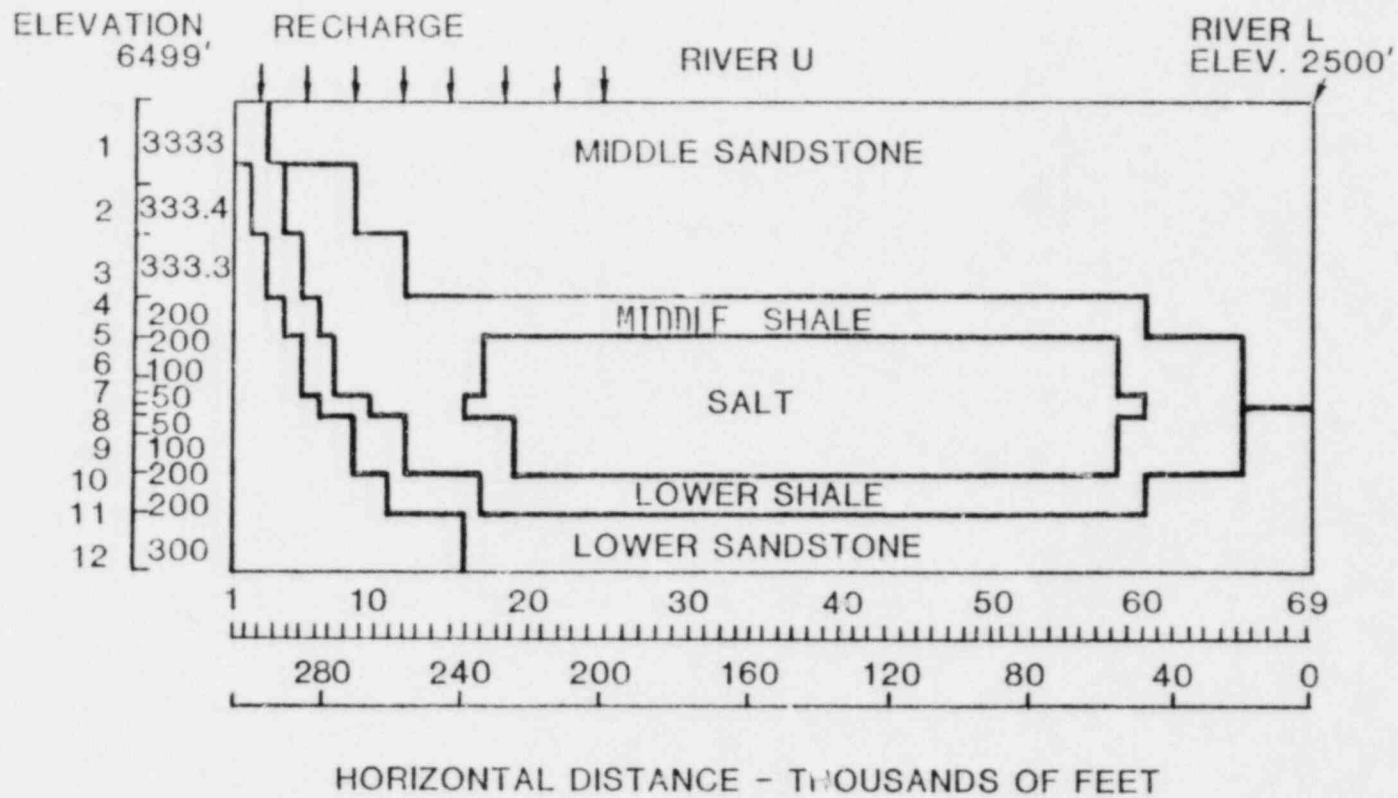


Figure 2-4. Reference Site as Gridded for Transport Calculations in this Document.

given at 2500 feet above sea level; therefore, the upper left-hand corner of the system is at 6446 feet above sea level. The total thickness of the system is 2400 feet; therefore, the lower right-hand corner of the system is 100 feet above sea level.

Various simplifications of the system are used for the sample problems. Problems 1, 2, 3 and 7 use only the middle sandstone layer in a one-dimensional approximation; thus, the three aquifer sections are combined into one. The result is an aquifer 305,000 feet long and 1000 feet thick with a dip angle of 0.0129 radians. Problem 5 uses a two-dimensional subsystem. This subsystem uses the entire thickness of the full system and 20,000 feet horizontally of the near-depository field of the full system (see Figure 2-5).

