
Verification of the Network Flow and Transport/Distributed Velocity (NWFT/DVM) Computer Code

Prepared by L. E. Duda

Sandia National Laboratories

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Prepared by
L. E. Duda

Sandia National Laboratories
Albuquerque, NM 87185

Prepared for
Division of Waste Management
Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
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ABSTRACT

The Network Flow and Transport/Distributed Velocity Method (NWFT/DVM) computer code was developed primarily to fulfill a need for a computationally efficient ground-water flow and contaminant transport capability for use in risk analyses where, quite frequently, large numbers of calculations are required. It is a semi-analytic, quasi-two-dimensional network code that simulates ground-water flow and the transport of dissolved species (radionuclides) in a saturated porous medium. The development of this code was carried out under a program funded by the U.S. Nuclear Regulatory Commission (NRC) to develop a methodology for assessing the risk from disposal of radioactive wastes in deep geologic formations (FIN: A-1192 and A-1266). In support of the methodology development program, the NRC has funded a separate Maintenance of Computer Programs project (FIN: A-1166) to ensure that the codes developed under A-1192 or A-1266 remain consistent with current operating systems, are as error-free as possible, and have up-to-date documentations for reference by the NRC staff. Part of this effort would include verification and validation tests to assure that a code correctly performs the operations specified and/or is representing the processes or system for which it is intended. This document contains four verification problems for the NWFT/DVM computer code. Two of these problems are analytical verifications of NWFT/DVM where results are compared to analytical solutions. The other two are code-to-code verifications where results from NWFT/DVM are compared to those of another computer code. In all cases NWFT/DVM showed good agreement with both the analytical solutions and the results from the other code.

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1. INTRODUCTION

The Network Flow and Transport/Distributed Velocity Method (NWFT/DVM) computer code was developed as part of a program, funded by the U.S. Nuclear Regulatory Commission (NRC), to develop a methodology for assessing the risk from disposal of radioactive wastes in deep geologic formations. The code was developed primarily to fulfill a need for a computationally efficient ground-water flow and contaminant transport capability for use in risk analyses where, quite frequently, large numbers of calculations are required. Its greatest strengths lie in its ability to include the combined effects of leaching and equilibrium solubility, treatment of transport path lengths much greater than the dispersivity, consideration of brine density effects on flow, and treatment of branching decay chains with contrasting half-lives and retardations.

In order to assess the accuracy of the NWFT/DVM computer code, several verification tests were performed and are included in this report. Generally, two types of tests are performed on a computer code to evaluate its accuracy, namely verification and validation tests. Verification tests are commonly used to provide "assurance that a computer code correctly performs the operations specified in a numerical code" (Silling, 1983). This is usually accomplished by comparison of code results with analytic solutions, although code-to-code comparisons may also be used. Validation tests are generally used to provide "assurance that a model as embodied in a computer code is a correct representation of the process or system for which it is intended" (Silling, 1983). This is usually done by comparison to field data or laboratory experiments. As NWFT/DVM is a network code designed to simulate two-dimensional flow and transport via one-dimensional path segments, many validation problems are beyond the scope of applicability of this code. Thus, for the present only verification problems are presented.

The purpose of this document is to present the results of four verification problems for NWFT/DVM. All four problems are verification of solute transport. The first two are one-dimensional radionuclide transport problems suggested as contaminant transport verification problems by Ross, et al. (1983). In addition, these problems were simulated by the SWIFT code (Reeves and Cranwell, 1981) and presented in the report on the validation and verification of that code by Ward, Reeves, and Duda (1983). The final two problems considered have already been reported in the NWFT/DVM User's Manual (Campbell, Longsine, and Cranwell, 1981). Both of these problems simulate quasi-two-dimensional solute transport. In one case (Problem 3) the results from NWFT/DVM are compared to those from an analytical solution (GETOUT), while in the other case (Problem 4) the results from NWFT/DVM are compared to those from the SWIFT computer code.

Additional verification tests of the Distributed Velocity Method may be found in Campbell, Longsine, and Reeves (1981a and b).

2. BRIEF DESCRIPTION OF NWFT/DVM

A detailed description of NWFT/DVM can be found in Campbell, Longsine, and Cranwell (1981). Briefly, the code simulates ground-water flow and the transport of dissolved species (radionuclides) in a saturated porous medium. Flow fields are represented as networks of one-dimensional path segments (or "legs"). The flow network used in NWFT/DVM (Figure 2.1) is loosely based on a hypothetical flow system, which, in the past, has served as a reference site for demonstrating a methodology for assessing the risk from disposal of radioactive wastes in bedded salt formations (Cranwell et al., 1982). The number of legs (15) and junctions (12) is currently fixed, but their location and properties are variable, providing some flexibility for simulating alternate flow fields.

Steady-state fluid flow is calculated in each leg of the network by first specifying (1) boundary pressures at the inlet junctions to the network (Junctions 1 and 2) and outlet junction (Junction 3), (2) hydraulic conductivity, cross-sectional area, length, porosity, and brine concentration of each leg, and (3) elevation (above datum) of each junction. Pressures at the remaining junctions are determined by solving conservation equations at each of the leg junctions. Fluid flow is then calculated by simultaneously solving, for each leg, the following equation:

$$Q_k = \frac{K_k A_k \mu_0}{\mu_k L_k \rho_0} [P_i - P_0 + \rho_k (D_i - D_0)] \quad (2-1)$$

where Q_k is the volumetric flow rate (ft³/day) in leg k ; P_i and P_0 are the pressures (lb/ft²) at the inlet and outlet junctions, respectively, of leg k ; D_i and D_0 are the junction elevations (ft) at the inlet and outlet junctions, respectively, of leg k , and

ρ_k = weight density of leg k (lb/ft³)
 K_k = hydraulic conductivity of leg k (ft/day)
 A = cross-sectional area of leg k (ft²)
 L = leg length (ft)
 μ = dynamic viscosity (in mixed units)

μ_0 and ρ_0 are the viscosity and density, respectively, of fresh water at the reference temperature (68°F).

Radionuclide transport in NWFT/DVM can be handled by either an analytic solution or by the Distributed Velocity Method (DVM)

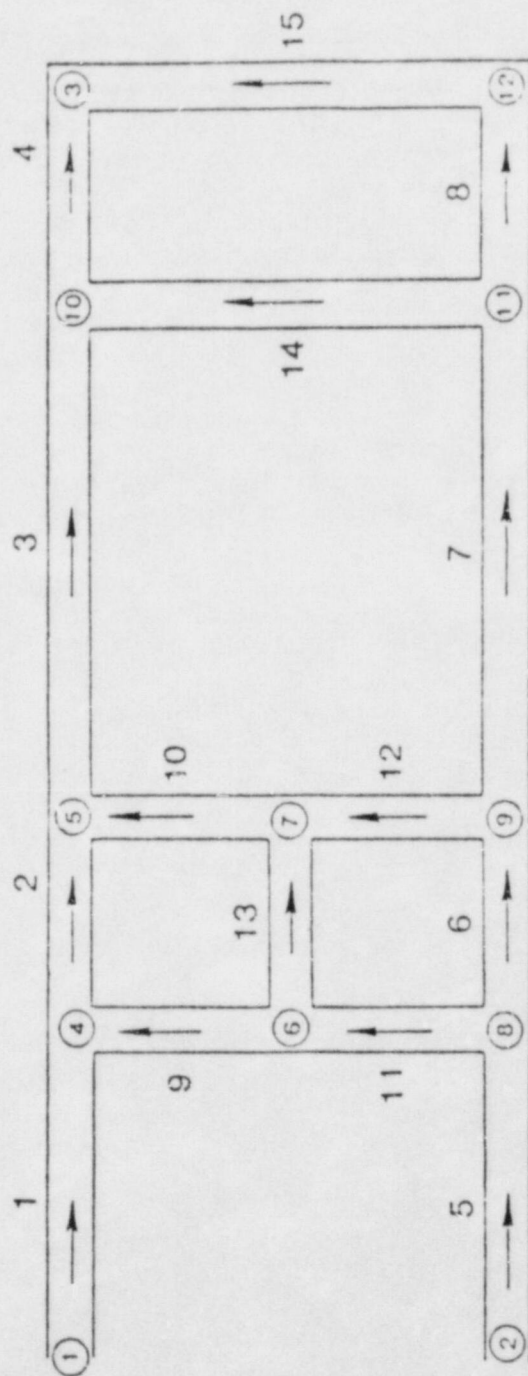


Figure 2-1. The Network Leg and Junction Numbering System.
Arrows indicate direction of positive flow.

which is unique to this code. The analytic solution is limited to decay chains of no more than three equally retarded isotopes and leach-limited source rates. The equations used are (see, e.g., Lester, Jansen, and Burkholder, 1975):

$$N_1(t) = \frac{N_1(0)}{2\tau} e^{-\lambda_1 t} [U(t) - U(t-\tau)H(t-\tau)] \quad (2-2)$$

$$N_2(t) = \left[\frac{N_2(0)}{2\tau} e^{-\lambda_2 t} + \frac{N_1(0)}{2\tau} \left(\frac{\lambda_1}{\lambda_2 - \lambda_1} \right) \left(e^{-\lambda_1 t} - e^{-\lambda_2 t} \right) \right] [U(t) - U(t-\tau)H(t-\tau)] \quad (2-3)$$

$$N_3(t) = \left[\frac{N_3(0)}{2\tau} e^{-\lambda_3 t} + \frac{N_2(0)}{2\tau} \left(\frac{\lambda_2}{\lambda_3 - \lambda_2} \right) (e^{-\lambda_2 t} - e^{-\lambda_3 t}) + \frac{N_1(0)}{2\tau} \lambda_1 \lambda_2 \left(\frac{e^{-\lambda_1 t}}{(\lambda_2 - \lambda_1)(\lambda_3 - \lambda_1)} + \frac{e^{-\lambda_2 t}}{(\lambda_1 - \lambda_2)(\lambda_3 - \lambda_2)} + \frac{e^{-\lambda_3 t}}{(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_3)} \right) \right] [U(t) - U(t-\tau)H(t-\tau)] \quad (2-4)$$

where

t = time (days)
 $N_r(0)$ = inventory of isotope r at time $t = 0$ (Ci)
 λ_r = decay constant of isotope r (days⁻¹)
 τ = leach time (days)
 $H(x) = 0$ for $x < 0$
 $H(x) = 1$ for $x \geq 0$

and

$$U(t) = \operatorname{erfc} \left(\frac{L_p - \bar{v}t}{\sqrt{4\alpha t \bar{v}}} \right) + e^{L_p/\alpha} \operatorname{erfc} \left(\frac{L_p + \bar{v}t}{\sqrt{4\alpha t \bar{v}}} \right) \quad (2-5)$$

where

α = dispersivity (ft)
 \bar{v} = average isotope velocity accounting for retardation (ft/day)
 L_p = distance from source to discharge point (ft).
 erfc = complementary error function

