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FRACVAL: Validation (Nonlinear Least Squares Method) of the Solution of One-Dimensional Transport of Decaying Species in a Discrete Planar Fracture With Rock Matrix Diffusion

Part 1: Analytical Solutions

Technical Report

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ABSTRACT

Analytical solutions based on the Laplace transforms are presented for the one-dimensional, transient, advective-dispersive transport of a reacting radionuclide through a discrete planar fracture with constant aperture subject to diffusion in the surrounding rock matrix where both regions of solute migration display residual concentrations. The dispersion-free solutions, which are of closed form, are also reported. The solution assumes that the ground-water flow regime is under steady-state and isothermal conditions and that the rock matrix is homogeneous, isotropic, and saturated with stagnant water. The flow region in both fracture and rock matrix are of the semi-infinite type. The initial conditions include a constant and a spatially varying distribution of solute in the case of the fracture region, and a constant in the case of the rock matrix region. The upstream boundary condition exclusive to the fracture corresponds to an exponentially decaying source of solute, which may be subject to a step or band release mode. The boundary condition corresponding to the rock matrix is implicit and corresponds to the space-time dependent concentration prevailing at the interface between fracture and rock. A zero flux condition is assumed at the downstream end of both fracture and rock.

The verification of the solution was performed by means of related analytical solutions dealing with particular aspects of the transport problem under investigation on the one hand, and a numerical solution capable of handling the complete problem on the other.

The integrals encountered in the general solution are evaluated by means of a composite Gauss-Legendre quadrature scheme.

FOREWORD

Following the passage of the Nuclear Waste Policy Act of 1982, the Civilian Radioactive Waste Management Program was organized in September 1983. The purpose of this program, managed by the U.S. Department of Energy (DOE), is to develop technology and provide facilities for safe, environmentally acceptable, permanent disposal of high-level waste (HLW). HLW includes wastes from both commercial and defense sources, such as spent (used) fuel from nuclear power reactors, accumulations of wastes from production of nuclear weapons, and solidified wastes from fuel reprocessing.

The information in this report pertains to analytical solutions based on Laplace transforms used in studying radionuclide transport in fractured geologic media for the Repository Technology Program. This work was sponsored by the DOE Repository Technology and Transportation Division.

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PART 1: ANALYTICAL SOLUTIONS

1.0 INTRODUCTION

1.1 PURPOSE

This report is presented in two parts. Part 1 gives the derivation and verification of the analytical solutions based on the Laplace transforms for the one-dimensional isothermal transport of a radionuclide in an idealized discrete planar fracture with constant aperture, including rock matrix diffusion, which accounts for non-zero residual concentrations. Part 2 gives a validation of the analytical solution restricted to the fracture (reported in Part 1) based on the nonlinear least squares method of optimization supplemented by a statistical method for analyzing the correlation between estimated parameters and their range of validity.

The verification of the portion of the computer code (i.e., FRACVAL) related to Part 1 is performed by means of available one-dimensional analytical and numerical solutions. The one-dimensional solution of van Genuchten and Alves (1982), which is restricted to a single medium system and which ignores the matrix diffusion process, will be used for benchmarking the performance of this solution. The solution of Gureghian (1990) will be used to verify the performance of the model for a zero residual concentration in both fracture and rock matrix. The verification of the total performance of the model will be carried out by means of a support program (STEFH). It is based on the numerical inversion of the Laplace transforms as proposed by Steffest (1970); its performance is first estimated by comparison with the benchmarking solutions used in this report.

1.2 APPLICATIONS

The solutions presented in this report are primarily related to performance assessment investigations of potential nuclear waste repository sites restricted to typical scenario analyses associated with long-term migration of radionuclides in an idealized fractured rock system. These solutions can be used to simulate the behavior of a decaying species in drill cores in a laboratory environment. Consequently, through a validation process (see Part 2 of this report) they may generate useful site-specific information regarding the various parameters gearing the transport process through fractured rock systems.

The model FRACVAL was written in VAX FORTRAN Version 4.8 using the G floating point option (REAL*16). An auxiliary graphics program XYLOT (see FRACVAL User's Guide, Gureghian and Steidl, 1990) was written using DISSPLA Version 10.5. The computation was executed on a VAX 8700 under VMS Version 4.7.

2.0 THE FRACVAL MODEL

The analytical solutions derived in Part 1 of FRACVAL are an extension of the ones related to the single fracture case reported in Gureghian (1990), and account for a non-zero residual concentration in both fracture and rock matrix. For the case of the fracture, the initial conditions may be described by either a constant value or a constant value plus a space-dependent exponential function. However, for the case of the rock matrix, the initial conditions are restricted to descriptions by a constant value.

To evaluate the semi-infinite solutions related to both fracture and rock matrix, based on the Laplace transforms, an integration must be performed by a composite Gauss-Legendre quadrature scheme. When the dispersion mechanism is neglected, closed-form solutions are derived. The documentation of the analytical solution is given in Section 2.1 and its verification in Section 2.2. The exact derivation of the first-order sensitivities of the concentration in the fracture with respect to the various parameters of the fracture-rock system required by the various optimization techniques used for the validation of FRACVAL are reported in Part 2 of this report.

2.1 GOVERNING EQUATIONS

The governing one-dimensional equation describing the movement of a typical nuclide in the fracture and rock matrix is given by Gureghian (1990) as follows:

(a) Fracture

$$R \frac{\partial A}{\partial t} - D_x \frac{\partial^2 A}{\partial x^2} + u \frac{\partial A}{\partial x} + \lambda R A + \frac{J}{b} = 0 \quad (2-1)$$

(b) Rock Matrix

$$R' \frac{\partial B}{\partial t} - D_p \frac{\partial^2 B}{\partial z^2} + \lambda R' B = 0 \quad (2-2)$$

where

- A is the concentration in the fracture (ML⁻³)
- R is the retardation factor in the fracture
- D_x is the hydrodynamic dispersion coefficient in the x direction of the fracture (L²T⁻¹)
- u is the average fluid velocity in the fracture (LT⁻¹)
- λ is the first-order rate constant for decay (T⁻¹)

- J is the diffusive rate of nuclide at surface of fracture per unit area of fracture surface (ML⁻²T⁻¹)
- b is half-thickness of the fracture (L)
- R' is the retardation factor in the rock matrix
- B is the concentration in the rock matrix (ML⁻³)
- D_p is the pore diffusivity (L²T⁻¹)
- t is the time (T).

The diffusive rate of a nuclide into the rock matrix is assumed to obey Fick's law of diffusion written as

$$J = - D_e \left. \frac{\partial B}{\partial z} \right|_{z=b} \quad (2-3)$$

where D_e is the effective diffusivity in the rock matrix (Neretnieks, 1980) defined as

$$D_e = \phi D_p \quad (2-4a)$$

and

$$D_p = D_d g_f \quad (2-4b)$$

where

- φ is the rock porosity
- D_d is the molecular diffusion of nuclide in water (L²T⁻¹)
- g_f is the geometric factor (i.e., δ_d/τ'²) where
- δ_d is the constrictivity for diffusion (L⁰)
- τ' is the tortuosity of the rock matrix (L⁰).