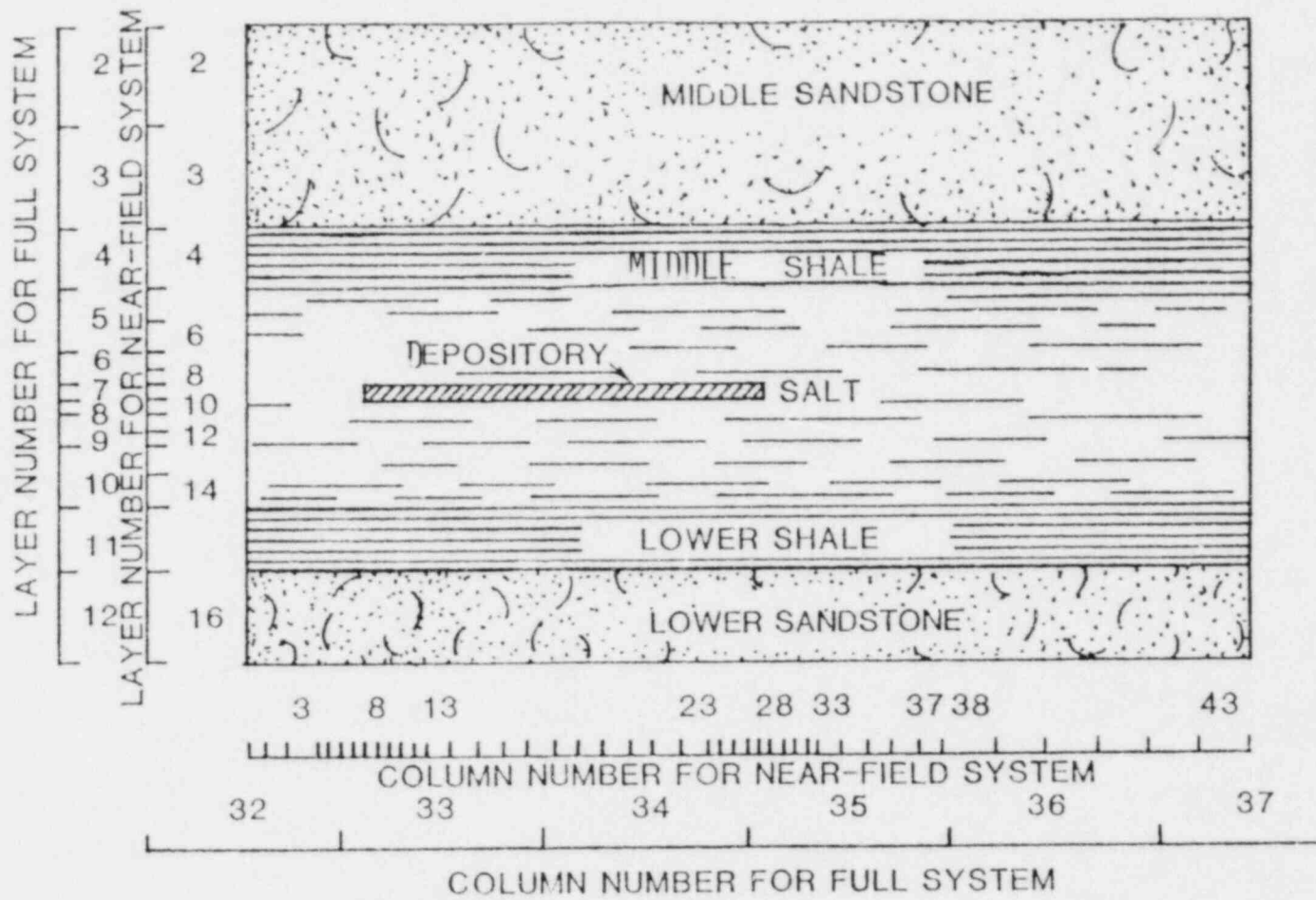


Figure 2-5. Near-Field System of the Reference Depository.

SWIFT/ESP STC

New Right Hand Page

Notebook Divider Should Read SIMPLE PROBLEMS

CHAPTER 3

SAMPLE PROBLEMS

3.1 PROBLEM 1.1-D FLOW WITH AQUIFER-INFLUENCE BOUNDARY CONDITIONS

3.1.1 Objectives

The objectives of this problem are:

1. Illustration of the use of aquifer-influence functions
2. Familiarity with input and output of the SWIFT/SSP program

Boundary conditions for the flow equation may be one of two types; i.e., either a prescribed constant value of the dependent variable or a prescribed derivative, typically a flux. The former is imposed by means of both aquifer-influence functions and "wells" (through a bottom-hole pressure limitation), and the latter is imposed only by means of "wells". This example illustrates the use of aquifer-influence functions.

3.1.2 Description of the Problem

Assumptions. The reference system described in Chapter 2 is grossly simplified here to satisfy problem objectives as simply as possible. First, only the middle sandstone layer is considered. Thus, all possible couplings to other parts of the system are ignored. Second, a one-dimensional approximation is used. Finally, radionuclide migration is not considered. Thus, the problem is to simulate one-dimensional fluid flow in a sandstone aquifer. The simplified system is shown schematically in Figure 3-1 and the appropriate hydrologic properties are presented in Table 3-1.

Table 3-1. Hydrologic Properties for Problems 1, 2 and 3

<u>Parameter</u>	<u>Symbol</u>	<u>Value</u>
Hydraulic Conductivity	K	
Problems 1 and 3		50 ft/day
Problem 2		25 ft/day
Porosity	ϕ	0.3
Rock Density	ρ_R	170 lb/ft ³
Compressibility of Water	c_w	$3.2 \times 10^{-6} \text{ psi}^{-1}$
Compressibility of Rock	c_R	$3.0 \times 10^{-6} \text{ psi}^{-1}$
Viscosity of Water	μ	1 cp
Density of Water	ρ	62.4 lb/ft ³

Boundary Conditions. Recharge occurs in the upland region and discharge occurs at River L (see Figure 2-1). For a relatively shallow river, the pressure condition

$$p(x=0) = 0 \quad (3.1-1)$$

is appropriate for the discharge. Furthermore, assuming that recharge is pressure limited with negligible puddling depths, then the condition

$$p(x=L) = 0 \quad (3.1-2)$$

is appropriate for recharge, where L is the length of the system.

Application of Aquifer-Influence Functions. Aquifer-influence functions are useful for treating both external and internal boundaries. Here they are used to characterize an external boundary of the system which is pressure controlled.

3.1.3 Preparation of Input Data

Figure 3-2 gives a partial data set with several blank fields, which are to be filled in by the reader with the aid of the User's Guide. The missing data pertain to aquifer-influence functions and hydrologic properties. In addition, parameters KOUT and IIPRT should be adjusted so that the initial arrays and Darcy velocities are printed. (Caution: pressure boundary conditions should be offset appropriately for the boundary blocks.)

PROBLEM NO. 1	SWIFT/SSP EXAMPLE	ENGLISH UNITS	
3/81			M-1-1
0 0 0			M-1-2
105 1 1 1 0 1	0.0 0.0	2 0 1 0 0 0	M-2
		1.0 1-4	R1-1
	0.0	67.4	R1-3
0.0	-6420.2	0.0	R1-16
305*1000.0			
1.0			
1000.0			
		-0.0129379 0.0	R1-20
		-2487.1	R1-20-BLNK
			R1-27
1 1 1 1 1 1			R1-28-1
			R1-28-2
105 305 1 1 1 1			R1-28-1
			R1-28-2
			R1-28-BLNK
			1-1
0 0 1 0 0 0			K2-1
1 0.5			K2-2
0 0			K2-13
0 0 1			K3-1

21

Figure 3-2. Partial Listing of SWIFT/SSP Input Data For Problem 1.

3.1.4 Examination of Results

A listing of output data is given in the enclosed microfiche. The reader will need to carefully examine the results given there. In particular, the following items should be verified:

- (1) initial arrays, especially transmissibilities (see note below)
- (2) summary table
- (3) pressure and Darcy velocity arrays

Transmissibilities. It is important to examine the fluid transmissibilities since these quantities control the block-to-block flows. Initially, they are calculated in the SWIFT code for the x-direction, from iteration invariant parameters by the relation

$$T_w^o, i+1/2, j, k = \frac{\Delta x_i \Delta y_j \Delta z_k}{\left(\frac{\Delta x}{k_x}\right)_i + \left(\frac{\Delta x}{k_x}\right)_{i+1}} \quad (3.1-3)$$

where T_w^o = initial transmissibility (ft³ · cp/psi · da)
 k_x = permeability in x direction (ft² · cp/psi · da)
 $\Delta x_i, \Delta y_j, \Delta z_k$ = spatial increments (ft)

Permeability k_x is calculated from initial data by the relation

$$k_x = K_x \mu_0 / \rho_0 \quad (3.1-4)$$

where

μ_0 = reference viscosity (cp)

ρ_0 = reference density (lb/ft³)

K_x = hydraulic conductivity (ft/da)

The significance of transmissibility is that after inclusion of its variable components through the relation

$$T_w = T_w^0 \rho / \mu_0 \quad (3.1-5)$$

the transmissibility controls all block-to-block flows within the system.