Details of the Distributed Velocity Method (DVM) can be found in either Campbell, Longsine, and Reeves (1980), Campbell, Longsine, and Reeves (1981a), or Campbell, Longsine, and Cranwell (1981). It is a direct simulation technique which, like other direct simulation methods, can simulate either convective or dispersive dominated regimes. Unlike other direct simulation techniques, DVM can treat radionuclide decay chains of arbitrary length and contrasting distribution coefficients. Furthermore, both leach- and/or solubility-limited sources are available using DVM.

Dispersion is treated in DVM by dividing the contaminant in each cell (grid block) into packets with different velocities. The velocities, of which there are N , are chosen so as to divide a Gaussian distribution of velocities into intervals of equal area. For a single specie, the amount $\rho(i,t)$ of the species arriving in cell i at time step t is given by

$$\rho(i,t) = \left[\frac{D}{N} \sum_j M_j \rho(i-k_j, t-1) + (1-M_j) \rho(i-k_j-1, t-1) \right] . \quad (2-6)$$

In this equation, D represents radioactive decay:

$$D = e^{-\lambda \Delta t} \quad (2-7)$$

where λ is the decay constant and Δt is the time step. k_j is the number of entire cells which can be traversed in one time step at velocity v_j :

$$k_j = \left\| \left\| \frac{v_j \Delta t}{\Delta x} \right\| \right\| . \quad (2-8)$$

The double bars indicate the integral part.

M_j is the fraction of cell $i-k_j$ which lies a distance $v_j \Delta t$ from points within cell i :

$$M_j = k_j + 1 - \frac{v_j \Delta t}{\Delta x} . \quad (2-9)$$

When a decay chain is involved, the creation of each species during the time interval by decay of its parents must be considered. The concentration of species r , ρ_r , is then given by

$$\rho_r(i, t) = \frac{1}{N} \sum_s D_{rs} \sum_j \left[M_j^{rs} \rho_s(i - k_j^{rs}, t-1) + (1 - M_j^{rs}) \rho_s(i - k_j^{rs} - 1, t-1) \right] \quad (2-10)$$

where s may be either r or any parent of r . When $r = s$, then D , k_j , and M are calculated from Equations (2-7)-(2-9). When $r \neq s$, D is the probability that an atom of species s at time $t - 1$ will have decayed into species r by time t . This is taken from the Bateman equation. k_j^{rs} and M_j^{rs} are calculated by replacing V_j in Equations (2-8) and (2-9) with

$$V_j^{rs} = \frac{1}{\Delta t} \sum_{n=s}^r T_n V_j^n \quad (2-11)$$

where n indicates the species in the decay chain from s to r , T_n is the mean time spent as species n , and V_j is the velocity of the j th packet of species n . This neglects the additional dispersion due to the range of possible decay times.

The amount of species r entering solution during a time step is the lesser of $C_r q \Delta t$, where C_r is the solubility and q the water flow rate, or the inventory of species r which has leached but, as yet, has not dissolved. This latter inventory is the sum of the amount of species r which leaches in the current interval and the amount which leached in previous intervals but did not dissolve.

3. PROBLEM 1: ONE-DIMENSIONAL TRANSPORT WITH CHAIN DECAY AND EQUAL RETARDATION PARAMETERS

3.1 Description of the Problem

In this problem a three component equally retarded radionuclide chain is released at a constant rate into a porous medium from a leach-limited source.

A schematic drawing of the problem is given in Figure 3-1.

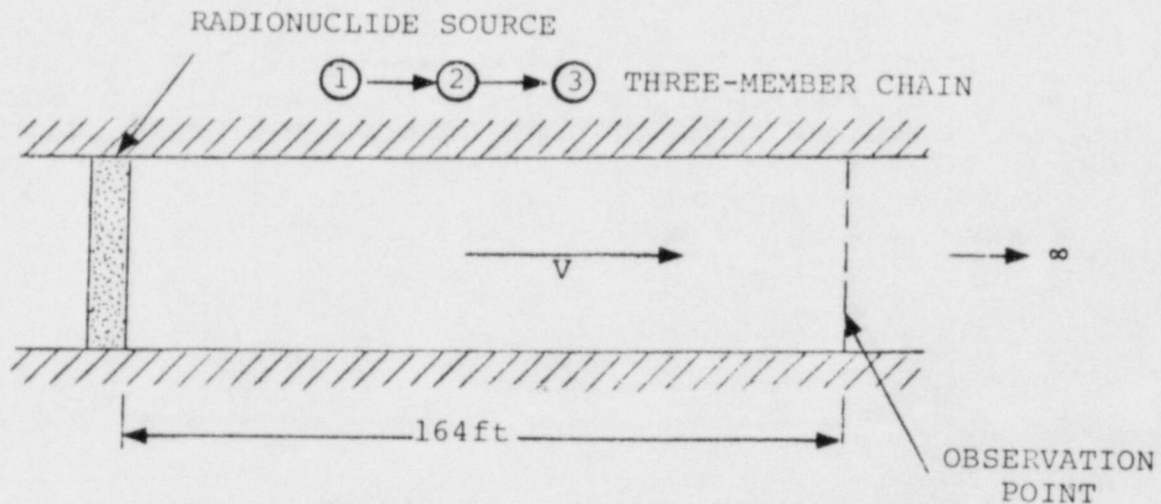


Figure 3-1. One-Dimensional Transport of a Three-Member Chain

The purpose of this problem is to compare the analytic solution for transport used in NWFT/DVM with the DVM solution. Both the analytic solution and DVM were briefly discussed in Chapter 2. The output by which the comparison is made consists of breakthrough curves of concentration versus time for each of the components at a distance of 164 ft from the source boundary.

3.2 Basic Assumptions

The following are assumptions that were invoked in the analysis of Problem 1:

- Hydraulic parameters are constant along the flow path.
- Radionuclide source is only leach limited (not solubility limited).
- Leach time and initial inventory of component 1 are essentially infinite.
- Leach rate is constant and nonzero.
- Dispersivity and retardation are constant along the flow path.

- f. All three radionuclide components have equal retardation.

3.3 Input Specifications

Input parameters used in NWFT/DVM for this problem are given in Tables 3-1, 3-2, and 3-3. Porosities, hydraulic conductivities (of Legs 1, 9, 13, 10, 3, and 4), retardation, leach time, dispersivity, boundary pressures (inlet and outlet pressures), migration path lengths, half-lives, and initial radionuclide inventories were all chosen to be consistent with those used in the SWIFT simulation of Problem 1 (see Ward, Reeves, and Duda, 1983).

In order to simulate Problem 1 using NWFT/DVM, the two-dimensional network of Figure 2-1 was collapsed to a one-dimensional system by placing all junctions at an elevation of zero feet. Flow was constrained primarily to Legs 1, 9, 13, 10, 3, and 4 by choosing low conductivities (1×10^{-20} ft/day) for the remaining legs of the network. Leg 13 serves as the source leg, with radionuclide migration beginning at the midpoint of this leg. Thus, the migration path begins at the midpoint of Leg 13 and continues through Legs 10, 3, and 4. As the total migration path length is 164 ft, the lengths of Legs 13, 10, 3, and 4 were set at 60 ft, 14 ft, 60 ft, and 60 ft, respectively. The remaining leg lengths are given in Table 3-1. The cross-sectional area of each leg was arbitrarily set at 1 ft². Variable fluid density and viscosity may be accounted for in NWFT/DVM by specifying brine concentrations for each leg of the network. For Problem 1, brine concentrations are assumed to be zero. The value of 2.747×10^7 years for leach time (Table 3-1) and 1.535×10^{17} curies for initial inventory of Component 1 (Table 3-2) are meant to represent infinite values for each of these parameters, and are consistent with those used in the SWIFT simulations.

Retardation in NWFT/DVM is approximated by a linear equilibrium sorption isotherm using the equation

$$R = 1 + K_d \rho / \phi \quad (3-1)$$

where

- R = retardation factor
- K_d = distribution coefficient (ft³/lb)
- ρ = rock density (lb/ft³)
- ϕ = porosity.