The hydrodynamic dispersion in the fracture (Bear, 1972) is given by

$$D_x = a_L u + \tau D_d \quad (2-5)$$

where

- a_L is the longitudinal dispersivity (L)
- τ is the tortuosity of the fracture (L⁰)

The retardation factor in the fracture (R) and in the rock matrix (R') (Neretnieks et al., 1982) are given by:

$$R = 1 + K_f/b \quad (2-6a)$$

$$R' = 1 + [(1 - \phi)/\phi] \rho_r K_r \quad (2-6b)$$

where

ρ_r is the rock density (ML^{-3})

K_f is the surface distribution coefficient in the fracture (L)

K_r is the distribution coefficient in the rock matrix (L^3M^{-1}).

2.1.1 Initial and Boundary Conditions

The set of differential equations, Equations 2-1 and 2-2, are subject to the initial conditions:

$$A(x,0) = a_1 + a_2 e^{-\alpha x}, 0 < x < \infty \quad (2-7)$$

$$B(x,z,0) = b_1, x > 0, z \geq b \quad (2-8)$$

where

a_1, a_2, b_1 (all ML^{-3}), and α (L^{-1}) are constant in space and time

and boundary conditions in the fracture and rock matrix. The boundary conditions in the fracture are given by

$$A(0,t) = A(t) U(t), t > 0 \quad (2-9a)$$

$$\frac{\partial A(\infty,t)}{\partial x} = 0, t > 0 \quad (2-9b)$$

where

$A(t)$ is the concentration at the source.

In the rock matrix, the boundary conditions are:

$$B(x,b,t) = A(x,t), x > 0 \quad (2-10a)$$

$$\frac{\partial B(x,\infty,t)}{\partial z} = 0, t > 0 \quad (2-10b)$$

For a step release mode (continuous decaying source), the concentration at the source for a typical nuclide may be written as

$$A(t) = A^0 e^{-\lambda t} \quad (2-11)$$

where A^0 is the concentration of the species at time equals zero. For a band release mode, the boundary condition at the inlet may be written as

$$A(0,t) = A(t)[U(t) - U(t-T)], \quad t > 0 \quad (2-12)$$

where T is the leaching time and $U(t-T)$ is the Heaviside unit function defined as

$$U(t-T) = \begin{cases} 1, & t \geq T \\ 0, & t < T \end{cases} \quad (2-13)$$

The general form of the solutions for the band release mode based on a boundary condition given by Equation 2-12 and which uses the superposition technique may be written as follows for the fracture and rock matrix:

$$A(x,t) = [A(x,t; A^0, A(x,0), B(x,z,0)) - A(x,t-T; A^0 e^{-\lambda T})]U(t-T) \quad (2-14a)$$

$$B(x,z,t) = [B(x,z,t; A^0, A(x,0), B(x,z,0)) - B(x,z,t-T; A^0 e^{-\lambda T})]U(t-T) \quad (2-14b)$$

2.1.2 Solution of Transport Equation for the Rock Matrix and Fracture

Rock Matrix

The Laplace transformation of Equation 2-2 with its associated initial and boundary condition Equations 2-7, 2-8, and 2-10 may be written as

$$D_p \frac{d^2 \bar{B}}{dz^2} - R'(s + \lambda) \bar{B} = -R'b_1 \quad (2-15)$$

$$\bar{B}(x,b,s) = \bar{A}(x,s) \quad (2-16)$$

where

$$\bar{B} = \int_0^\infty B e^{-st} dt \quad (2-17)$$

The general solution of Equation 2-15 is given by

$$\bar{B}(x,z,s) = \left(\bar{A} - \frac{b_1}{s+\lambda} \right) e^{r_b(z-b)} + \frac{b_1}{s+\lambda} \quad (2-18)$$

with

$$r_b = -c_r(s+\lambda)^{1/2} \quad (2-19a)$$

and

$$c_r = \left(R'/D_p \right)^{1/2} \quad (2-19b)$$

Note that the inverse Laplace transform of $\bar{B}$ might be sought once $\bar{A}$ is identified as shown in the subsequent section.

The transformed diffusive flux (Equation 2-3) at the interface of the fracture and rock matrix is given by

$$\bar{J} = -\phi D_p \frac{\partial \bar{B}}{\partial z}(x,b,s) = -\phi D_p r_b \left(\bar{A}(x,s) - \frac{b_1}{s+\lambda} \right) \quad (2-20)$$

Note that r_b in the above equation is given by Equation 2-19a.

Fracture

After proper substitution of the transform of the diffusive flux given by Equation 2-20 into the Laplace transformation of Equation 2-1,

$$D_x \frac{d^2 \bar{A}}{dx^2} - u \frac{\partial \bar{A}}{\partial x} - \left[R(s+\lambda) + c_r(s+\lambda)^{1/2} \right] \bar{A} = -R(a_1 + a_2 e^{-ax}) - \frac{c_r b_1}{(s+\lambda)^{1/2}} \quad (2-21)$$

with

$$c_r = \frac{\phi}{b} \left(R'D_p \right)^{1/2} \quad (2-22)$$

The Laplace transforms of the boundary conditions (Equations 2-9b and 2-11) associated with Equation 2-10 are given by:

$$\bar{A}(0,s) = \frac{\Lambda^0}{s+\lambda} \quad (2-23a)$$

$$\frac{\partial \bar{A}}{\partial x} = 0, \quad x = \infty \quad (2-23b)$$

The general solution of Equation 2-21 subject to its initial and boundary conditions given by Equations 2-7b and 2-9 may be written as

$$\bar{A}(x,s) = \left[\frac{A^0}{s+\lambda} - R \left[\frac{a_1}{r_a} + \frac{a_2}{r_a-p} \right] - \frac{c_f b_1}{r_c} \right] e^{a_n x} + R \left[\frac{a_1}{r_a} + \frac{a_2 e^{-\alpha x}}{r_a-p} \right] + \frac{c_f b_1}{r_c} \quad (2-24)$$

where

$$a_n x = \frac{1}{2D_x} \left[u - \left(u^2 + 4r_a D_x \right)^{1/2} \right] x \quad (2-25)$$

and

$$p = D_x \alpha^2 + u\alpha \quad (2-26a)$$

$$r_a = R(s+\lambda) + c_f (s+\lambda)^{1/2} \quad (2-26b)$$

$$r_c = r_a (s+\lambda)^{1/2} \quad (2-26c)$$

Recognizing the following integral (see Gradshteyn and Ryzhik, 1980)

$$\int_0^\infty \exp\left(-\sigma^2 - \frac{\gamma^2}{\sigma^2}\right) d\sigma = \frac{\sqrt{\pi}}{2} \exp(-2\gamma) \quad (2-27)$$