This flow is given by

$$F = T_w \Delta p \quad (3.1-6)$$

where

F = inter-block flow (lb/da)

T_w = transmissibility (lb/psi.da)

Δp = inter-block pressure change (psi)

Equation (3.1-5) is implemented for individual grid-block interfaces by using the average density of the neighboring grid blocks. Viscosity is assumed to remain constant at the reference value over the entire system. The numbers appearing in the array entitled "X-Direction Transmissibility" should be verified for accuracy, using this equation.

3.2 PROBLEM 2. 1-D FLOW WITH PRESSURE-LIMITED WELL BOUNDARY CONDITIONS

3.2.1 Objectives

The objectives of this problem are:

1. Simulation of recharge with a pressure-limited well
2. Simulation of discharge with a pressure-limited well

The major differences between Problem 1 and Problem 2 are the boundary conditions. In the former, aquifer-influence functions were used, whereas in the latter, wells are used. The term "well", as used in the documentation of the SWIFT code, simply denotes a source or a sink. Thus, wells may be used to simulate aquifer recharge and discharge boundary conditions as well as injection and production wells. Physically, such wells may be controlled either by a maximum pressure limit or by a maximum rate limit. This problem illustrates discharge to a river as controlled by the elevation of that river, which is a pressure limit condition. It also illustrates recharge for which the water-table elevation in the upland area is roughly equivalent to the surface elevation. Thus recharge is also pressure limited.

3.2.2 Description of the Problem

The physical setting here is much the same as for Problem 1. As in Problem 1, the focus is on fluid flow within the middle sandstone which, in the reference site, overlays the bedded-salt formation containing the

depository. Furthermore, a one-dimensional approximation is used to satisfy problem objectives as simply as possible. The simplified system is shown in Figure 3-1, and the hydrologic properties are presented in Table 3-1. Here, in contrast to Problem 1, the hydraulic conductivity is lowered by a factor of two to 25 ft/day.

3.2.3 Preparation of Input Data

Figure 3-3 gives a partial data set, which is to be completed by the reader. The missing data pertain to the hydraulic conductivity of the sandstone and the well parameters.

Well Data. The Well Cards R2-4, R2-6 and R2-7 are described in the User's Guide. The input provided gives the number of wells, rates of injection (minus sign) and production (plus sign), location and additional descriptive information, which includes well index, specification index and bottom-hole pressure. The well index WI_o simply gives the transmissibility of the so-called skin region which immediately surrounds the well. (For recharge, this quantity typically is identical to the transmissibility of the surrounding formation.) The model for injection then relates a volumetric flow to a head drop between bottom hole (H_{bh}) and grid-block center (H) through the relation

$$q = WI_o (H_{bh} - H) \quad (3.2-1)$$

PROBLEM NO. 2	SWIFT/SSP EXAMPLE	ENGLISH UNITS	
1781			M-1-1
0 0 0			M-1-2
305 1 1 1 0 1 1		2 0 0 1 0 0	M-2
3.2E-6 1.0E-6 0.0 0.0		1.0 1-4	R1-1
170.0 0.0 0.0 0.0			R1-3
0.0 -4900.0 0.0			R1-16
105*1000.0			
1.0			
1000.0			
	0.3	-0.0129379 0.0	-2487.1
			M1-20
			K1-26-BLNK
			K1-27-BLNK
			I-1-BLNK
2 1 1 0 0			K2-1
1 0.5			K2-2
2			K2-4
1			K2-6
2			K2-6
			K2-6-BLNK
1 305 1 1 1			R2-7-1
			K2-7-2
2 1 1 1 1			K2-7-1
			K2-7-2
			K2-7-BLNK
0 1 0			R2-13
0 0 1			K3-1

Figure 3-3. Partial Listing of SWIFT/SSP Input Data For Problem 2.

With regard to specification option, there is one difference between steady state (SSP) and fully transient (PTC) versions of SWIFT. For the former $|IINDWI| = 3$ means pressure control only; whereas for the latter $|IINDWI| = 3$ implies a time-dependent switching between rate and pressure limitations depending upon the relation between calculated and prescribed bottom-hole pressures.

3.2.4 Examination of Results

The following items should be verified:

- (1) well data
- (2) consistency between well rates and pressure drops
- (3) pressure-at-depth array

3.3 PROBLEM 3. 1-D TRANSPORT OF A DECAYING RADIONUCLIDE

3.3.1 Objectives

1. To calculate the spatial distribution for a decaying radionuclide at 1161 days after initiation of release
2. To compare numerical and analytical solutions by determining an effective dispersivity from the calculated results

3.3.2 Description of the Problem

The Physical Setting. The physical setting here is much the same as for Problems 1 and 2. As in those problems, only the middle sandstone formation is of interest (see Figure 2-2). Further, the hydrologic properties are given by Table 3-1. Here, however, radionuclide migration is the focus of this problem.

Assumptions. It is assumed that the containment of radionuclides by the depository itself and by the bedded salt which surrounds it is breached, resulting in a release of radionuclides to the middle sandstone. For convenience, only one component of this release is considered, and a solubility limit is hypothesized. The assumed geochemical properties are given in Table 3-2.

Table 3-2. Radionuclide Parameters for Problem 3

Dispersivity (ft)	100
Half-Life (yr)	3.18
Distribution Coefficient (ft ³ /lb)	0
Solubility Limit (ppm)	1
Molecular Diffusivity (ft ² /da)	10 ⁻⁴

In order to model this problem and to satisfy problem objectives as simply as possible, a one-dimensional representation of the middle sandstone is used which extends only a distance

$$L = 5000 \text{ ft} \quad (3.3-1)$$

down-dip from the depository. Further, the simulation time is taken to be

$$t = 1161 \text{ days} \quad (3.3-2)$$

Boundary Conditions. At the extreme down-dip end of this near-field system, the flux, F , is simply that due to convection, i.e.,

$$F(x=0) = uC(x=0) \quad (3.3-3)$$

a condition which is invoked by default in the SWIFT computer model.

Quantity u in Eq. (3.3-3) is the Darcy velocity of the flow field, which is virtually identical to that obtained in Problem I. To establish such a flow field, the following boundary conditions are used:

$$q(x=L) = 646.3 \text{ ft}^3/\text{day} \quad (3.3-4)$$

and

$$p(x=0) = 0 \quad (3.3-5)$$

3.3.3 Preparation of Input Data

Figure 3-4 gives a partial data set which is to be completed by the reader. The missing data pertain to four items, namely

- (1) characterization of radionuclides in terms of half life and distribution coefficient
- (2) dispersivities and molecular diffusion coefficient
- (3) radioactive sources
- (4) time differencing

Data for Items (1) - (3) may be determined from the above information. For Item (4), it is desired that the CIT-CIS method be used since it is the least restrictive for this problem. Thus, it is necessary for the reader to consider the numerical criterion from Table 3-3. In general, one should also consider the half-life limitation on the time-step, as discussed in Chapter 4 of the User's Manual. For this problem, however, the latter criteria are nonrestrictive, and only the transport criteria of Table 3-3 need be invoked.