The rock density value selected for each leg of the network was 120 lb/ft³. A distribution coefficient value of 7.793 ft³/lb was chosen for each of the radionuclide components. Thus, with a porosity of 0.1, the retardation factor is ≈ 9352 , which is

Table 3-1
Flow and Transport Parameters for Problem 1

Parameter	Value
Porosity	0.1 (all legs)
Hydraulic Conductivity (ft/day)	1.9 (Legs 1, 3, 4, 9, 10, and 13) 1×10^{-20} (remaining legs)
Cross-sectional area (ft ²)	1 (all legs)
Leg Length (ft)	60 (Legs 1-8, and 13) 14 (Legs 9-12) 28 (Legs 14 and 15)
Density (lb/ft ³)	120 (all legs)
Brine Concentration	0 (all legs)
Junction Elevation (ft)	0 (all junctions)
Dispersivity (ft)	8.5 (all legs of transport path)
Distribution Coefficient (ft ³ /lb)	7.793 (all components and all legs of transport path)
Migration Path Length (ft)	164
Leach Time (yrs)	2.747×10^7
Inlet Pressure (psi)	48.27 (Junctions 1 and 2)
Outlet Pressure (psi)	10.0 (Junction 3)

Table 3-2
Half-Lives and Initial Inventory
of Radionuclides for Problem 1

Name	Half-Life (y)	Decay Constant (y ⁻¹)	Initial Amount (Curies)
COMP1	433	1.6×10^{-3}	1.535×10^{17}
COMP2	15	4.62×10^{-2}	0.0
COMP3	6540	1.06×10^{-4}	0.0

Table 3-3
Time- and Space-Step Parameters
for Problem 1

Δx	5.0 ft
Δt	100.0 yrs
C	4.9 ^a

^a For all components.

consistent with the value used in the SWIFT simulation of Problem 1.

As is the case with finite-difference and finite-element implementations, the Courant number is important in DVM for controlling numerical dispersion. The Courant number C , is given by

$$C(r) = \bar{v}(r) \frac{\Delta t}{\Delta x} \quad (3-2)$$

where r is the isotope, \bar{v} is the mean velocity of isotope r , Δt is the time step, and Δx is the grid-block size. For centered-in-time, finite-difference implementations, C is typically limited (to first order) by:

$$C < 2 \quad (3-3)$$

However, in DVM, the dependence of effective dispersivity on the Courant number is an inverse dependence (see, e.g., Campbell, Longsine, and Reeves, 1981b). Thus, rather than bounding the Courant numbers from above, as in Equation 3-3, it must be bounded from below in DVM. Typically, for DVM, $C \geq 1$ (Campbell, Longsine, and Reeves, 1981b) and should be adjusted so that each isotope, if possible, satisfies this criterion. Thus, from Equation 3-2, it is advantageous to maximize the time step and minimize the grid-block size in NWFT/DVM.

There is a space- and time-step selection subroutine in NWFT/DVM which takes into account not only minimization of numerical dispersion, as discussed above, but also source-pulse length (in space and time), radionuclide half-lives, desired resolution of discharge curves, and machine storage and execution time (see Campbell, Longsine, and Cranwell, 1981). However, the user may choose to input Δx and Δt . This was the case for Problem 1, as it was desired to have output at specified times. The time step and space step (and corresponding Courant number) used in Problem 1 are given in Table 3-3. These were arrived at by an iterative process of running the code, observing the isotope velocities, adjusting Δt (and Δx if necessary), rerunning the code, etc., until the criterion

$$\min_r \{C(r) \geq 1\}$$

was satisfied, where r is the isotope. Other guidelines are recommended for user input of Δx and Δt (see Campbell, Longsine, and Cranwell, 1981) but these were not applicable in this problem.

3.4 Results

Calculated breakthrough curves for Problem 1 from DVM and the analytic solution are shown in Figure 3-2. As this figure indicates, the analytic and DVM results agree extremely well. More precise agreement would probably have been possible if the space- and time-step selection subroutine in NWFT/DVM would have been used. However, as output at specified times and location was desired, it would have been difficult to compare the two results if the automatic space- and time-step option had been selected.

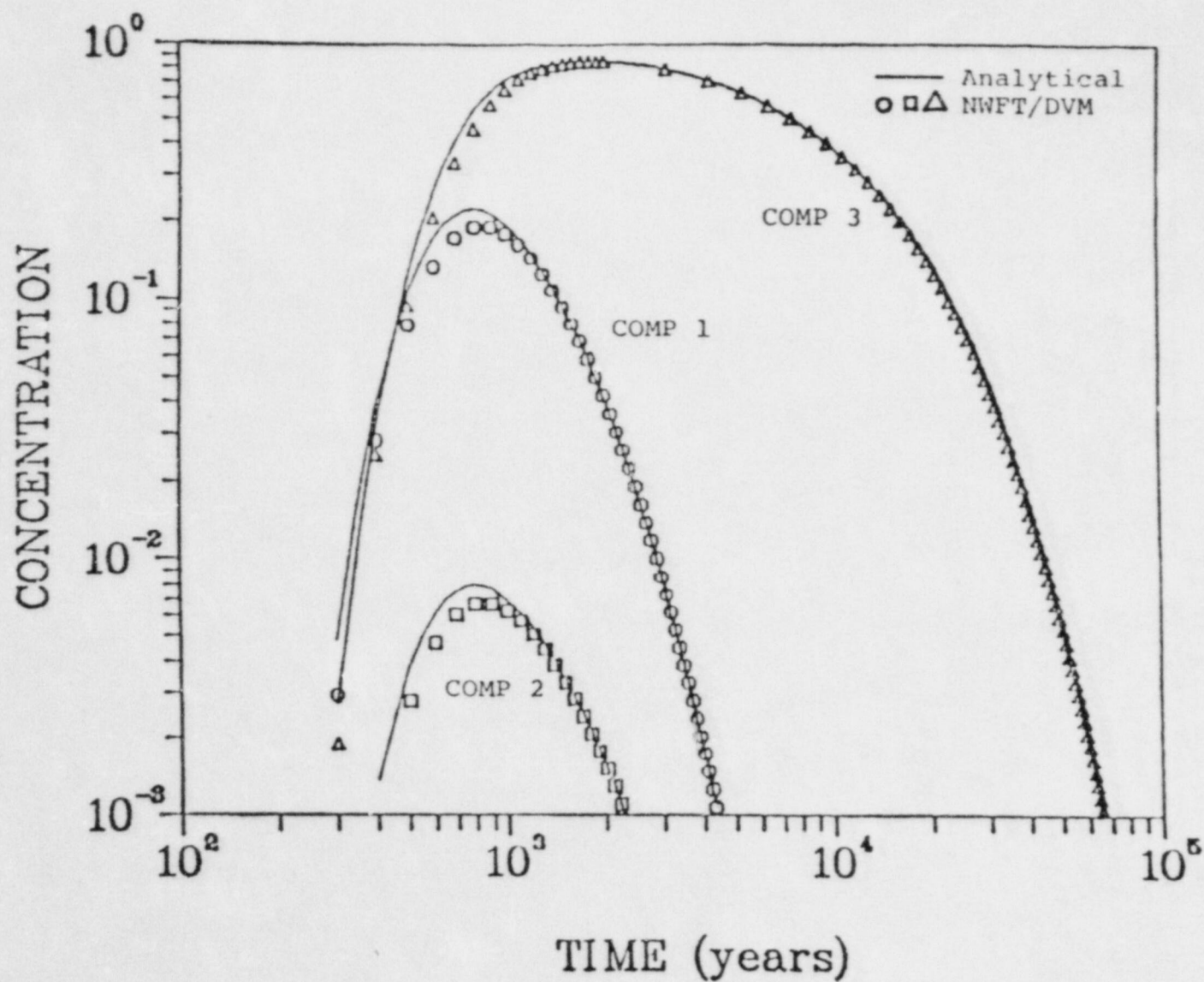


Figure 3-2. Comparison of Results for Problem 1 for DVM and the Analytical Solution

4. PROBLEM 2: ONE-DIMENSIONAL TRANSPORT WITH CHAIN DECAY AND UNEQUAL RETARDATION PARAMETERS

4.1 Description of the Problem

Problem 2 is designed to test the capability of NWFT/DVM to handle radionuclides with contrasting retardations. It is equivalent to Problem 1 of the International Nuclide Transport Code Intercomparison study (INTRACOIN) (INTRACOIN, 1981, 1982) and was suggested by Ross et al. (1982) as a second contaminant transport verification problem.

In this problem, a one-dimensional system is simulated similar to that described in Problem 1. Here, however, the migration path length is 1640 ft, and two independent 3-member decay chains, each with contrasting retardation factors, are transported. Two sets of retardation factors are considered, resulting in a total of four separate runs of NWFT/DVM. (Since NWFT/DVM is currently not designed to handle multiple decay chains, each of the decay chains has to be run for each set of retardation factors). The two chains, half-lives, initial inventories, and two sets of retardation factors are given in Table 4.1. The four cases considered are: Case 1: I_1 , R_1 ; Case 2: I_1 , R_2 ; Case 3: I_2 , R_1 ; and Case 4: I_2 , R_2 .

4.2 Basic Assumptions

The following assumptions were invoked in the analysis of Problem 2.

- a. Hydraulic parameters are constant along the flow path.
- b. Radionuclide source is leach limited only.
- c. Leach rate is constant and nonzero for $t < T$ (leach time).
- d. Dispersivity and retardation are constant along flow path.
- e. Radionuclide components have contrasting retardations.

4.3 Input Specifications

Table 4-2 contains values of the flow and transport parameters used in the simulation of Problem 2. These values are the same for all four cases of Problem 2 and are consistent with those specified in INTRACOIN and used in the SWIFT simulations of this problem (Ward, Reeves, and Duda, 1983). As with Problem 1, the network of Figure 2-1 was collapsed to a one-dimensional system and transport was through Legs 13, 10, 3, and 4. Set 1 of the distribution coefficient corresponds to set R_1 of the retardation factors of Table 4-1. Similarly, set 2 of the distribution coefficient corresponds to set R_2 .