Equation 2-24 may now be written in the form

$$\bar{A}(x,s) = \int_0^\infty \psi(x,\sigma) \left(\frac{A^0}{s+\lambda} - R \left[\frac{a_1}{r_a} + \frac{a_2}{r_a-p} \right] - \frac{c_f b_1}{r_c} \right) e^{-r_a x} d\sigma + R \left[\frac{a_1}{r_a} + \frac{a_2 e^{-\alpha x}}{r_a-p} \right] + \frac{c_f b_1}{r_c} \quad (2-28)$$

where

$$\psi(x,\sigma) = \frac{2}{\sqrt{\pi}} \exp \left[- \left(\sigma - \frac{ux}{4D_x \sigma} \right)^2 \right] \quad (2-29a)$$

and

$$\chi = \frac{x^2}{4D_x \sigma^2} \quad (2-29b)$$

Note that c_f in Equation 2-26b is given by Equation 2-22. Substitution from Equations 2-26a and 2-26b into Equation 2-28 and using the Laplace inversion formulae (Appendix A), after some manipulation the final solution of the concentration in the fracture may be written as

$$\begin{aligned}
A(x,t) = & e^{-\lambda t} \int_0^\infty \psi(X,\sigma) \left\{ (A^0 - b_1) \operatorname{erfc} \left(\frac{c_f X}{2(t-R_X)^{1/2}} \right) \right. \\
& - (a_1 - b_1) \exp \left[\left(\frac{c_f}{R} \right)^2 t \right] \operatorname{erfc} \left[\frac{c_f}{R} (t-R_X)^{1/2} + \frac{c_f X}{2(t-R_X)^{1/2}} \right] \\
& \left. - \frac{a_2}{q} \beta_2 \exp \left[\beta_2 c_f X + \beta_2^2 (t-R_X) \right] \operatorname{erfc} \left[\beta_2 (t-R_X)^{1/2} + \frac{c_f X}{2(t-R_X)^{1/2}} \right] \right\} U(t-R_X) d\sigma \\
& + e^{-\lambda t} \left[b_1 + (a_1 - b_1) \exp \left[\left(\frac{c_f}{R} \right)^2 t \right] \operatorname{erfc} \left[\frac{c_f}{R} t^{1/2} \right] + \frac{a_2 e^{-\alpha x}}{q} \beta_2 \exp(\beta_2^2 t) \operatorname{erfc}(\beta_2 t^{1/2}) \right. \\
& \left. + \frac{a_2}{q} \beta_1 \exp[\beta_1^2 t - \lambda t] [F_1(x,t) - F_2(x,t)] \right] \quad (2-30)
\end{aligned}$$

where

$$F_1(x,t) = \int_0^\infty \psi(x,\sigma) \exp \left[\beta_1 c_f X - \beta_1^2 R_X \right] \operatorname{erfc} \left[\beta_1 (t-R_X)^{1/2} + \frac{c_f X}{2(t-R_X)^{1/2}} \right] U(t-R_X) d\sigma \quad (2-30a)$$

$$F_2(x,t) = \exp(-\alpha x) \operatorname{erfc}(\beta_1 t^{1/2}) \quad (2-30b)$$

and

$$q = 2 \left[\left(\frac{c_f}{2R} \right)^2 + \frac{p}{R} \right]^{1/2} \quad (2-31)$$

and

$$\beta_1 = \frac{c_f}{2R} - \frac{q}{2} \quad (2-32a)$$

$$\beta_2 = \frac{c_f}{2R} + \frac{q}{2} \quad (2-32b)$$

Substitution of Equation 2-28 in Equation 2-18 gives

$$\begin{aligned} \bar{B}(x, z, s) = & \int_0^\infty \psi(x, \sigma) \left(\frac{A^0}{s + \lambda} - R \left[\frac{a_1}{r_a} + \frac{a_2}{r_a - p} \right] - \frac{c_f b_1}{r_c} \right) \exp \left[r_b(z-b) - r_a x \right] d\sigma \\ & + \left(R \left[\frac{a_1}{r_a} + \frac{a_2 e^{-\alpha x}}{r_a - p} \right] + \frac{c_f b_1}{r_c} \right) \exp[r_b(z-b)] + \frac{b_1}{s + \lambda} (1 - \exp[r_b(z-b)]) \end{aligned} \quad (2-33)$$

and the final solution of the concentration in the rock matrix may be written as

$$\begin{aligned} B(x, z, t) = & e^{-\lambda t} \int_0^\infty \psi(x, \sigma) \left\{ (A^0 - b_1) \left[\operatorname{erfc} \left(\frac{c_f x + c_r(z-b)}{2(t-Rx)^{1/2}} \right) \right] \right. \\ & - (a_1 - b_1) \exp \left[(c_f x + c_r(z-b)) \frac{c_f}{R} + \left(\frac{c_f}{R} \right)^2 (t-Rx) \right] \operatorname{erfc} \left[\frac{c_f}{R} (t-Rx)^{1/2} + \frac{c_f x + c_r(z-b)}{2(t-Rx)^{1/2}} \right] \\ & \left. - \frac{a_2}{q} \beta_2 \exp \left[\beta_2 (c_f x + c_r(z-b)) + \beta_2^2 (t-Rx) \right] \operatorname{erfc} \left[\beta_2 (t-Rx)^{1/2} + \frac{c_f x + c_r(z-b)}{2(t-Rx)^{1/2}} \right] \right\} U(t-Rx) d\sigma \\ & + e^{-\lambda t} \left[b_1 + (a_1 - b_1) \exp \left[c_r(z-b) \frac{c_f}{R} + \left(\frac{c_f}{R} \right)^2 t \right] \operatorname{erfc} \left[\frac{c_f}{R} t^{1/2} + \frac{c_r(z-b)}{2t^{1/2}} \right] \right. \\ & + \frac{a_2}{q} e^{-\alpha x} \beta_2 \exp \left[\beta_2 c_r(z-b) + \beta_2^2 t \right] \operatorname{erfc} \left[\beta_2 t^{1/2} + \frac{c_r(z-b)}{2t^{1/2}} \right] \\ & \left. + \frac{a_2}{q} \beta_1 \exp [\beta_1^2 t - \lambda t] [G_1(x, t) - G_2(x, t)] \right] \end{aligned} \quad (2-34)$$

where

$$\begin{aligned} G_1(x, t) = & \int_0^\infty \psi(x, \sigma) \exp \left[\beta_1 (c_f x + c_r(z-b)) - \beta_1^2 Rx \right] \operatorname{erfc} \left[\beta_1 (t-Rx)^{1/2} \right. \\ & \left. + \frac{c_f x + c_r(z-b)}{2(t-Rx)^{1/2}} \right] U(t-Rx) d\sigma \end{aligned} \quad (2-34a)$$

$$G_2(x,t) = \exp[-\alpha x + \beta_1 c_r(z-b)] \operatorname{erfc} \left[\beta_1 t^{1/2} + \frac{c_r(z-b)}{2t^{1/2}} \right] \quad (2-34b)$$

Note that c_r , c_f , $\psi(x,\sigma)$, and χ in Equations 2-30 and 2-34 are given by Equations 2-19b, 2-22, 2-29a, and 2-29b, respectively.

After setting appropriate finite integration limits (see Appendix B), the integration of Equations 2-30, 2-30a, 2-34, and 2-34a is then performed using a Gauss-Legendre quadrature scheme.