3.3.4 Examination of Results

The numerical solution corresponding to an elapsed time of 1161 days is given in the microfiche listing and may be compared with the analytic solution in a straightforward manner. To do this, one uses the formula

PROBLEM NO. 3	SWIFT/SSP EXAMPLE						ENGLISH UNITS						
3/81													M-1-1
0 0 0													M-1-2
50 1 1													M-2
100 RAD													K0-1
<hr/>													
3.2E-6													K0-2
170.0	0.0												K1-1
0.0	-4015.0	0.0					62.4	62.4					K1-3
50*100.0													K1-16
1.0													
1000.0													
50.0	50.0	50.0	0.3				-0.0129379	0.0			-4000.0		
<hr/>													
2 1 1 0 0 0													K1-20
1 0.5													K1-20-BLNK
2													K1-27-BLNK
1 -646.1													I-1-BLNK
2 1.0E10													K2-1
<hr/>													
1 50 1 1 1 1													K2-2
25.0	0.0001												K2-4
2 1 1 1 1 -1													K2-6
1000.0	0.0001												K2-6
<hr/>													
0 1 0													K2-6-BLNA
													K2-7-1
<hr/>													
1 50 1 1													K2-7-2
<hr/>													
0.5													K2-7-1
1101.0	10.0												K2-7-2
5 1 0 0 0													K2-7-BLNA
0 0 1													K2-13
<hr/>													
													K3-1
													K3-2
													K3-3-1
													K3-3-2
													K3-3-BLNA
													K3-4
													K3-6
													K3-7
													K3-1

Figure 3-4. Partial Listing of SWIFT/SSP Input Data For Problem 3.

35

Table 3-3. Numerical Criteria for Radionuclide Transport⁺

<u>Scheme</u>	<u>Numerical Dispersion</u>	<u>Dispersion Criterion</u>	<u>Overshoot Criteria</u>
CIT-CIS	None	None	$\frac{v\Delta t}{2\Delta x} + \frac{\alpha v\Delta t}{\Delta x^2} \leq 1$
CIT-BIS	$\frac{v\Delta x}{2}$	$\frac{\Delta x}{2\alpha} \ll 1$	$\frac{\Delta x}{2\alpha} \leq 1$ $\frac{vt}{2x} \leq 1$
BIT-CIS	$\frac{v^2\Delta t}{2}$	$\frac{v\Delta t}{2\alpha} \ll 2$	$\frac{\Delta x}{2\alpha} \leq 1$
BIT-BIS	$\frac{v\Delta x}{2} + \frac{v^2\Delta t}{2}$	$\frac{\Delta x + v\Delta t}{2\alpha} \ll 1$	None

+ Here CIT means central in time, CIS means central in space, BIT refers to backward in time, and BIS refers to backward in space. In addition,

v = retarded interstitial velocity

Δx = space increment in direction of flow

Δt = time increment

α = dispersivity

$$\alpha_{\text{eff}} = (x_{16} - x_{84})^2 / 8x_{50} \quad (3.3-6)$$

The various distances x_p are defined by the distribution of relative concentrations:

$$C(x_p)/C_o = (p)f(x_p)/100, \quad p = 16, 50, 84 \quad (3.3-7)$$

here the decay factor f is given by

$$f(x) = \exp -(x/2D)(w-v) \quad (3.3-8)$$

Here the effective retarded velocity is given by

$$w = \left\{ v^2 + 4D\lambda \right\}^{1/2} \quad (3.3-9)$$

where D is the dispersion ($D = \alpha v$) and λ is the decay constant. As shown, Eq. (3.3-7) is nonlinear in x_p . However, it may be solved relatively easily in this case by taking

$$x_{50} = wt \quad (3.3-10)$$

and

$$f \approx f(x_{50}) = \text{constant} \quad (3.3-11)$$

The latter will permit the evaluation of x_{16} and x_{84} from the numerical profiles. The effective dispersivity α_{eff} may be then evaluated from Eq. (3.3-7) for comparison with the physical dispersivity α .

3.4 PROBLEM 4. 2-D FLOW FOR A REFERENCE BEDDED-SALT DEPOSITORY SITE

3.4.1 Objectives

1. Simulation of steady-state flow in a two-dimensional reference site
2. Illustration of the use of heterogeneous block specification with the R1-21 Cards
3. Illustration of zero pore-volume block modification with the R1-26 Cards
4. Illustration of two-dimensional printer maps and their specification with the R2-14 and R2-15 Cards
5. Demonstration of the use of wells to simulate recharge

In Problem 3, a grid limitation was necessary for both time and space domains. In the solution of the flow equation, however, there are no such limitations, and less restrictive conditions, such as geometry and the desired resolution, are controlling. For depository evaluations, an efficient procedure is to first simulate flow on the entire domain with a relatively coarse grid. Pressure boundary conditions can then be prescribed for a near-field simulation of both flow and transport which, of course, typically requires a much finer grid. The objective of this problem and of Problem 5 is to illustrate such a procedure.

3.4.2 Description of the Problem

The Physical Setting. The physical setting here is the same as that for Problems 1 through 3. In those problems the middle sandstone only was considered since the objective was primarily to demonstrate various features of the SWIFT code and various numerical artifacts. Here the physical system described in Chapter 2 is characterized in much more detail. Figure 2-4 shows the geologic cross section with the various sedimentary layers and gives the vertical and horizontal gridding, as well as the recharge and discharge areas. Aquifer and fluid properties are given in Tables 2-1 and 2-2.

Assumptions. Four assumptions are made for purposes of the flow modeling. They are given in Section 2-2. These assumptions mean that a two-dimensional model may be used and that the upper sand and gravel zones have no influence on the flow domain in which the depository is located. Thus, those two zones are omitted in Figure 2-4.

Boundary Conditions. In addition, the assumptions give the recharge boundary condition. Since the flow is two-dimensional, we arbitrarily take the width (into the plane of Figure 2-4) to be 1 ft. Thus, for the recharge area shown in Figure 2-4, of length 135,000 ft, the total inflow is

$$q = 740 \text{ ft}^3/\text{day} \text{ (recharge)} \quad (3.4-1)$$

The two rivers are simulated in the same manner as in Problem 2. Thus, the depth of each river is taken to be identical to the local elevations, yielding the pressure condition

$$p = 0 \quad (\text{rivers}) \quad (3.4-2)$$

All remaining boundaries have no flow conditions due to an impermeable bedrock below, the lack of flow through the upper shale above, a ground-water divide at the extreme up-dip boundary and symmetry for the boundary below River L. Such conditions all follow from the assumptions given.