Table 4-1

Isotope Half-Lives, Inventories, and
Retardation Factors for Each of the
Four Cases of Problem 2

Isotope Set	Nuclides	Half-Life (y)	Inventory (Ci)	Retardation	
				Set R ₁	Set R ₂
I ₁	U234	2.445×10^5	1.0	300	60
	Th230	7.700×10^4	0.01	20,000	500
	Ra226	1.600×10^3	0.004	10,000	20
I ₂	Cm245	8.500×10^3	0.7	5,000	60
	Np237	2.140×10^6	1.0	700	200
	U233	1.592×10^5	0.004	300	60

Table 4-2
Flow and Transport Parameters
for Problem 2

Parameter	Value	
Porosity	0.01 (all legs)	
Hydraulic Conductivity (ft/day)	2.835 x 10 ⁻¹ (legs 1, 3, 4, 9, 10, 13) 1 x 10 ⁻²⁰ (remaining legs)	
Cross-sectional Area (ft ²)	1076.5 (all legs)	
Leg Lengths (ft)	520 (Legs 1 and 5) 600 (Legs 2-4, 6-8, and 13) 140 (Legs 9-12) 280 (Legs 14 and 15)	
Density (lb/ft ³)	170 (all legs)	
Brine Concentration	0 (all legs)	
Junction Elevation (ft)	0 (all junctions)	
Dispersivity (ft)	164	
Distribution Coefficient (ft ³ /lb)	<u>Set 1</u>	<u>Set 2</u>
U234	.01759	.003471
TH230	1.176	.02935
RA226	.5882	.001118
CM245	.2941	.003471
NP237	.04112	.01171
U233	.01759	.003471
Migration Path Length (ft)	1640	
Leach Time (y)	10 ⁵	
Inlet Pressure (psi)	10.361 (Junctions 1 and 2)	
Outlet Pressure (psi)	10 (Junction 3)	

of the retardation factor. These values are constant in all legs of the migration path. The space- and time-steps used in each of the four cases are given in Table 4-3 and were chosen to minimize numerical dispersion per the discussion in Section 3.

4.4 Results

The results of Problem 2 are presented in terms of discharge concentrations at a distance of 1640 ft. from the source and are compared to those of the SWIFT simulation of the same problem (Ward, Reeves, and Duda, 1983). Since the analytical solution for transport in NWFT/DVM cannot handle decay chains with contrasting retardation factors, a comparison with the analytical solution was not possible.

Plots showing comparisons between NWFT/DVM and SWIFT for the four cases are shown in Figures 4-1 through 4-4. Table 4-4 shows the comparisons between NWFT/DVM and SWIFT for the four parameters:

C_{max} ,	maximum concentration;
T_{max} ,	time corresponding to C_{max} ;
$T+50\%$,	time of the first occurrence of the concentration $C_{max}/2$;
$T-50\%$,	time of the last occurrence of the concentration $C_{max}/2$.

These were the parameters suggested by INTRACON to facilitate comparison of the results of different codes (INTRACON, 1981, 1982).

This set of four cases, as evidenced by the variety of shapes shown in Figures 4-1 through 4-4, constitutes a rather stringent test of the treatment of radionuclide-chain decay and transport within NWFT/DVM. The agreement with SWIFT is reasonably good. Differences seen are possibly due to the different space- and time-step criteria of each code. Concentration values are somewhat sensitive to these criteria.