In the composite quadrature formula adopted in this work, 60 integration points were found to yield a converging quadrature. An exception is made of the integrals given by Equations 2-30a and 2-34a. In the latter case, particularly when the Peclet number (i.e., ux/D) is less than 2, convergence could be met by subdividing the selected intervals into two more subintervals using 60 integration points each.

Zero Dispersion

When the hydrodynamic dispersion effects are neglected, Equation 2-21 becomes

$$u \frac{\partial \bar{A}}{\partial x} + \left[R(s+\lambda) + c_f(s+\lambda)^{1/2} \right] \bar{A} = R(a_1 + a_2 e^{-\alpha x}) + \frac{c_f b_1}{r_c} \quad (2-35)$$

The solution of the above equation subject to its initial and boundary conditions given by Equations 2-9b and 2-11 may be written as

$$\bar{A}(x,s) = \left(\frac{A^0}{s+\lambda} - R \left(\frac{a_1}{r_a} + \frac{a_2}{r_a - p} \right) - \frac{c_f b_1}{r_c} \right) e^{-r_a x'} + R \left(\frac{a_1}{r_a} + \frac{a_2 e^{-\alpha x}}{r_a - p} \right) + \frac{c_f b_1}{r_c} \quad (2-36)$$

where

$$x' = \frac{x}{u} \quad (2-37)$$

The inverse Laplace transforms of $\bar{A}(x,s)$ yielding the solution in the fracture and the rock matrix are given by expressions similar to Equations 2-30 and 2-34 after substitution of x by x' and setting

$$\int_0^\infty \psi(x,\sigma) d\sigma = 1 \quad (2-38)$$

Note

General Case. For large values of the time parameter or small values of the Peclet number, the β_1 , which is a negative constant for a typical problem (see Equation 2-32a), is a parameter associated with the nonlinear part of the model describing the residual concentration in the fracture (see Equation 2-7). This may tend to cause overflow problems when the components of the solution that include this parameter are not evaluated independently of the remaining ones. Consequently, the two components of the solution which include parameter β_1 (where one is subject to integration) are combined and represented by the last terms in Equations 2-30 and 2-34, hence made subject to an independent evaluation. The latter are assumed to correspond to zero when either of the following criteria are said to be satisfied.

$$\frac{|F1 - F2|}{\text{Max}(|F1|, |F2|)} \leq 10^{-8} \quad (2-39a)$$

$$|F1 - F2| \leq 10^{-12} \quad (2-39b)$$

In this particular instance, the significant maximum absolute value of the exponential argument used in the computation was restricted to 30. The implication is that, typically, exponential terms with arguments exceeding this number in absolute value are automatically set to zero.

Zero Dispersion. When dispersion effects are neglected and in view of Equations 2-37 and 2-38, it may be easily shown that the arguments of the exponential functions in Equations 2-30a and 2-30b are identical. Consequently, when the values of the complementary error function in both these equations will tend to 2 (i.e., for negative arguments less than or equal to -3), the contribution of the component of the solution in the fracture associated to parameter β_1 becomes zero. A similar conclusion may be drawn for the solution corresponding to the rock matrix, which will involve in this case Equations 2-34a and 2-34b.

The evaluation of the components of the solution presented in this section associated to the product of an exponential and complementary error function is given in Appendix C.

2.2 DISCUSSION OF RESULTS

The analytical solutions presented in this section of the report were verified by comparison with available one-dimensional closed-form analytical and numerical solutions. The one-dimensional closed-form analytical solution reported by van Genuchten and Alves (1982) through their mathemati-

cal model EXACT, restricted to a porous medium system, enabled a check of the performance of the solution strictly pertaining to the initial conditions, i. e., at time $t = 0$ in the fracture, when the spatial concentration distribution is non-uniform (Case 1). In addition, the solution referred to the two types of solute release modes at the source, namely step and band release, that were also investigated. The one-dimensional version of the analytical solution of Cureghian (1990) for both fracture and rock matrix was also used to verify the solution referred to in the case where the residual concentration in the fracture corresponds to zero and where the concentration at the source was subject to a step release mode (Case 2). The solution scheme proposed by Steffest (1970) based on the numerical inversion of the Laplace transforms whose performance was first evaluated in the above-mentioned test cases by means of the model STEFH (1990) was subsequently selected as a viable alternative for benchmarking the general form of the new analytical solution presented in this section. In this instance, the selected test case (Case 3) assumes a non-zero residual concentration in both fracture and rock matrix (spatially varying in the former and constant in the latter location). The solute release mode is the band release type. Finally, the general test case is presented as Case 4.

2.2.1 Case 1 Results

Case 1 examines the concentration of Cs-135 in a one-dimensional domain for a non-zero residual concentration distribution in the absence of rock matrix diffusion. In order to compare our results adequately with the solution reported by van Genuchten and Alves (1982), which neglects transfer of solute from the fracture to the rock matrix, the key parameter controlling this particular physical process (i. e., the pore diffusivity D_p) is consequently set to zero. The solution proposed by Steffest (1970), which in this instance operates on the Laplace transforms of Equation 2-28 with parameter c_f set to zero, was also used in the current investigation. In the simulations reported here, three values of the retardation factor were considered; the type of solute release mode at the source encompasses a step and band release mode. The general form of the model simulating the non-zero residual concentration condition in the fracture (see Equation 2-7) giving way to a non-uniform concentration distribution at time zero is adopted in these simulations. Based on the data presented in Table 2-1, the numerical results reported in Tables 2-2 through 2-4 (step release mode) and 2-5 through 2-7 (band release mode) show excellent agreement between our solution and those generated by the ones reported by both van Genuchten and Alves (1982) and Steffest (1970). Note that in the latter case 36 integration points were required in order to generate a stable and satisfactory solution.

Figures 2-1 and 2-2 show the relative spatial distribution of Cs-135 at time corresponding to 3,000 years for the step and band release modes and three values of the retardation factor ($R = 50$, 100, and 200).

Table 2-1. Input Parameters for Case 1

Species	Cs-135
$T_{1/2}$	2.3×10^6 yr
T (Case 1A: Step Release Mode)	N/A
(Case 1B: Band Release Mode)	10^3 yr
A_0^*	1.0
a_1^*	0.1
a_2^*	$-(0.1)^{**}$
α	0.02 1/m
D_p	0.0 m ² /yr
u	2.0 m/yr
D_x	5.0 m ² /yr
R	50, 100, 200

*(arbitrary units of activity/L³)

**This indicates that in Equation 2-7 the constant $+ a_2$ becomes $- a_2$.

2.2.2 Case 2 Results

Case 2 examines the concentration of Np-237 for a zero residual concentration distribution in both fracture and rock including rock matrix diffusion. This test case is meant to verify the associated mathematical model and to estimate the performance of the Stefhest (1970) solution scheme, and to characterize the conditions when the residual concentration in both fracture and matrix is assumed to be zero. In the simulations reported here, three values of the retardation factor were considered; the solute injected at the source is subjected to a step release mode. Based on the data presented in Table 2-8, the numerical results reported in Tables 2-9 through 2-11 (fracture) and Tables 2-12 through 2-14 (rock matrix) show that the two solutions FRACVAL and STEFH are in excellent agreement with those generated by FRACFLO (see Gureghian, 1990).