3.4.3 Preparation of Input Data

Figure 3-5 gives a partial data set which is to be completed by the reader. The missing data pertain to Items (2) - (5) of the objectives listed above. The reader is expected to supply this data using the data given herein and the User's Manual with an occasional reference to the SWIFT Curriculum.

3.4.4 Examination of Results

In examining the computed printout (see microfiche listing), one should take note of several questions:

1. Was a steady-state mass balance achieved?

2. Considering that the positive z axis is directed downward, what is the direction and magnitude of the Darcy velocity through the depository zone? (Assume the depository is located in Row 7 of Column 34.)

3. What would be the total flow through a depository with horizontal dimensions 3200 ft x 400 ft?

Figure 3-5. Partial Listing of SWIFT/SSP Input Data for Problem 4.

PROBLEM NO. 5 REDUCED-SALT REFERENCE SITE SWIFF/SSP EXAMPLE

U	0	0	0	0	1	1	2	0	0	1	0	0	0	0	M-1
69	1	17													M-1-1
.0000032	.0000031	0.													M-1-2
170.	15.7	62.3													M-2
15.7	-5582.9	0.													M-1-1
295500.	405500.														M-1-3
1.0															M-1-16
333.1	333.4	333.1	200.0	100.0	0.2	50.0	100.0	100.0	200.0	0.3	100.0	0.3	100.0		M-1-20
50.	50.	1.4													M-1-21-1
40.	40.	7.													M-1-21-2
40.	40.	7.													M-1-21-3
40.	40.	7.													M-1-21-4
.01	.01	.001													M-1-21-5
40.	40.	7.													M-1-21-6
.01	.01	.001													M-1-21-7
40.	40.	7.													M-1-21-8
40.	40.	7.													M-1-21-9
5	6	1	1	5											M-1-21-10
40.	40.	7.													M-1-21-11
.01	.01	.001													M-1-21-12
15	55	1	1	5											M-1-21-13
56	64	1	1	5											M-1-21-14
.01	.01	.001													M-1-21-15
65	69	1	1	5											M-1-21-16
50.	50.	1.4													M-1-21-17
40.	40.	7.													M-1-21-18
.01	.01	.001													M-1-21-19
15	55	1	1	5											M-1-21-20
59	64	1	1	5											M-1-21-21
.01	.01	.001													M-1-21-22
65	69	1	1	5											M-1-21-23
50.	50.	1.4													M-1-21-24
40.	40.	7.													M-1-21-25
.01	.01	.001													M-1-21-26
14	58	1	1	5											M-1-21-27
59	64	1	1	5											M-1-21-28
.01	.01	.001													M-1-21-29
65	69	1	1	5											M-1-21-30
50.	50.	1.4													M-1-21-31
40.	40.	7.													M-1-21-32
.01	.01	.001													M-1-21-33
17	55	1	1	5											M-1-21-34
56	64	1	1	5											M-1-21-35
.01	.01	.001													M-1-21-36

-6413.7

3.5 PROBLEM 5. 2-D NEAR-FIELD TRANSPORT FROM A BEDDED-SALT
REFERENCE DEPOSITORY

3.5.1 Objectives

The objectives of this problem are:

1. To calculate the steady-state fluid flow and the transient-state radionuclide transport which would result from a U-tube breachment scenario for a depository
2. To understand the use of aquifer-influence functions for near-field simulations
3. To illustrate the use of rock-dependent distribution coefficients
4. To illustrate the use of the waste-leach model
5. To demonstrate the intentional violation of numerical criteria

With knowledge of the steady-state hydraulic potentials at the depository site from the previous example, one is able to extract fluid-flow boundary conditions for more detailed near-field radionuclide transport calculations. It is, of course, desirable to restrict the spatial domain for the transport simulation to the near field whenever possible because of the storage and time requirements necessary to satisfy the numerical criteria of Table 3-3. The object of this problem is to perform such a near-field simulation as a demonstration.

3.5.2 Description of the Problem

The Physical Setting. Figure 3-6 shows a cross-sectional view of the system. As shown, this is simply a subsystem of the regional system used in Problem 4 (Figure 2-4). The near field includes the entire thickness of the full system. However, its length has been truncated to 20,000 ft. Relative to the regional simulation, the left-hand boundary is located at the centerline of Column 32. Hydraulic parameters are the same as for the previous problem and are given in Tables 2-1 and 2-2.

Depository Breachment Scenario. The depository is located at a depth of 1500 feet from the interface between upper shale and middle sandstone, and its centerline is located 6500 feet to the right of the left-hand boundary for the near-field system. It is assumed to measure 8,000 feet in length by 50 feet in height. As is indicated, two vertical connections to the middle sandstone are present. These connecting legs, together with the depository, would constitute a U-tube breachment scenario. Due to the slope of the system (not shown in Figure 3-6), there is a pressure drop between the two legs, resulting in a flow through the U-tube. The vertical connections are taken to be 250 feet in width with a lateral extent (into the page of Figure 3-6) comparable to that of the depository itself. The hydraulic conductivity and porosity of the entire U-tube are arbitrarily taken to be