Table 4-3
Time-and Space-Step Parameters for Problem 2

Case	Δt (y)	Δx (ft)
1	3,000	2 5
2	500	25.0
3	2,000	10.0
4	500	25.0

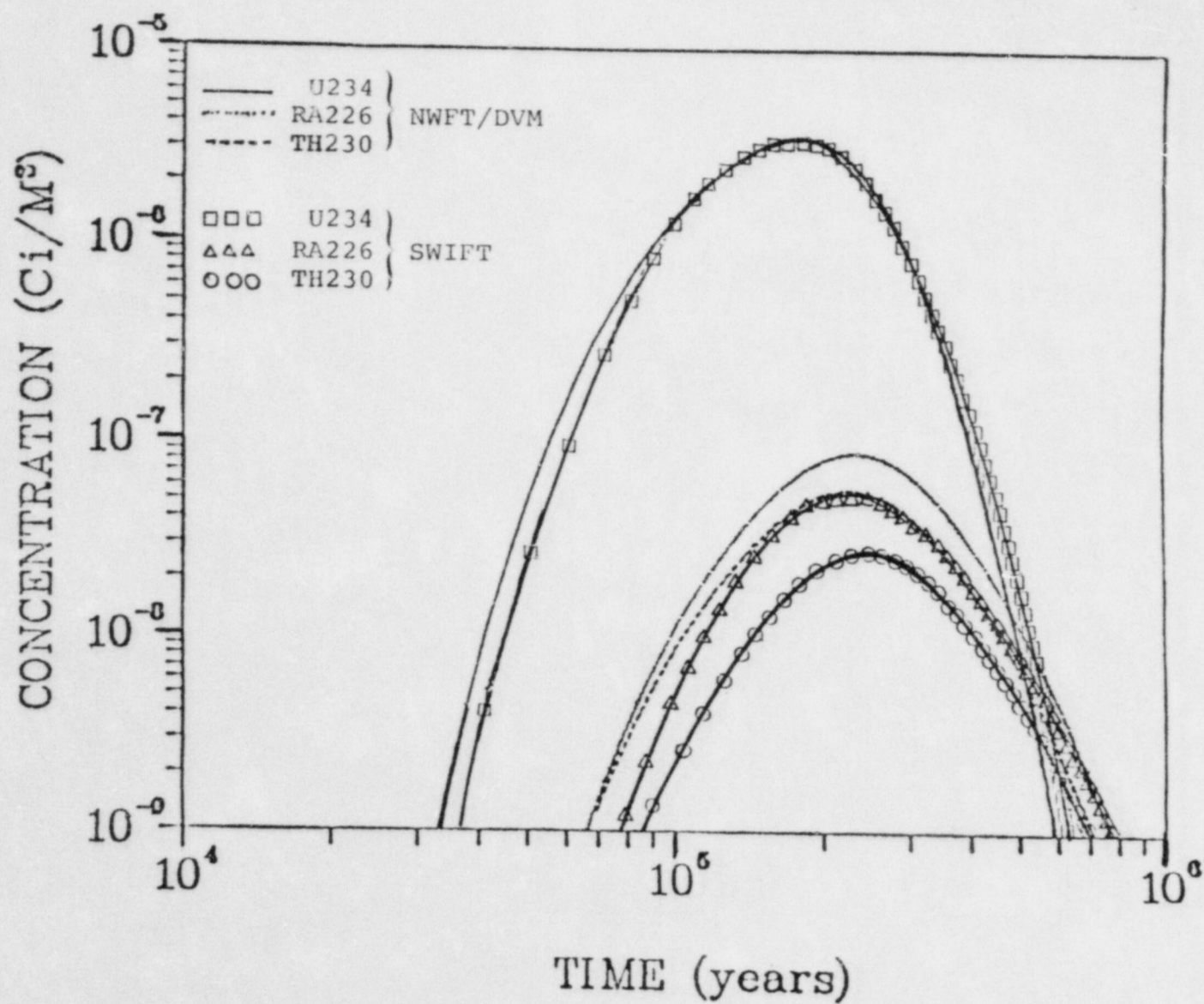


Figure 4-1. Radionuclide Discharge Concentrations for Problem 2, Case 1

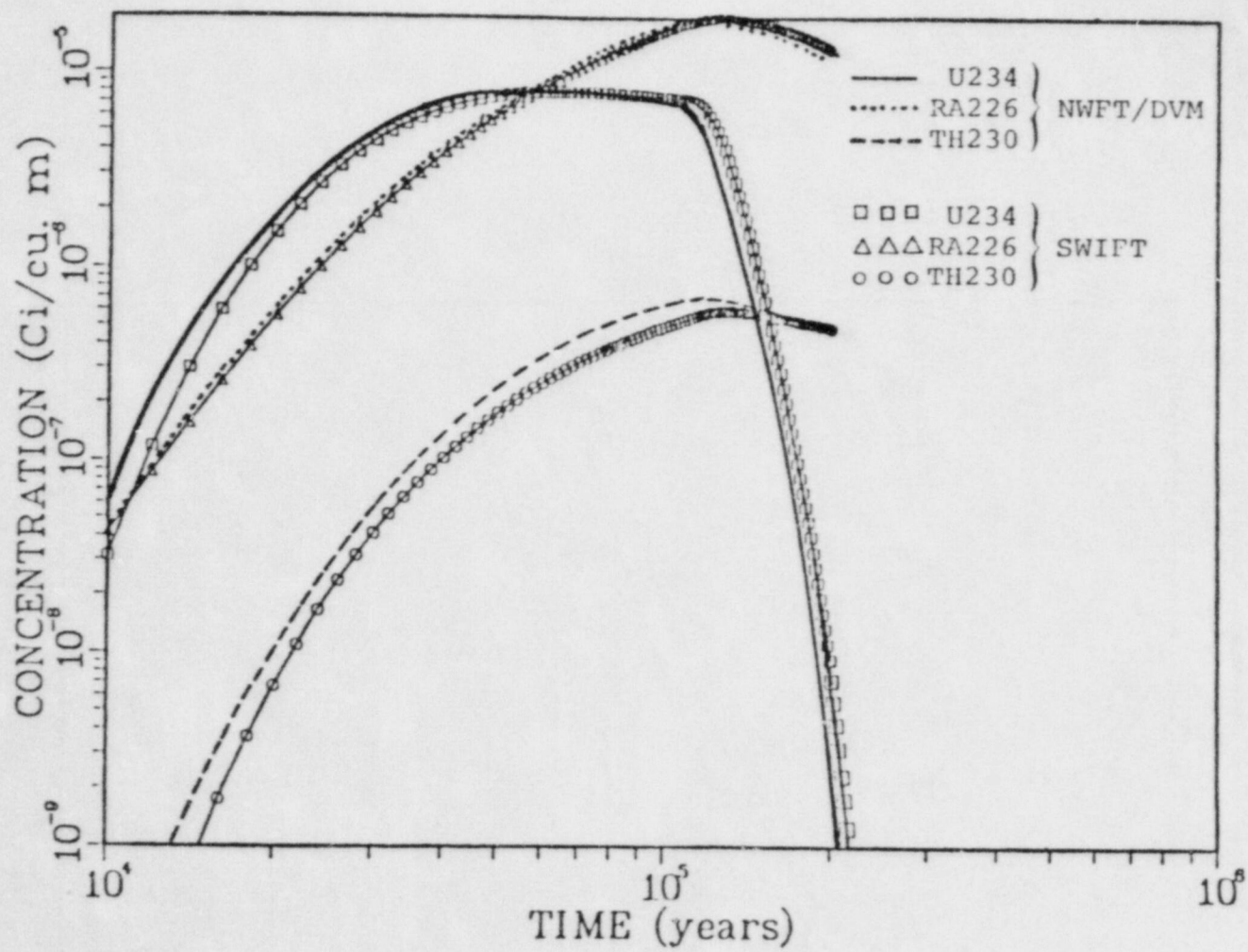


Figure 4-2. Radionuclide Discharge Concentrations for Problem 2, Case 2

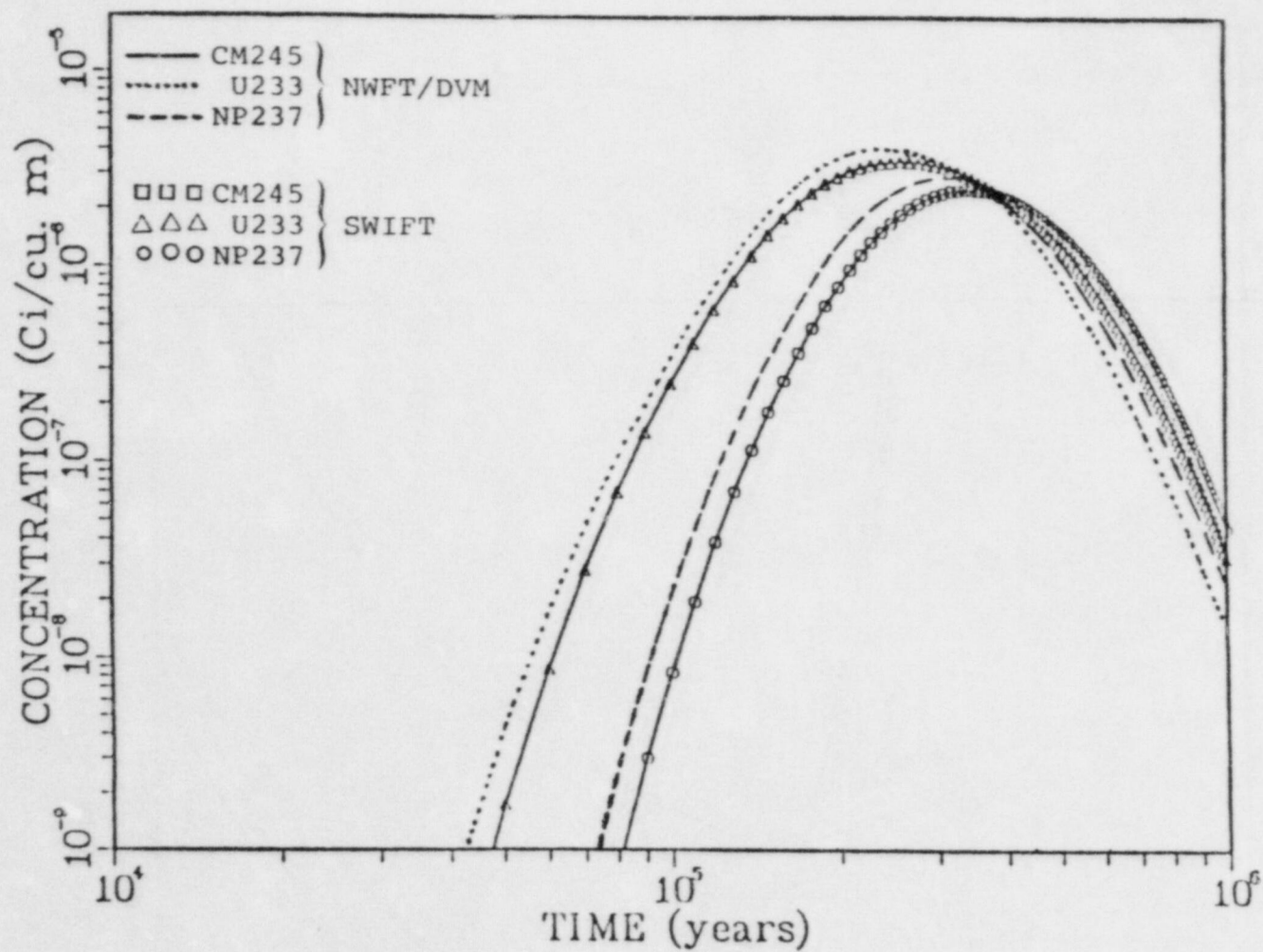


Figure 4-3. Radionuclide Discharge Concentrations for Problem 2, Case 3

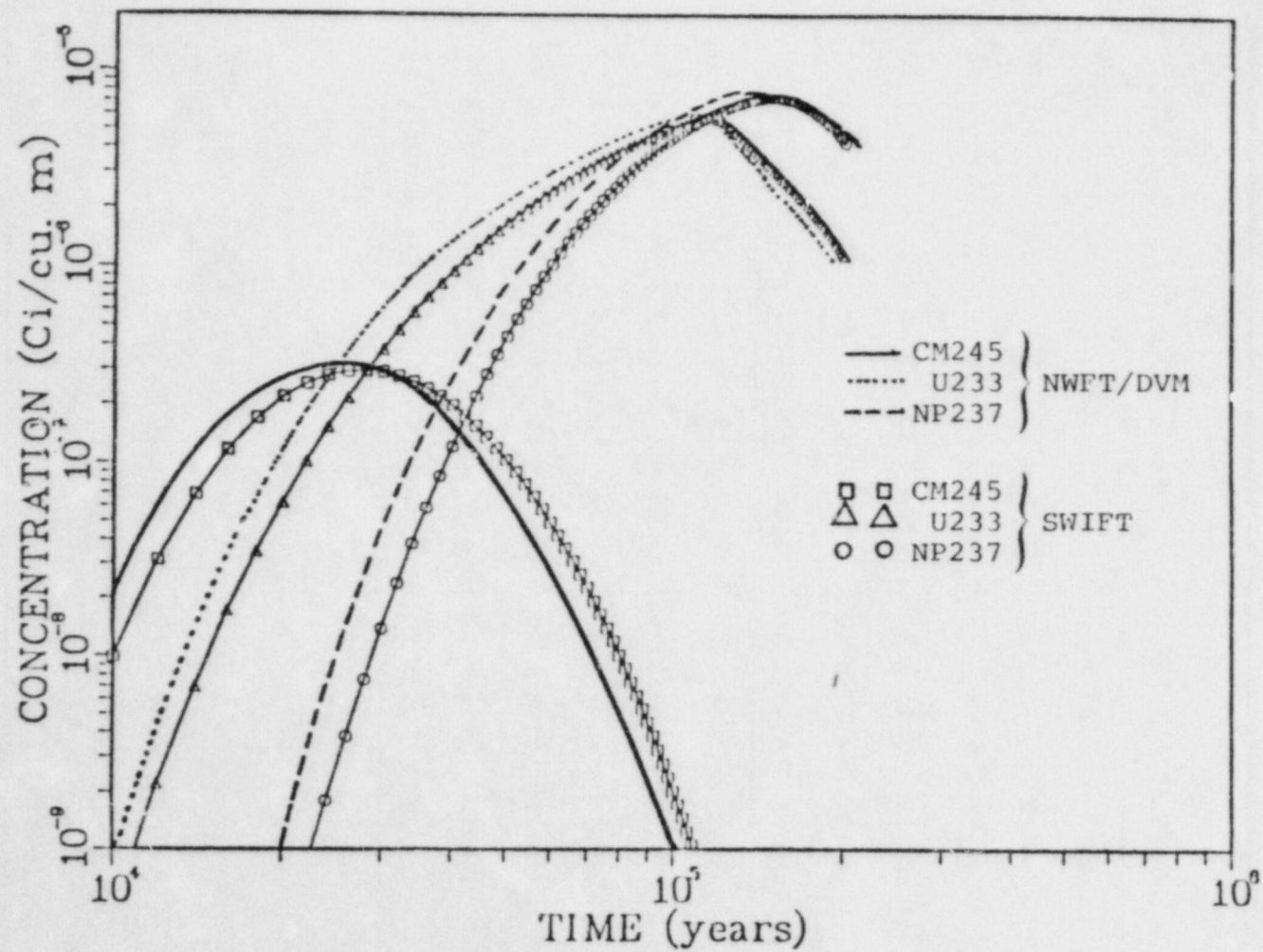


Figure 4-4. Radionuclide Discharge Concentrations for Problem 2, Case 4

Table 4-4

Comparison of NWFT/DVM and SWIFT
for the Four Cases of Problem 2

Case	Nuclide	Code	C_{\max} (Ci/m ³)	T_{\max} (y)	T+50% (y)	T-50% (y)
I_1, R_1	U234	NWFT	3.44×10^{-6}	1.80×10^5	1.11×10^5	2.58×10^5
		SWIFT	3.53×10^{-6}	1.77×10^5	1.14×10^5	2.57×10^5
	Th230	NWFT	5.66×10^{-8}	2.28×10^5	1.44×10^5	3.51×10^5
		SWIFT	3.21×10^{-8}	2.43×10^5	1.56×10^5	3.86×10^5
	Ra226	NWFT	8.77×10^{-8}	2.34×10^5	1.48×10^5	3.60×10^5
		SWIFT	6.42×10^{-8}	2.46×10^5	1.57×10^5	3.88×10^5
I_1, R_2	U234	NWFT	7.74×10^{-6}	7.10×10^4	2.83×10^4	1.31×10^5
		SWIFT	8.03×10^{-6}	6.59×10^4	2.85×10^4	1.28×10^5
	Th230	NWFT	6.42×10^{-7}	1.32×10^5	6.65×10^4	2.67×10^5
		SWIFT	5.93×10^{-7}	1.31×10^5	6.61×10^4	4.80×10^5
	Ra226	NWFT	1.81×10^{-5}	1.28×10^5	6.70×10^4	2.32×10^5
		SWIFT	1.93×10^{-5}	1.26×10^5	6.53×10^4	2.20×10^5
I_2, R_1	Cm245	NWFT	0.	-	-	-
		SWIFT	0.	-	-	-
	Np237	NWFT	2.60×10^{-6}	3.40×10^5	2.18×10^5	5.18×10^5
		SWIFT	2.49×10^{-6}	3.44×10^5	2.25×10^5	5.37×10^5
	U233	NWFT	3.54×10^{-6}	2.54×10^5	1.57×10^5	4.32×10^5
		SWIFT	3.45×10^{-6}	2.61×10^5	1.58×10^5	4.52×10^5