Figures 2-3 and 2-4 show the relative spatial distribution of Np-237 in both fracture and rock matrix at time corresponding to 10,000 years for the three values of the rock retardation factor ($R = 1$, 100, and 10,000).

Table 2-2. Case 1A Results: Concentration of Cs-135 at Time
 $t = 3,000$ Years, Zero Matrix Diffusion, Step
 Release Mode, Retardation Factor $R = 50$

Distance x (m)	FRACVAL	EXACT*	STEFH**
0.000E+00	9.991E-01	9.991E-01	9.991E-01
1.000E+01	9.991E-01	9.991E-01	9.991E-01
2.000E+01	9.991E-01	9.991E-01	9.991E-01
3.000E+01	9.991E-01	9.991E-01	9.991E-01
4.000E+01	9.988E-01	9.988E-01	9.988E-01
5.000E+01	9.979E-01	9.979E-01	9.979E-01
6.000E+01	9.947E-01	9.947E-01	9.947E-01
7.000E+01	9.851E-01	9.851E-01	9.851E-01
8.000E+01	9.614E-01	9.614E-01	9.614E-01
9.000E+01	9.126E-01	9.126E-01	9.126E-01
1.000E+02	8.280E-01	8.281E-01	8.281E-01
1.100E+02	7.050E-01	7.051E-01	7.050E-01
1.200E+02	5.544E-01	5.545E-01	5.543E-01
1.300E+02	3.993E-01	3.994E-01	3.994E-01
1.400E+02	2.653E-01	2.653E-01	2.655E-01
1.500E+02	1.685E-01	1.685E-01	1.685E-01
1.600E+02	1.109E-01	1.109E-01	1.106E-01
1.700E+02	8.365E-02	8.374E-02	8.343E-02
1.800E+02	7.487E-02	7.495E-02	7.492E-02
1.900E+02	7.482E-02	7.491E-02	7.509E-02
2.000E+02	7.787E-02	7.796E-02	7.808E-02
2.100E+02	8.144E-02	8.153E-02	8.142E-02
2.200E+02	8.469E-02	8.478E-02	8.449E-02
2.300E+02	8.743E-02	8.752E-02	8.723E-02
2.400E+02	8.969E-02	8.978E-02	8.963E-02
2.500E+02	9.154E-02	9.163E-02	9.163E-02
2.600E+02	9.306E-02	9.315E-02	9.321E-02
2.700E+02	9.430E-02	9.439E-02	9.441E-02
2.800E+02	9.532E-02	9.541E-02	9.534E-02
2.900E+02	9.615E-02	9.624E-02	9.610E-02
3.000E+02	9.683E-02	9.692E-02	9.676E-02

* EXACT is the name of the mathematical model
 (van Genuchten and Alves, 1982)

** Based on Stefhest, 1970

Table 2-3. Case 1A Results: Concentration of Cs-135 at Time
 $t = 3,000$ Years, Zero Matrix Diffusion, Step
Release Mode, Retardation Factor $R = 100$

Distance x (m)	FRACVAL	EXACT*	STEFH**
0.000E+00	9.991E-01	9.991E-01	9.991E-01
5.000E+00	9.990E-01	9.990E-01	9.990E-01
1.000E+01	9.986E-01	9.986E-01	9.986E-01
1.500E+01	9.974E-01	9.974E-01	9.974E-01
2.000E+01	9.945E-01	9.945E-01	9.945E-01
2.500E+01	9.878E-01	9.878E-01	9.878E-01
3.000E+01	9.745E-01	9.745E-01	9.745E-01
3.500E+01	9.504E-01	9.504E-01	9.504E-01
4.000E+01	9.112E-01	9.112E-01	9.112E-01
4.500E+01	8.530E-01	8.530E-01	8.530E-01
5.000E+01	7.743E-01	7.743E-01	7.743E-01
5.500E+01	6.769E-01	6.770E-01	6.769E-01
6.000E+01	5.670E-01	5.670E-01	5.670E-01
6.500E+01	4.534E-01	4.534E-01	4.534E-01
7.000E+01	3.460E-01	3.461E-01	3.460E-01
7.500E+01	2.532E-01	2.533E-01	2.532E-01
8.000E+01	1.801E-01	1.802E-01	1.801E-01
8.500E+01	1.278E-01	1.279E-01	1.278E-01
9.000E+01	9.405E-02	9.414E-02	9.404E-02
9.500E+01	7.487E-02	7.496E-02	7.486E-02
1.000E+02	6.578E-02	6.587E-02	6.579E-02
1.050E+02	6.293E-02	6.302E-02	6.294E-02
1.100E+02	6.347E-02	6.356E-02	6.348E-02
1.150E+02	6.560E-02	6.569E-02	6.561E-02
1.200E+02	6.832E-02	6.841E-02	6.831E-02
1.250E+02	7.112E-02	7.121E-02	7.110E-02
1.300E+02	7.379E-02	7.388E-02	7.377E-02
1.350E+02	7.625E-02	7.634E-02	7.625E-02
1.400E+02	7.849E-02	7.858E-02	7.850E-02
1.450E+02	8.053E-02	8.062E-02	8.054E-02
1.500E+02	8.237E-02	8.246E-02	8.238E-02
1.550E+02	8.404E-02	8.413E-02	8.405E-02
1.600E+02	8.555E-02	8.564E-02	8.555E-02
1.650E+02	8.692E-02	8.701E-02	8.691E-02
1.700E+02	8.815E-02	8.825E-02	8.815E-02

Table 2-3. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
1.750E + 02	8.927E - 02	8.936E - 02	8.927E - 02
1.800E + 02	9.029E - 02	9.038E - 02	9.028E - 02
1.850E + 02	9.120E - 02	9.129E - 02	9.120E - 02
1.900E + 02	9.203E - 02	9.212E - 02	9.203E - 02
1.950E + 02	9.278E - 02	9.287E - 02	9.278E - 02
2.000E + 02	9.346E - 02	9.355E - 02	9.346E - 02
2.050E + 02	9.407E - 02	9.416E - 02	9.407E - 02
2.100E + 02	9.463E - 02	9.472E - 02	9.463E - 02
2.150E + 02	9.513E - 02	9.522E - 02	9.513E - 02
2.200E + 02	9.559E - 02	9.568E - 02	9.558E - 02
2.250E + 02	9.600E - 02	9.609E - 02	9.600E - 02
2.300E + 02	9.637E - 02	9.646E - 02	9.637E - 02
2.350E + 02	9.671E - 02	9.680E - 02	9.671E - 02
2.400E + 02	9.701E - 02	9.710E - 02	9.701E - 02
2.450E + 02	9.729E - 02	9.738E - 02	9.729E - 02
2.500E + 02	9.754E - 02	9.763E - 02	9.754E - 02
2.550E + 02	9.776E - 02	9.785E - 02	9.776E - 02
2.600E + 02	9.797E - 02	9.806E - 02	9.797E - 02
2.650E + 02	9.815E - 02	9.824E - 02	9.815E - 02
2.700E + 02	9.832E - 02	9.841E - 02	9.832E - 02
2.750E + 02	9.847E - 02	9.856E - 02	9.847E - 02
2.800E + 02	9.861E - 02	9.870E - 02	9.861E - 02
2.850E + 02	9.873E - 02	9.882E - 02	9.873E - 02
2.900E + 02	9.884E - 02	9.893E - 02	9.884E - 02
2.950E + 02	9.894E - 02	9.904E - 02	9.894E - 02
3.000E + 02	9.904E - 02	9.913E - 02	9.904E - 02