$$K_U = 1.0 \text{ ft/da and } \phi = 0.5 \quad (3.5-1)$$

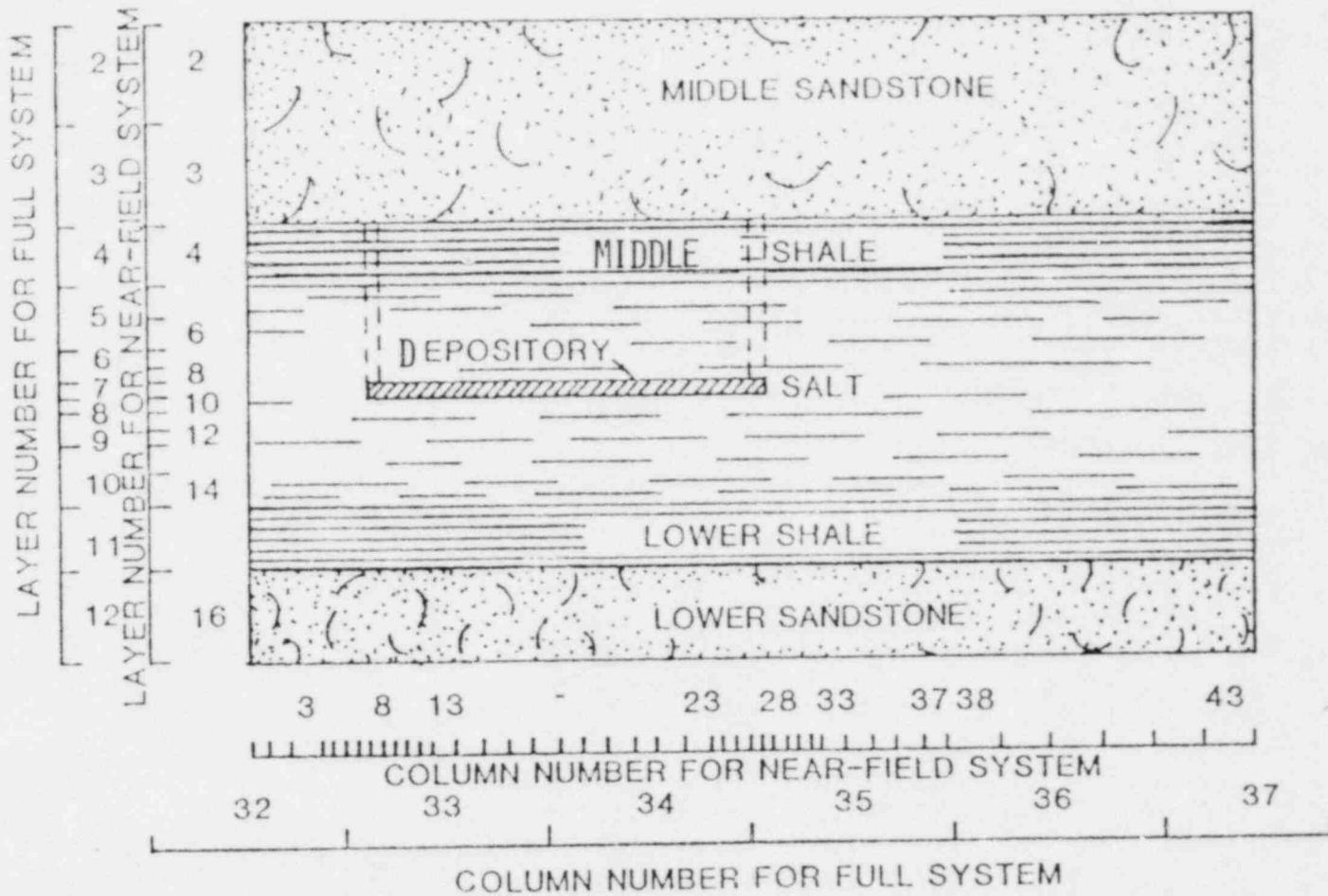


Figure 3-6. The U-Tube Breachment Scenario.

Thus, the two vertical legs represent a rather massive communication between depository and aquifer and could possibly result from a thermal fracturing process. Our intent here, however, is not to formulate a realistic U-tube breachment scenario but to demonstrate the SWIFT/SSP code and to develop physical concepts for such a scenario. Properties of the radioactive-waste component are given in Table 3-4.

Boundary Conditions. The basic idea here is to reproduce on a local scale the flow obtained in the previous problem. This may be done quite easily. First of all, no-flow boundaries are prescribed along the upper and lower horizontal bounding surfaces just as they were along the same surfaces for Problem 4. Calculated pressures are taken from the previous problem and used as boundary conditions for the two vertical surfaces (with some linear interpolation for the fine-mesh region of the near-field grid). As for the radioactive component, a source is provided by the waste-leach model in its simulation of the depository. A constant leach rate is assumed such that the leach time is 10,000 y.

3.5.3 Preparation of Input Data

Figure 3-7 gives a partial data set which is to be completed by the reader. The missing items are intended to direct the reader's attention to certain items which are illustrated by this problem. Aquifer-influence boundary conditions may be obtained from the pressures given in Columns 32 and 37 for Problem 4, using interpolation where required. Distribution coefficient and waste-leach parameters may be obtained from Table 3-4.

Table 3-4. Properties of a Hypothetical Radioactive-Waste Component

<u>Property</u>	<u>Value</u>
Initial waste density within depository	5 lb/ft ³
Leach time	10,000 y
Solubility	∞
Distribution coefficient in salt	0
Distribution coefficient in shale and sandstone	1.6 ft ³ /lb
Longitudinal dispersivity	150 ft
Transverse dispersivity	50 ft

Figure 3-7. Partial Listing of SWIFT/SSP Input Data for Problem 5.

K3-7
 K3-1
 K3-0
 K3-7
 K3-6
 K3-9
 K3-1-EMO

1 1 1 1 0 0
 0 0 0 0
 375.125105 1.0
 -1 -1 1 1 0
 1 0.7489 1 0.
 19 53 1 1 15 10.0 E-5 1.0 E-5
 0 0 0 1

3.5.4 Examination of Results

There are several questions which may be asked concerning the computer output.

1. What is the interpretation of the pressure map?
2. Based on a comparison of the Darcy-velocity field here with that of Problem 4, do you think that the presence of the U-tube has perturbed the near-field boundary appreciably?
3. Can the reader verify the concentrations within the depository at 10,000 y with a rough hand calculation?
4. What is the significance of the print-out time of 400 y, 10,000 y and 10,250 y?
5. Have the CIS-CIT criteria of Table 3-3 been violated by the chosen space steps? If so, what is the significance of such a violation?
6. Have the CIS-CIT criteria of Table 3-3 been violated by the chosen time-steps? If so, what is the significance of such a violation?

The reader may wish to consult the discussion for Problem 5 in the SWIFT Curriculum before answering Questions 5 and 6.

3.6 PROBLÉM 7. 1-D TRANSPORT OF A 5-MEMBER RADIONUCLIDE CHAIN

3.6.1 Objectives

The objectives of this problem are:

1. Simulation of the transport of a 5-member chain
2. Application of numerical criteria to the transport of a chain
3. Restarting the SWIFT code

Numerical criteria were introduced in Problem 3. They apply rigorously to the case of one-species transport. For the case of daughter products, however, these criteria may, at times, be relaxed to great advantage.

In performing lengthy and complex computations such as those sometimes encountered for radionuclide chains, it usually is advisable to restart the SWIFT/SSP code several times. If a problem develops, it is necessary then only to return to the last restart record, rather than to redo the entire calculation. Numerical criteria and creation of a restart record are considered here in conjunction with the simulation of transport for a 5-nuclide chain.

3.6.2 Description of the Problem

The Physical Setting. The underlying physical picture here is the bedded-salt reference site discussed in Chapter 2. The basic idea is that depository containment is somehow breached, resulting in release to an overlying aquifer, and that transport occurs to a biosphere-discharge point. Details of the simplified hydrological system are given in Table 3-5.