Table 4-4 (Continued)

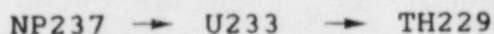
Case	Nuclide	Code	C_{\max} (Ci/m ³)	T_{\max} (y)	T+50% (y)	T-50% (y)
I ₂ , R ₂	Cm245	NWFT	2.95×10^{-7}	2.65×10^4	1.60×10^4	4.37×10^4
		SWIFT	2.96×10^{-7}	2.76×10^4	1.73×10^4	4.47×10^4
	Np237	NWFT	7.04×10^{-6}	1.52×10^5	8.70×10^4	2.12×10^5
		SWIFT	7.32×10^{-6}	1.47×10^5	8.94×10^4	2.00×10^5
	U233	NWFT	5.65×10^{-6}	1.18×10^5	6.67×10^4	1.56×10^5
		SWIFT	5.74×10^{-6}	1.14×10^5	6.54×10^4	1.65×10^5

5. PROBLEM 3: QUASI-TWO-DIMENSIONAL TRANSPORT WITH CHAIN DECAY AND UNEQUAL RETARDATION PARAMETERS

5.1 Description of the Problem

Problem 3 simulates what is generally referred to as a "U-tube" breachment scenario of an underground waste repository. In this case, the repository is assumed to be located in a layer of bedded salt. A schematic representation of this scenario is given in Figure 5-1. Fresh water enters the repository through the vertical conduit on the up-gradient side of the repository, dissolves leached radionuclides in the repository, and exits through the vertical conduit on the down-gradient side of the repository.

The three-member decay chain



was transported from the repository to a discharge location 142,500 ft from the source. This problem is identical to Problem 2 in the NWFT/DVM User's Manual (Campbell, Longsine, and Cranwell, 1981). The results from NWFT/DVM are compared to those of the analytic computer code GETOUT (DeMier, Cloninger, and Burkholder, 1979). Briefly, GETOUT uses analytical solutions of the solute transport equation for one-, two-, or three-member chains. Longer chains are approximated by using these solutions. The analytic solution may be written as

$$B_i \frac{\partial C_i}{\partial t} = D \frac{\partial^2 C_i}{\partial x^2} - V \frac{\partial C_i}{\partial x} - B_i \lambda_i C_i + B_{i-1} \lambda_{i-1} C_{i-1} \quad (5-1)$$

where C is concentration, B is retardation factor, D is dispersion coefficient, V is pore velocity, and λ is the radioactive decay constant. The subscripts refer to position in the decay chain.

The equations are solved for an impulse release, for a decaying band release, and for a decaying step function release. The solutions are too complicated to display here, but are given in the paper by Burkholder and Rosinger (1980).

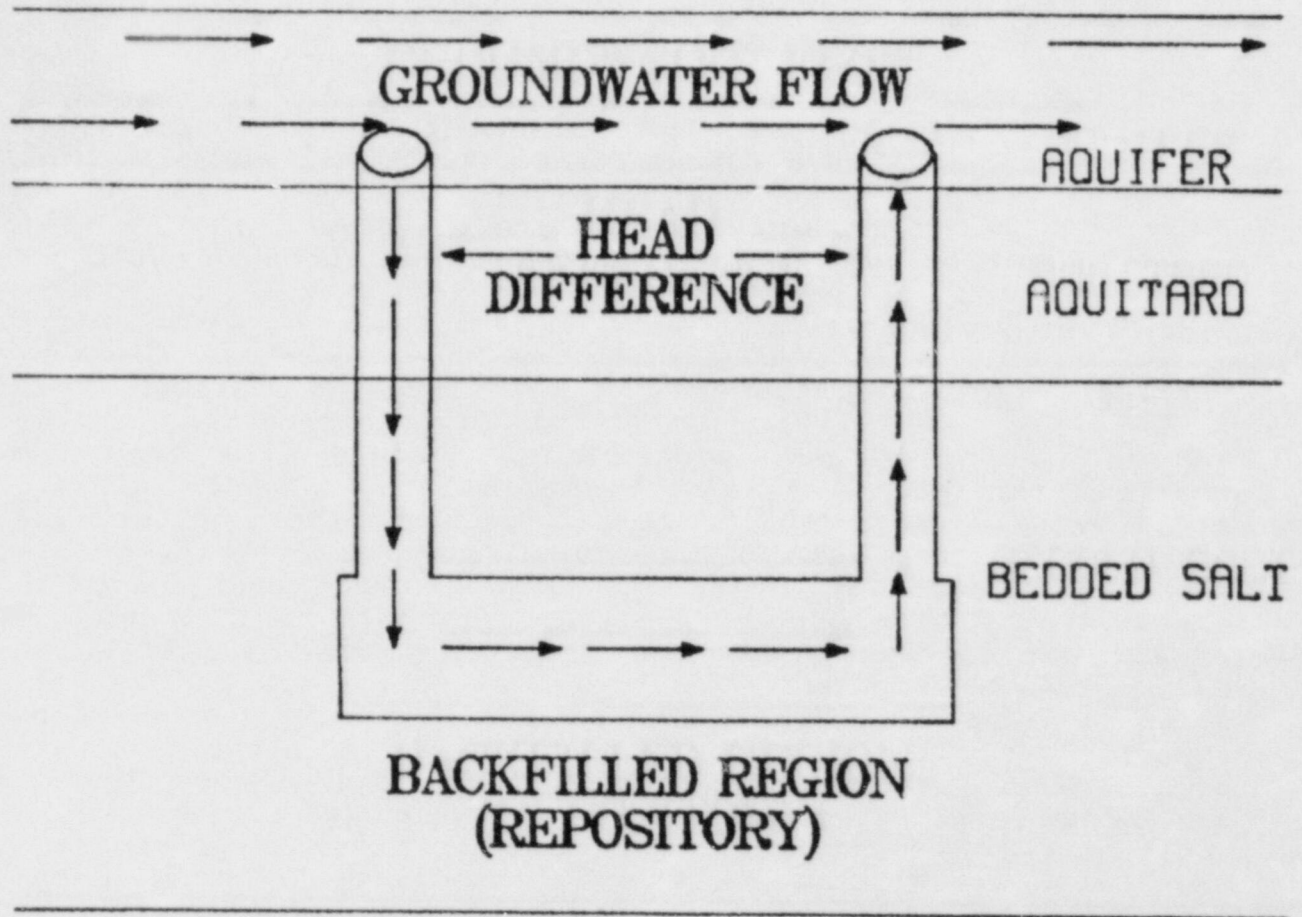


Figure 5-1. U-tube Scenario of Problem 3

Problem 3 was simulated using NWFT/DVM and the network of Figure 2-1 in the following manner: Legs 1, 2, 3, and 4 were used to represent an overlying aquifer, and Legs 5, 6, 7, and 8 an underlying aquifer. Leg 15 represents a hydraulic communication from the lower aquifer to a discharge point at Junction 3. Leg 9 was used to represent the up-gradient vertical conduit to the overlying aquifer and Leg 10 the down-gradient conduit. In this problem, Leg 9 was chosen as a 30-foot diameter shaft and Leg 10 a 13.5-inch diameter borehole. Leg 13 represents the repository. Legs 11, 12, and 14 were assigned low hydraulic conductivities so as to restrict flow in these legs.

5.2 Basic Assumptions

The following assumptions were invoked in the simulation of Problem 3.

- a. Hydraulic parameters vary along the flow path.
- b. Radionuclide source is leach limited only.
- c. Leach rate is constant for $t < T$ (leach time).
- d. Dispersivity is constant along the flow path.
- e. Retardation factors vary along the flow path.
- f. Radionuclide components have contrasting retardations.

5.3 Input Specifications

Input parameters for Problem 3 are given in Tables 5-1 and 5-2. Table 5-1 contains values of input parameters for flow and transport. These values were obtained from the hypothetical reference bedded-salt site which was used in demonstrating the Bedded-Salt Risk Assessment Methodology (see Cranwell et al., 1982). The upper and lower aquifer inlet pressures (Junctions 1 and 2, respectively), and the outlet pressure (Junction 3) were obtained from the SWIFT simulation of the hypothetical site (see, e.g., Campbell, Longsine, and Cranwell, 1981). Rock densities were not read in for this problem. When not read in, the rock density in NWFT/DVM defaults to $170 \text{ lb/ft}^3 \times (1-\phi)$, where ϕ is the porosity. Brine concentrations of zero for Legs 1-8 and 15 come from the assumption that both aquifers are fresh water. Brine concentrations of 1 for Legs 11-14 come from the assumption that these legs are through bedded-salt formations. The brine concentration of .67 for Leg 9 was determined by assuming that fresh water enters from the overlying aquifer and remains fresh throughout the aquitard located between the aquifer and the salt (see Figure 5-1). The remaining portion of Leg 9 is assumed to be through the bedded salt. Thus, it is assumed that the fresh water becomes saturated brine at this point. Hence, the brine concentration of Leg 9 is estimated as (length of Leg 9 in salt)/(total length of Leg 9). In this problem, the thickness of the aquitard is assumed to be 200 ft. (see Cranwell et al., 1982). From Table 5-1, the total length of Leg 9 is 600 ft. Thus, the brine concentration of Leg 9 is $600-200/600 = 400/600 = 0.67$. The brine concentration of 1 in Leg 10 comes from the assumption that saturated brine is exiting through this leg.