* EXACT is the name of the mathematical model
(van Genuchten and Alves, 1982)

** Based on Stefhest, 1970

Table 2-4. Case 1A Results: Concentration of Cs-135 at Time
 $t = 3,000$ Years, Zero Matrix Diffusion, Step
 Release Mode, Retardation Factor $R = 200$

Distance x (m)	FRACVAL	EXACT*	STEFH**
0.000E+00	9.991E-01	9.991E-01	9.991E-01
3.000E+00	9.971E-01	9.971E-01	9.971E-01
6.000E+00	9.923E-01	9.923E-01	9.923E-01
9.000E+00	9.827E-01	9.827E-01	9.827E-01
1.200E+01	9.656E-01	9.656E-01	9.656E-01
1.500E+01	9.379E-01	9.379E-01	9.379E-01
1.800E+01	8.967E-01	8.967E-01	8.967E-01
2.100E+01	8.401E-01	8.402E-01	8.401E-01
2.400E+01	7.678E-01	7.678E-01	7.678E-01
2.700E+01	6.817E-01	6.818E-01	6.817E-01
3.000E+01	5.860E-01	5.860E-01	5.860E-01
3.300E+01	4.863E-01	4.864E-01	4.863E-01
3.600E+01	3.893E-01	3.894E-01	3.893E-01
3.900E+01	3.009E-01	3.010E-01	3.009E-01
4.200E+01	2.254E-01	2.255E-01	2.254E-01
4.500E+01	1.652E-01	1.653E-01	1.652E-01
4.800E+01	1.204E-01	1.205E-01	1.204E-01
5.100E+01	8.942E-02	8.950E-02	8.942E-02
5.400E+01	6.978E-02	6.986E-02	6.978E-02
5.700E+01	5.860E-02	5.869E-02	5.860E-02
6.000E+01	5.326E-02	5.335E-02	5.326E-02
6.300E+01	5.161E-02	5.170E-02	5.161E-02
6.600E+01	5.212E-02	5.221E-02	5.212E-02
6.900E+01	5.375E-02	5.384E-02	5.375E-02
7.200E+01	5.590E-02	5.599E-02	5.590E-02
7.500E+01	5.823E-02	5.832E-02	5.823E-02
7.800E+01	6.056E-02	6.065E-02	6.055E-02
8.100E+01	6.281E-02	6.290E-02	6.281E-02
8.400E+01	6.496E-02	6.505E-02	6.496E-02
8.700E+01	6.699E-02	6.708E-02	6.699E-02
9.000E+01	6.890E-02	6.899E-02	6.890E-02
9.300E+01	7.071E-02	7.080E-02	7.071E-02
9.600E+01	7.241E-02	7.250E-02	7.241E-02
9.900E+01	7.401E-02	7.410E-02	7.401E-02
1.020E+02	7.552E-02	7.561E-02	7.552E-02

Table 2-4. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
1.050E+02	7.694E-02	7.703E-02	7.694E-02
1.080E+02	7.828E-02	7.837E-02	7.828E-02
1.110E+02	7.954E-02	7.963E-02	7.954E-02
1.140E+02	8.072E-02	8.081E-02	8.072E-02
1.170E+02	8.184E-02	8.193E-02	8.184E-02
1.200E+02	8.289E-02	8.298E-02	8.289E-02
1.230E+02	8.388E-02	8.397E-02	8.388E-02
1.260E+02	8.482E-02	8.491E-02	8.482E-02
1.290E+02	8.570E-02	8.579E-02	8.570E-02
1.320E+02	8.652E-02	8.661E-02	8.652E-02
1.350E+02	8.730E-02	8.739E-02	8.730E-02
1.380E+02	8.804E-02	8.813E-02	8.804E-02
1.410E+02	8.873E-02	8.882E-02	8.873E-02
1.440E+02	8.938E-02	8.947E-02	8.938E-02
1.470E+02	8.999E-02	9.008E-02	8.999E-02
1.500E+02	9.057E-02	9.066E-02	9.057E-02
1.530E+02	9.111E-02	9.120E-02	9.111E-02
1.560E+02	9.163E-02	9.172E-02	9.163E-02
1.590E+02	9.211E-02	9.220E-02	9.211E-02
1.620E+02	9.256E-02	9.265E-02	9.256E-02
1.650E+02	9.299E-02	9.308E-02	9.299E-02
1.680E+02	9.339E-02	9.348E-02	9.339E-02
1.710E+02	9.377E-02	9.386E-02	9.377E-02
1.740E+02	9.413E-02	9.422E-02	9.413E-02
1.770E+02	9.447E-02	9.456E-02	9.447E-02
1.800E+02	9.478E-02	9.487E-02	9.478E-02
1.830E+02	9.508E-02	9.517E-02	9.508E-02
1.860E+02	9.536E-02	9.545E-02	9.536E-02
1.890E+02	9.563E-02	9.572E-02	9.563E-02
1.920E+02	9.588E-02	9.597E-02	9.588E-02
1.950E+02	9.611E-02	9.620E-02	9.611E-02
1.980E+02	9.633E-02	9.642E-02	9.633E-02
2.010E+02	9.654E-02	9.663E-02	9.654E-02
2.040E+02	9.674E-02	9.683E-02	9.674E-02
2.070E+02	9.692E-02	9.701E-02	9.692E-02