The radioactive chain which is considered here is the following:



Table 3-6 gives the (assumed) initial inventory of these components, and their (assumed) constant leach rate is characterized by the leach time

$$\tau = 10^5 \text{ y} \quad (3.6-1)$$

Table 3-6 also gives the retardations chosen for these radionuclides in this demonstration problem.

Assumptions and Extensions. As was mentioned in connection with Problem 4, flow can be modeled on a much larger scale than can transport since the restrictive numerical criteria, due to convection, do not apply to flow calculations. One alternative for treating the transport is to focus multidimensionally upon the near field of the depository, as

Table 3-5. Geometric and Hydrological Parameters for Problem 7

<u>Parameter</u>	<u>Value</u>
Length	10,000 ft.
Interstitial velocity	10 ft/y
Flow rate	0.0274 ft ³ /day

Table 3-6. Properties of the Radionuclide Chain Used in Problem 7

Nuclide	Half Life (y)	Solubility	Retardation ⁺⁺	Inventory		Conversion (Ci/lb)
				(Ci)	(lbs)	
Pu 242	3.79×10^5	1.0×10^{-5}	500	1.36×10^3	7.85×10^2	1.73
U 238	4.51×10^9	$2.0 \times 10^{-4+}$	2500	1.07×10^2	7.01×10^5	1.53×10^{-4}
U 234	2.48×10^5	$5.3 \times 10^{-7+}$	2500	4.83×10^3	1.70×10^3	2.84
Th 230	7.7×10^4	2.5×10^5	1000	4.02×10^1	4.39	9.16
Ra 226	1.6×10^3	1.0×10^{-5}	100	7.03	1.57×10^{-2}	4.49×10^2

+ The solubility for uranium has been partitioned via the initial inventories (in lbs) in order to satisfy the input demands of SWIFT.

++ Retardation is defined as the ratio of groundwater velocity to radionuclide velocity.

was done in Problem 5. A second alternative is to define a dominant flow path through, say, point tracking, and then perform a one-dimensional transport simulation on that path. Thus, one-dimensional simulation of transport can be a very useful tool in safety assessment of a nuclear-waste depository.

3.6.3 Preparation of Input Data

If one were to blindly proceed to apply numerical criteria in this case, he would find the half life of Ra (1600 y) to be restrictive. The resulting data deck would lead to an inefficient execution, however, since computer times may be reduced by about a factor of about 20 by applying some physical insight to the problem.

The rationale used here may be seen from Table 3-7. This table ignores both dispersion and production after discharge from the depository. It is, nevertheless, quite useful for purposes of organizing the calculations. As is indicated, Ra is expected to break through first, followed by Pu, Th and the two isotopes of U. The half life of Ra (1.6×10^3 y) is much less than its breakthrough time (10^5 y). Thus, a negligible quantity of that Ra released from the depository will actually be discharged from the system. Therefore, Ra is ignored in constructing our data sets.

Table 3-7. Migration Times and Time-Step Criteria^{1,2}

Nuclide	Migration (y x 10 ⁶)	Time ³ (d x 10 ⁸)	Order of Breakthrough	Time-Step y x 10 ⁴	Control ⁴ y x 10 ⁴
Pu 242	0.5-0.6	1.8-2.2	2	1.0	1.0
U 238	2.5-2.6	9.1-9.5	4,5	5.0	5.0
U 234	2.5-2.6	9.1-9.5	4,5	5.0	5.0
Th 230	1.0-1.1	3.7-4.0	3	2.0	2.0
Ra 226	0.1-0.2	0.4-0.6	1	0.16	0.19

¹ Assuming (1) no dispersion and (2) no production after discharge from depository.

² This table is used only for planning the simulation. It does not represent calculated results.

³ Leach time is taken to be 10⁵ y.

⁴ As required by the numerical criteria.

As a precautionary measure, slugs of the various nuclide components, which are released from the depository, are tracked by separate restarts. There are therefore four input data sets, the primary data set shown in Figure 3-8 and two restart data sets. The primary data set is set up to resolve the slug of Pu as it breaks through. The first restart data set captures the behavior of the thorium released from the depository, and the second captures that of the two U isotopes. Time-steps are prescribed via Table 3-7 within each restart relative to only those components which remain in the system.

For each component, a distinction is made between the portion which is released from the depository and the portion which is produced by radioactive decay. For all radionuclides other than Ra, numerical criteria must be applied to that portion which is released directly from the depository. For Ra, that portion has decayed to negligible amounts by the time release to the biosphere occurs. Thus, the only Ra which is released from the system is that portion which is produced by the decay of Th. The importance of the distinction between that released and that produced is that numerical criteria need not be applied to a daughter product which is in secular equilibrium with its parent.

Figure 3-8 presents a partial listing of the primary data set which is to be completed by the reader. Furthermore, the reader is asked to construct the first restart data set for the SWIFT/SSP code. It may be helpful here to refer to the SWIFT Curriculum (Problem 7).

Figure 3-8. Partial Listing of SWIFT/SSP Input Data for Problem 7.

2-19	ER	1	0	0	0
		-1	0	0	0
2-225	ER	1	0	0	0
		-1	0	0	0
2-255	ER	1	0	0	0
		-1	0	0	0

K3-6
 K3-7
 K3-1
 K3-6
 K3-7
 K3-1
 K3-6
 K3-7
 K3-1-END

3.6.4 Examination of Results

The missing data refer both to time-step and restart specifications. (Note that recurrent data sets are prescribed so as to resolve the dispersed slug of Pu as it breaks through.)

It is instructive to track the peak value of Pu242 from 10^5 y to 7×10^5 y. It is also instructive to note the peak value of each radionuclide at the latter time. Can the reader explain such behavior in each case?

3.7 PROBLEM 10. 2-D FLOW INCLUDING BRINE FOR A REFERENCE
BEDDED-SALT DEPOSITORY SITE

3.7.1 Objectives

To calculate steady-state, fluid pressures based on brine concentrations within the reference system

3.7.2 Description of the Problem

The entire bedded-salt reference site is used here, just as in Problem 4. This system is described in Chapter 2. In particular, however, the reader is referred to a cross-sectional view of the sedimentary sequence in Figure 2-4 and aquifer and fluid parameters in Tables 2-1 and 2-2. Additional brine-transport data are given in Table 3-8. In Problem 4, pressures are calculated based on fresh-water fluid densities throughout the system. Here, it is desired to include a variable density based on brine concentrations so that the effect upon flow through the depository may be assessed. To solve such a problem, one would normally do a steady-state calculation for flow and brine. Here, however, because of the nature of the system, an acceptable approximation consists of setting brine concentrations to saturation within the bedded salt and zero elsewhere and performing a steady-state calculation only for pressure using the resulting variable-density field.