It was assumed that no sorption of radionuclides took place in Legs 13 and 10. Thus, a distribution coefficient of 0 was placed in these legs for all three radionuclides. This results in a retardation of 1 for Legs 13 and 10 (see Equation 3-1). Distribution coefficients of 10, 1.6, and 1 were assigned to NP237, U233, and TH229, respectively, for the remainder of the legs in the transport path. These values are based

Table 5-1
Flow and Transport Parameters
for Problem 3

Parameter	Value
Porosity	0.30 (Legs 1-8, 13, and 15) 0.15 (Legs 9 and 10) 0.03 (Legs 11, 12, and 14)
Hydraulic Conductivity (ft/day)	50 (Legs 1-4) 40 (Legs 5-8) 0.1 (Leg 9) 10 (Legs 10 and 13) 1.67×10^{-6} (Leg 11) 1.5×10^{-6} (Leg 12) 1.57×10^{-6} (Leg 14) 2.5 (Leg 15)
Cross-sectional Area (ft ²)	6×10^6 (Legs 1-4) 1.8×10^6 (Legs 5-8) 707 (Leg 9) 1 (Legs 10-12 and 14) 540 (Leg 13) 1.2×10^8 (Leg 15)
Leg Length (ft)	14,500 (Legs 1 and 5) 8000 (Legs 2, 6, and 13) 38,000 (Legs 3 and 7) 1×10^5 (Legs 4 and 8) 600 (Leg 9) 496.5 (Leg 10) 500 (Leg 11) 603.5 (Leg 12) 1100 (Legs 14 and 15)
Brine Concentration	0 (Legs 1-8 and 15) 0.67 (Leg 9) 1 (Legs 10-14)
Junction Elevation (ft)	3602.41 (Junction 1) 2502.41 (Junction 2) 1525.89 (Junction 3) 3414.81 (Junction 4) 3311.31 (Junction 5) 2814.81 (Junctions 6 and 7)

Table 5-1 (Continued)

Parameter	Value
Junction Elevation (ft) (Cont.)	2314.81 (Junction 8) 2211.31 (Junction 9) 2819.67 (Junction 10) 1717.67 (Junction 11) 425.89 (Junction 12)
Dispersivity (ft)	500 (all legs of transport path)
Distribution Coefficient (ft ³ /lb)	0 (all components, Legs 13 and 10) 10 (NP237, Legs 3 and 4) 1.6 (U233, Legs 3 and 4) 1.0 (Th229, Legs 3 and 4)
Migration Path Length (ft)	142,500
Leach Time (y)	10 ⁵
Upper Aquifer Pressure (psi)	432.70 (Junction 1)
Lower Aquifer Pressure (psi)	646.10 (Junction 2)
Outlet Pressure (psi)	432.70 (Junction 3)

Table 5-2

Isotope Half-Lives, Initial Inventory,
and Retardation Factors for Problem 3

Isotope	Half-Life (y)	Inventory (Ci)	Retardation	
			Legs 13 & 10	Legs 3 & 4
NP237	2.140×10^6	1.00×10^3	1	3968
U233	1.620×10^5	1.00×10^3	1	636
Th229	7.300×10^3	1.00×10^3	1	398

on typical values for clean sandstone (see, e.g., Cranwell et al., 1982). Using Equation 3-1, retardation values of 3968, 636, and 398 are obtained for NP237, U233, and TH229, respectively.

The half-lives, initial inventories, and retardation factors of the three isotopes are given in Table 5-2. Space and time steps were set by the code for this problem. The values chosen by the code were $\Delta t = 1.20 \times 10^4$ (years) and $\Delta x = 2.45 \times 10^3$ (ft).

5.4 Results

The comparison between NWFT/DVM and GETOUT for Problem 3 is shown in Figure 5-2. As can be seen, the agreement between these two codes is excellent.

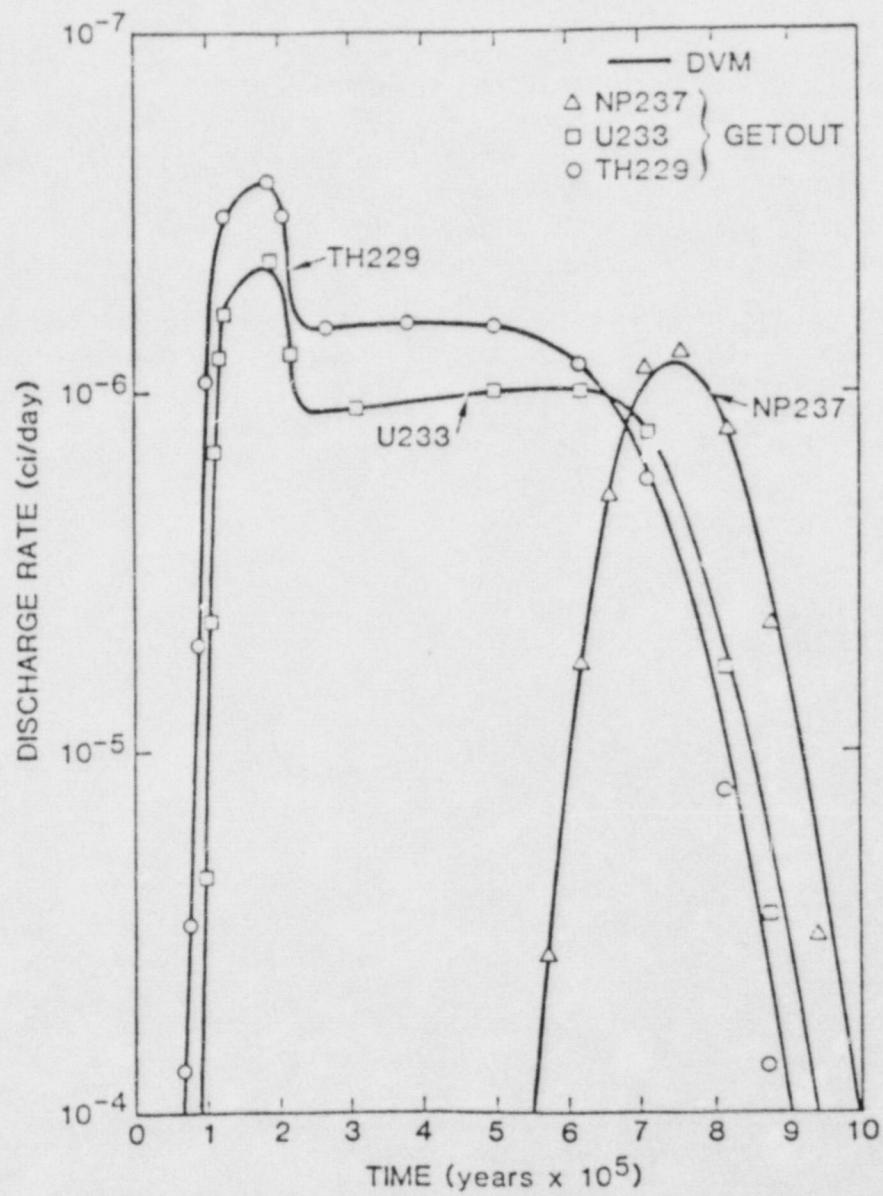


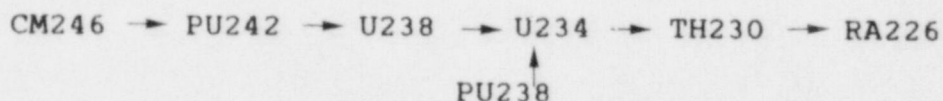
Figure 5-2. Graphed Output of Problem 3

6. PROBLEM 4: QUASI-TWO-DIMENSIONAL TRANSPORT OF A SEVEN-MEMBER CHAIN WITH UNEQUAL RETARDATION PARAMETERS AND SOLUBILITY-LIMITED SOURCE

6.1 Description of the Problem

Problem 4 is designed to test the ability of NWFT/DVM to handle multiple-branching decay chains and solubility-limited sources. The scenario analyzed assumes the existence of a hydraulic communication from an overlying aquifer to an underlying aquifer and passing through the repository (Figure 6-1). The communication is assumed to result from a single 13.5-inch diameter borehole. Water enters the borehole from the overlying aquifer, passes through the repository, and discharges dissolved radionuclides into the underlying aquifer. Water from the overlying aquifer is assumed to circulate through the entire repository.

The seven-member decay chain



is transported from the repository to a discharge point 143,700 ft from the source. This problem is identical to Problem 3 in the NWFT/DVM 'User's Manual.

For comparison purposes, the GETOUT code cannot be used, as there are both leach- and solubility-limited sources (GETOUT assumes an infinite solubility for all radionuclides). Thus, results from the SWIFT code were used for comparison.

Legs 10 and 12 of the network in Figure 2-1 were used to represent the borehole in the NWFT/DVM simulation of this problem. Thus, the migration path is through Legs 13, 12, 7, 8, and 15, with migration beginning at the midpoint of Leg 13.

6.2 Basic Assumptions

The following assumptions were invoked in the simulation of Problem 4.