Table 2-4. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
2.100E + 02	9.710E - 02	9.719E - 02	9.710E - 02
2.130E + 02	9.726E - 02	9.735E - 02	9.726E - 02
2.160E + 02	9.741E - 02	9.751E - 02	9.741E - 02
2.190E + 02	9.756E - 02	9.765E - 02	9.756E - 02
2.220E + 02	9.770E - 02	9.779E - 02	9.770E - 02
2.250E + 02	9.783E - 02	9.792E - 02	9.783E - 02
2.280E + 02	9.795E - 02	9.804E - 02	9.795E - 02
2.310E + 02	9.806E - 02	9.815E - 02	9.806E - 02
2.340E + 02	9.817E - 02	9.826E - 02	9.817E - 02
2.370E + 02	9.827E - 02	9.836E - 02	9.827E - 02
2.400E + 02	9.837E - 02	9.846E - 02	9.837E - 02
2.430E + 02	9.846E - 02	9.855E - 02	9.846E - 02
2.460E + 02	9.854E - 02	9.863E - 02	9.854E - 02
2.490E + 02	9.862E - 02	9.871E - 02	9.862E - 02
2.520E + 02	9.870E - 02	9.879E - 02	9.870E - 02
2.550E + 02	9.877E - 02	9.886E - 02	9.877E - 02
2.580E + 02	9.883E - 02	9.892E - 02	9.883E - 02
2.610E + 02	9.890E - 02	9.899E - 02	9.890E - 02
2.640E + 02	9.895E - 02	9.904E - 02	9.895E - 02
2.670E + 02	9.901E - 02	9.910E - 02	9.901E - 02
2.700E + 02	9.906E - 02	9.915E - 02	9.906E - 02
2.730E + 02	9.911E - 02	9.920E - 02	9.911E - 02
2.760E + 02	9.916E - 02	9.925E - 02	9.916E - 02
2.790E + 02	9.920E - 02	9.929E - 02	9.920E - 02
2.820E + 02	9.924E - 02	9.933E - 02	9.924E - 02
2.850E + 02	9.928E - 02	9.937E - 02	9.928E - 02
2.880E + 02	9.932E - 02	9.941E - 02	9.932E - 02
2.910E + 02	9.935E - 02	9.944E - 02	9.935E - 02
2.940E + 02	9.939E - 02	9.948E - 02	9.939E - 02
2.970E + 02	9.942E - 02	9.951E - 02	9.942E - 02
3.000E + 02	9.944E - 02	9.954E - 02	9.944E - 02

* EXACT is the name of the mathematical model
(van Genuchten and Alves, 1982)

** Based on Stefhest, 1970

Table 2-5. Case 1B Results: Concentration of Cs-135 at Time
 $t = 3,000$ Years, Zero Matrix Diffusion, Band
Release Mode, Retardation Factor $R = 50$.

Distance x (m)	FRACVAL	EXACT*	STEFH**
1.000E+01	6.251E-09	6.251E-09	6.274E-09
2.000E+01	7.730E-08	7.730E-08	7.735E-08
3.000E+01	6.368E-07	6.368E-07	6.214E-07
4.000E+01	4.142E-06	4.142E-06	3.949E-06
5.000E+01	2.244E-05	2.246E-05	2.353E-05
6.000E+01	1.038E-04	1.038E-04	1.066E-04
7.000E+01	4.150E-04	4.151E-04	4.040E-04
8.000E+01	1.447E-03	1.447E-03	1.425E-03
9.000E+01	4.425E-03	4.425E-03	4.461E-03
1.000E+02	1.191E-02	1.191E-02	1.202E-02
1.100E+02	2.836E-02	2.836E-02	2.835E-02
1.200E+02	5.985E-02	5.986E-02	5.958E-02
1.300E+02	1.124E-01	1.124E-01	1.121E-01
1.400E+02	1.882E-01	1.882E-01	1.884E-01
1.500E+02	2.820E-01	2.820E-01	2.828E-01
1.600E+02	3.795E-01	3.795E-01	3.801E-01
1.700E+02	4.601E-01	4.602E-01	4.598E-01
1.800E+02	5.047E-01	5.048E-01	5.034E-01
1.900E+02	5.031E-01	5.032E-01	5.017E-01
2.000E+02	4.582E-01	4.583E-01	4.581E-01
2.100E+02	3.842E-01	3.843E-01	3.857E-01
2.200E+02	3.001E-01	3.002E-01	3.022E-01
2.300E+02	2.226E-01	2.227E-01	2.239E-01
2.400E+02	1.619E-01	1.620E-01	1.615E-01
2.500E+02	1.209E-01	1.210E-01	1.190E-01
2.600E+02	9.709E-02	9.724E-02	9.483E-02
2.700E+02	8.578E-02	8.593E-02	8.433E-02
2.800E+02	8.211E-02	8.226E-02	8.212E-02
2.900E+02	8.239E-02	8.254E-02	8.371E-02
3.000E+02	8.431E-02	8.446E-02	8.622E-02
3.100E+02	8.665E-02	8.680E-02	8.829E-02
3.200E+02	8.888E-02	8.903E-02	8.966E-02
3.300E+02	9.082E-02	9.097E-02	9.060E-02
3.400E+02	9.244E-02	9.259E-02	9.147E-02
3.500E+02	9.378E-02	9.393E-02	9.251E-02

Table 2-5. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
3.600E+02	9.438E-02	9.503E-02	9.375E-02
3.700E+02	9.578E-02	9.593E-02	9.510E-02
3.800E+02	9.652E-02	9.667E-02	9.638E-02
3.900E+02	9.712E-02	9.727E-02	9.746E-02
4.000E+02	9.762E-02	9.777E-02	9.824E-02

* EXACT is the name of the mathematical model
(van Genuchten and Alves, 1982)

** Based on Stefhest, 1970

Table 2-6. Case 1B Results: Concentration of Cs-135 at Time
 $t = 3,000$ Years, Zero Matrix Diffusion, Band
Release Mode, Retardation Factor $R = 100$.

Distance x (m)	FRACVAL	EXACT*	STEFH**
5.000E+00	8.496E-06	8.526E-06	8.496E-06
1.000E+01	4.234E-05	4.238E-05	4.234E-05
1.500E+01	1.493E-04	1.494E-04	1.493E-04
2.000E+01	4.419E-04	4.419E-04	4.419E-04
2.500E+01	1.157E-03	1.157E-03	1.157E-03
3.000E+01	2.746E-03	2.746E-03	2.746E-03
3.500E+01	5.981E-03	5.981E-03	5.981E-03
4.000E+01	1.205E-02	1.205E-02	1.205E-02
4.500E+01	2.259E-02	2.259E-02	2.259E-02
5.000E+01	3.951E-02	3.951E-02	3.951E-02
5.500E+01	6.469E-02	6.469E-02	6.469E-02
6.000E+01	9.934E-02	9.934E-02	9.933E-02
6.500E+01	1.433E-01	1.433E-01	1.433E-01
7.000E+01	1.947E-01	1.947E-01	1.947E-01
7.500E+01	2.492E-01	2.492E-01	2.492E-01
8.000E+01	3.012E-01	3.012E-01	3.012E-01
8.500E+01	3.440E-01	3.441E-01	3.441E-01
9.000E+01	3.721E-01	3.721E-01	3.721E-01
9.500E+01	3.816E-01	3.817E-01	3.815E-01
1.000E+02	3.719E-01	3.720E-01	3.718E-01
1.050E+02	3.453E-01	3.454E-01	3.453E-01
1.100E+02	3.065E-01	3.066E-01	3.065E-01
1.150E+02	2.613E-01	2.614E-01	2.614E-01
1.200E+02	2.155E-01	2.157E-01	2.157E-01
1.250E+02	1.738E-01	1.739E-01	1.738E-01
1.300E+02	1.390E-01	1.391E-01	1.389E-01
1.350E+02	1.123E-01	1.124E-01	1.121E-01
1.400E+02	9.346E-02	9.361E-02	9.329E-02
1.450E+02	8.145E-02	8.160E-02	8.133E-02
1.500E+02	7.472E-02	7.487E-02	7.470E-02
1.550E+02	7.174E-02	7.188E-02	7.183E-02
1.600E+02	7.119E-02	7.134E-02	7.135E-02
1.650E+02	7.210E-02	7.225E-02	7.227E-02
1.700E+02	7.376E-02	7.391E-02	7.388E-02
1.750E+02	7.574E-02	7.589E-02	7.578E-02