Table 3-8. Brine Transport Data

<u>Parameter</u>	<u>Symbol</u>	<u>Value</u>
Product of dissolution rate and solubility fraction	k_{fs}	$1.0 \times 10^{-3}/d$
Longitudinal dispersivity	α_L	500 ft
Transverse dispersivity	α_T	50 ft

3.7.3 Preparation of Input Data

A partial listing of the data is shown in Figure 3-9. The reader is requested to fill in the blanks, which refer to density variation and (assumed) brine concentrations.

3.7.4 Examination of Results

In examining the computed printout (see microfiche), it is useful to consider the following questions:

1. How is the pressure changed relative to the simulation of Problem 4 in the vicinity of the depository (Row 7, Column 34)?
2. What is the dominant direction and magnitude of the Darcy velocity within the depository? How does this differ from Problem 4, where the density of fresh water was used?

Figure 3-9. Partial Listing of SWIFT/SSP Input Data for Problem 10.

APPENDIX

COMPLETED DATA SETS

PROBLEM NO. 1	SWISS/SSP	EXAMPLE	ENGLISH	UNITY		
3/81	0	0			M-1-1	
	305	1	1	1	0	M-1-2
	3.2E-6	3.0E-6	0.3	0.0	1	0
	170.0	0.0	62.4	62.4	2	1
	0.0	-0.020.7	0.0		4	0
	405*1000.0					
	1.0					
	1000.0					
	50.0	50.0	0.3	-0.0129379	0.0	-2.897.1
	N	0				
	1	1	1	1	1	
	1.0	-2.8				
	305	305	1	1	1	
	2.0	2.0				
	0	0	1	3	0	0
	1	0.5				
	0	1	0			
	0	0	1			

PROBLEM NO.	3	SWIFT/SP	EXAMPLE	ENGLISH UNITS	
3701	0	0			M-1-1
	50	1	1	1	M-1-2
	100	MAD	1	0	M-2
	0.0				R0-1
	3.22-6	3.0E-6	107.0	1.0	R0-2
	170.0	0.0	62.5		M-1-1
	0.0	-5015.0	0.0		M-1-3
	50*100.0				M-1-16
	1.0				
	1000.0				
	50.0	50.0	0.3	-0.0128179	0.0
					-4000.0
	2	1	1	0	0
	1	2.5			
	2				
	1	-556.3			
	2	1.0E10			
	1	50	1	1	1
	25.0	0.0001			
	2	1	1	1	-1
	1000.0	0.0001			
	0	1	0		
	1	1	0		
	1				
	1	50	1	1	
	-0.00033				
	-1	0.5			
	1161.0	30.0			
	5	1	0	0	0
	0	0	1		

K3-7
K3-1
K3-6
K3-7
K3-8
K3-9
K3-1-END

1 1 1 1 0
0 0 0 0
J/S=1.25165 1.0
-1 -1 1 1 0
1 8.5999 1 1
19 43 1 1 15 10.0 F-5 1.0 1-2
0 0 0 1

K1-6
K3-7
K1-1
K3-6
K3-7
K1-1
K1-6
K3-7
K3-1-ENO

2.17	1	EB	3.05	EB	0
	0	0	0	0	0
2.1725	1	EB	3.05	EB	0
	0	0	0	0	0
2.555	1	EB	3.05	EB	1
	0	0	0	0	1

PROBLEM NO.	10	SWIFT/SSP	EXAMPLE	ENGLISH	UNITS	M-1-1										
3701						M-1-2										
	0	0	0			M-2										
	49	1	12	2	0	1	1	2	0	0	1	0	0	0	0	M-3
	.0000032	.000001	0.	0.	0.001	R1-1										
	170.	14.7	62.3	73.98		R1-3										
	14.7	-4482.9	0.			R1-16										
	24*5000.	40*4000.														
	1.0															
	333.3	333.4	333.3	2*200.0	100.0	2*50.0	100.0	2*200.0	300.0							
	50.	50.	1.5	.3	.012937864	0.0	-0413.7	R1-20								
	1	2	1	1	1	1		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	2	3	1	1	2	2		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	4	7	1	1	2	2		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	3	4	1	1	3	3		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	5	10	1	1	3	3		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	4	5	1	1	4	4		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	6	50	1	1	4	4		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	5	6	1	1	5	5		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	7	14	1	1	5	5		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	15	55	1	1	5	5		R1-21-1								
	1.00E-05	1.00E-05	1.00E-05	0.01				R1-21-2								
	50	64	1	1	5	5		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	65	64	1	1	5	5		R1-21-1								
	50.	50.	1.5	.3				R1-21-2								
	5	6	1	1	6	6		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	7	14	1	1	6	6		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	15	55	1	1	6	6		R1-21-1								
	1.00E-05	1.00E-05	1.00E-05	0.01				R1-21-2								
	50	64	1	1	6	6		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	65	69	1	1	6	6		R1-21-1								
	50.	50.	1.5	.3				R1-21-2								
	8	6	1	1	7	6		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	9	13	1	1	7	6		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	14	58	1	1	7	6		R1-21-1								
	1.00E-05	1.00E-05	1.00E-05	0.01				R1-21-2								
	59	64	1	1	7	6		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	65	64	1	1	7	7		R1-21-1								
	50.	50.	1.5	.3				R1-21-2								
	65	69	1	1	8	4		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	8	10	1	1	4	4		R1-21-1								
	40.	40.	7.	.3				R1-21-2								
	11	16	1	1	4	4		R1-21-1								
	.01	.01	.001	.3				R1-21-2								
	17	55	1	1	4	4		R1-21-1								
	1.00E-05	1.00E-05	1.00E-05	0.01				R1-21-2								
	50	64	1	1	4	4		R1-21-1								
	.01	.01	.001	.3				R1-21-2								

SWIFT/SSP STC

New Right Hand Page

Network Divide. Eureka Kernel. REFERENCES

REFERENCES

Cranwell, R. M., and Reeves, M., User's Manual for SWIFT/SSP, SAND81-2047, 1981.

Finley, N. C., and Reeves, M., SWIFT Self-Teaching Curriculum, NUREG/CR-1968, SAND81-0410, 1981.

Trescott, Peter C., Documentation of Finite Difference Model for Simulation of Three-Dimensional Groundwater Flow, U.S. Geol. Survey, Open File Report 75-438, 1975.

Trescott, P. C., and Larson, S. P., Supplement to Open File Report 75-438 (Trescott, 1975), U.S. Geol. Survey Open File Report 76-571, 1976.

Franke, O. L., and Cohen, Philip, "Regional Rates of Groundwater Movement on Long Island, New York," U.S. Geol. Survey Prof. Paper 800-C, p. C271-277, 1972.