- Hydraulic parameters vary along the flow path.
- Radionuclide source is both solubility and leach limited.
- Leach rate is constant for $t < T$ (leach time).
- Dispersivity is constant along the flow path.
- Retardation factors vary along the flow path.
- Radionuclide components have contrasting retardations.

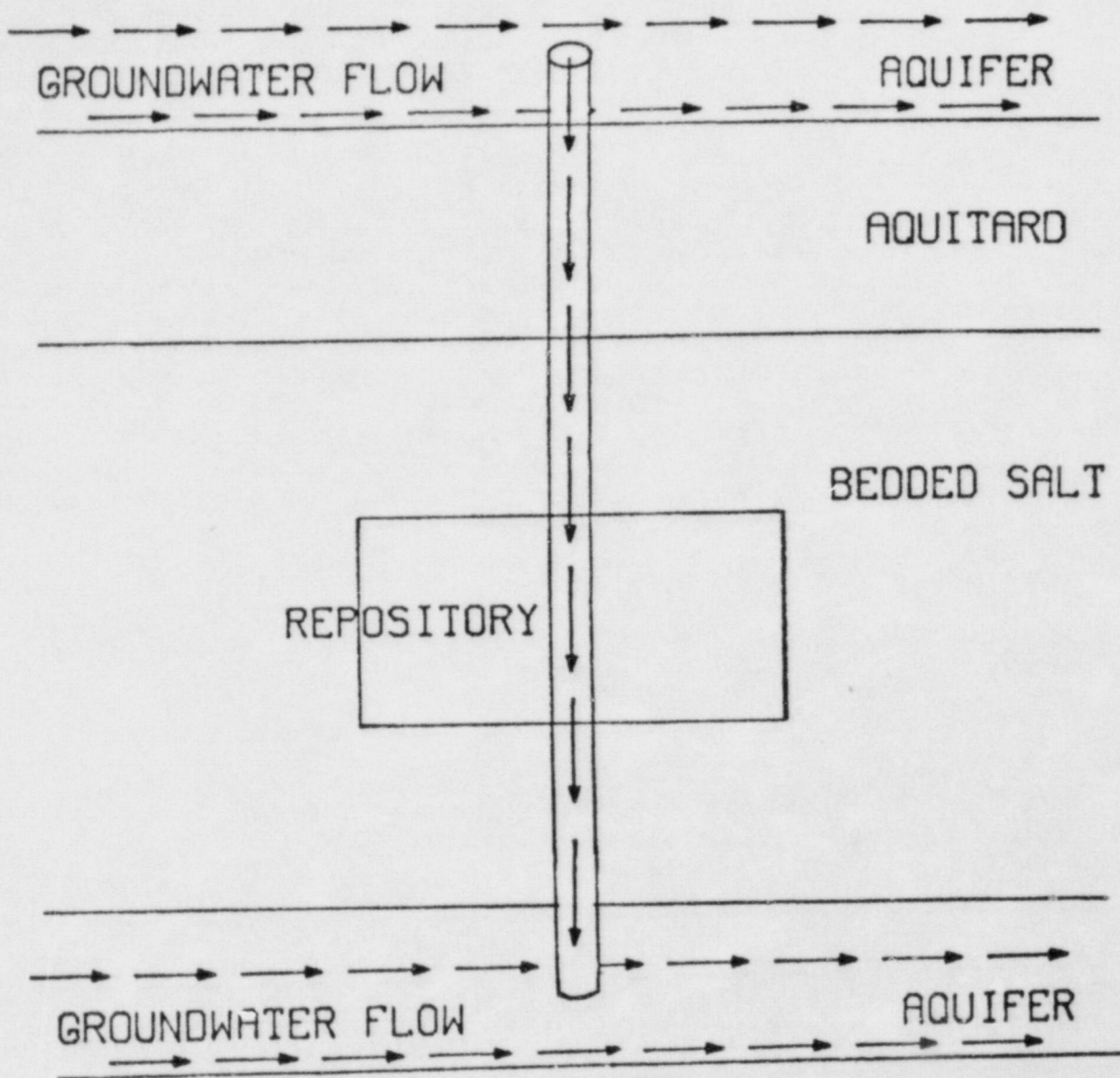


Figure 6-1. Borehole Scenario of Problem 4

6.3 Input Specifications

The majority of the input parameter values for Problem 4 are identical to those of Problem 3. Those for which the values have changed are given in Tables 6-1 and 6-2. The cross-sectional area of Leg 13 was obtained by assuming a 25 percent extraction ratio. That is, $AREA(13) = 6,000 \times 18 \times .25$, where repository width is 6,000 ft and height is 18 ft (see Cranwell et al., 1982).

The values for distribution coefficients were obtained by random sampling from reasonable ranges of distribution coefficients for each isotope. It was assumed that no sorption of radionuclides took place in Legs 13 and 12. Thus, a distribution coefficient of zero was used in these legs for all radionuclides.

The initial inventory (curies) in Table 6-2 were taken from low-growth projections of Blomeke and Kee (1976). As was the case with distribution coefficients, the solubility limits were obtained by a random sampling over reasonable ranges of solubility limits.

6.4 Results

The output from NWFT/DVM and SWIFT is plotted in Figure 6-2. As can be seen, the agreement between the two codes is very good.

Table 6-1
Flow and Transport Parameters
for Problem 4

Parameter	Value
Porosity	.03 (Leg 9) .15 (Leg 12) .1 (Leg 13)
Hydraulic Conductivity (ft/day)	1.5×10^{-6} (Leg 9) 10 (Leg 12)
Cross-sectional Area (ft ²)	1 (Leg 9) 2.7×10^4 (Leg 13)
Brine Concentration	1 (Leg 9) .67 (Leg 10)
Distribution Coefficient (ft ³ /lb) Legs 7, 8, and 15	5.2 (CM246) .96 (PU242) .15 (U238) .96 (PU238) .15 (U234) 7.35 (TH230) .02 (RA226)
Distribution Coefficient (ft ³ /lb) Legs 13 and 12	0 (all radionuclides)
Migration Path Length (ft)	143,700

Table 6-2

Isotope Half-Lives, Initial Inventory
Retardation Factors, and Solubility
Limits for Problem 4

Inventory	Half-Life (y)	Inventory (Ci)	Retardation		Solubility Limit (g/g)
			Legs 13 & 12	Legs 7, 8, & 5	
^{246}Cm	4.710×10^3	3.22×10^4	1	2064	1.00×10^1
^{242}Pu	3.790×10^5	1.28×10^3	1	382	1.55×10^{-13}
^{238}U	4.510×10^9	1.06×10^2	1	60.5	2.57×10^{-5}
^{238}Pu	8.900×10^1	1.11×10^7	1	382	4.54×10^{-13}
^{234}U	2.470×10^5	7.89×10^2	1	60.5	5.14×10^{-8}
^{230}Th	8.000×10^4	1.74×10^0	1	2917	5.35×10^{-8}
^{226}Ra	1.600×10^3	1.40×10^{-2}	1	8.9	6.74×10^{-9}

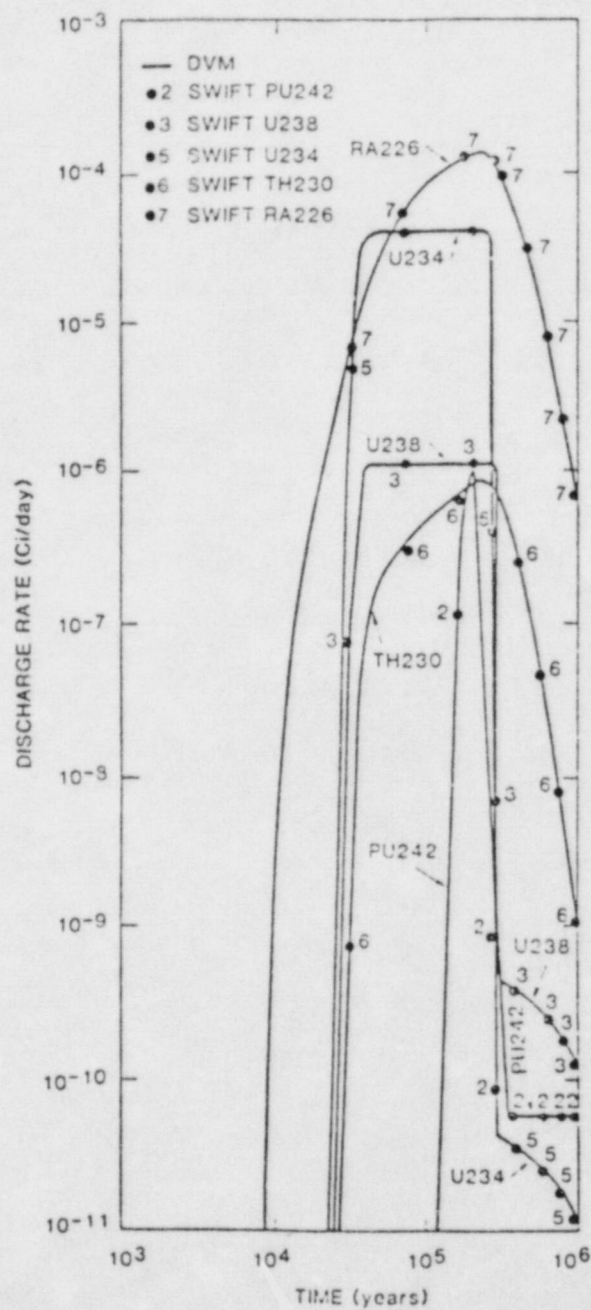


Figure 6-2. Graphed Output of Problem 4

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VERIFICATION OF THE NETWORK FLOW AND TRANSPORT/DISTRIBUTED VELOCITY
(NWFT/DVM) COMPUTER CODE

MAY 1984