Table 2-6. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
1.800E+02	7.780E-02	7.795E-02	7.774E-02
1.850E+02	7.979E-02	7.994E-02	7.967E-02
1.900E+02	8.165E-02	8.180E-02	8.150E-02
1.950E+02	8.336E-02	8.351E-02	8.323E-02
2.000E+02	8.492E-02	8.507E-02	8.484E-02
2.050E+02	8.634E-02	8.649E-02	8.632E-02
2.100E+02	8.762E-02	8.777E-02	8.766E-02
2.150E+02	8.879E-02	8.894E-02	8.886E-02
2.200E+02	8.984E-02	8.999E-02	8.993E-02
2.250E+02	9.079E-02	9.094E-02	9.088E-02
2.300E+02	9.165E-02	9.180E-02	9.172E-02
2.350E+02	9.243E-02	9.258E-02	9.247E-02
2.400E+02	9.314E-02	9.329E-02	9.314E-02
2.450E+02	9.378E-02	9.393E-02	9.375E-02
2.500E+02	9.436E-02	9.451E-02	9.431E-02
2.550E+02	9.488E-02	9.503E-02	9.483E-02
2.600E+02	9.535E-02	9.550E-02	9.530E-02
2.650E+02	9.578E-02	9.593E-02	9.574E-02
2.700E+02	9.617E-02	9.632E-02	9.614E-02
2.750E+02	9.652E-02	9.667E-02	9.651E-02
2.800E+02	9.683E-02	9.698E-02	9.684E-02
2.850E+02	9.712E-02	9.727E-02	9.713E-02
2.900E+02	9.738E-02	9.753E-02	9.740E-02
2.950E+02	9.762E-02	9.777E-02	9.764E-02
3.000E+02	9.783E-02	9.798E-02	9.785E-02
3.050E+02	9.802E-02	9.817E-02	9.804E-02
3.100E+02	9.819E-02	9.835E-02	9.821E-02
3.150E+02	9.835E-02	9.850E-02	9.836E-02
3.200E+02	9.849E-02	9.865E-02	9.850E-02
3.250E+02	9.862E-02	9.877E-02	9.862E-02
3.300E+02	9.874E-02	9.889E-02	9.874E-02
3.350E+02	9.885E-02	9.900E-02	9.884E-02
3.400E+02	9.894E-02	9.909E-02	9.893E-02
3.450E+02	9.903E-02	9.918E-02	9.902E-02
3.500E+02	9.911E-02	9.926E-02	9.910E-02

Table 2-6. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
3.550E + 02	9.918E - 02	9.933E - 02	9.917E - 02
3.600E + 02	9.924E - 02	9.939E - 02	9.924E - 02
3.650E + 02	9.930E - 02	9.945E - 02	9.930E - 02
3.700E + 02	9.935E - 02	9.950E - 02	9.935E - 02
3.750E + 02	9.940E - 02	9.955E - 02	9.940E - 02
3.800E + 02	9.944E - 02	9.959E - 02	9.944E - 02
3.850E + 02	9.948E - 02	9.963E - 02	9.948E - 02
3.900E + 02	9.952E - 02	9.967E - 02	9.952E - 02
3.950E + 02	9.955E - 02	9.970E - 02	9.955E - 02
4.000E + 02	9.958E - 02	9.973E - 02	9.958E - 02

* EXACT is the name of the mathematical model
(van Genuchten and Alves, 1982)

** Based on Stefhest, 1970

Table 2-7. Case 1B Results: Concentration of Cs-135 at Time
 $t = 3,000$ Years, Zero Matrix Diffusion, Band
 Release Mode, Retardation Factor $R = 200$.

Distance x (m)	FRACVAL	EXACT*	STEFH**
4.000E+00	6.107E-04	6.106E-04	6.107E-04
8.000E+00	2.436E-03	2.436E-03	2.436E-03
1.200E+01	6.778E-03	6.776E-03	6.778E-03
1.600E+01	1.558E-02	1.558E-02	1.558E-02
2.000E+01	3.125E-02	3.125E-02	3.125E-02
2.400E+01	5.596E-02	5.596E-02	5.596E-02
2.800E+01	9.070E-02	9.071E-02	9.070E-02
3.200E+01	1.341E-01	1.341E-01	1.341E-01
3.600E+01	1.820E-01	1.820E-01	1.820E-01
4.000E+01	2.274E-01	2.275E-01	2.274E-01
4.400E+01	2.628E-01	2.629E-01	2.628E-01
4.800E+01	2.818E-01	2.818E-01	2.818E-01
5.200E+01	2.812E-01	2.812E-01	2.812E-01
5.600E+01	2.623E-01	2.624E-01	2.623E-01
6.000E+01	2.300E-01	2.301E-01	2.300E-01
6.400E+01	1.911E-01	1.912E-01	1.911E-01
6.800E+01	1.525E-01	1.526E-01	1.525E-01
7.200E+01	1.191E-01	1.192E-01	1.191E-01
7.600E+01	9.353E-02	9.367E-02	9.353E-02
8.000E+01	7.616E-02	7.631E-02	7.616E-02
8.400E+01	6.590E-02	6.605E-02	6.590E-02
8.800E+01	6.098E-02	6.113E-02	6.099E-02
9.200E+01	5.964E-02	5.979E-02	5.964E-02
9.600E+01	6.041E-02	6.056E-02	6.041E-02
1.000E+02	6.229E-02	6.244E-02	6.229E-02
1.040E+02	6.464E-02	6.479E-02	6.463E-02
1.080E+02	6.711E-02	6.726E-02	6.711E-02
1.120E+02	6.953E-02	6.969E-02	6.953E-02
1.160E+02	7.183E-02	7.198E-02	7.183E-02
1.200E+02	7.397E-02	7.412E-02	7.397E-02
1.240E+02	7.596E-02	7.611E-02	7.596E-02
1.280E+02	7.779E-02	7.794E-02	7.780E-02
1.320E+02	7.949E-02	7.964E-02	7.949E-02
1.360E+02	8.105E-02	8.120E-02	8.105E-02
1.400E+02	8.250E-02	8.265E-02	8.250E-02

Table 2-7. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
1.440E + 02	8.383E - 02	8.398E - 02	8.383E - 02
1.480E + 02	8.506E - 02	8.521E - 02	8.506E - 02
1.520E + 02	8.620E - 02	8.635E - 02	8.620E - 02
1.560E + 02	8.725E - 02	8.740E - 02	8.725E - 02
1.600E + 02	8.822E - 02	8.837E - 02	8.822E - 02
1.640E + 02	8.911E - 02	8.926E - 02	8.911E - 02
1.680E + 02	8.994E - 02	9.009E - 02	8.994E - 02
1.720E + 02	9.070E - 02	9.085E - 02	9.070E - 02
1.760E + 02	9.140E - 02	9.155E - 02	9.140E - 02
1.800E + 02	9.205E - 02	9.220E - 02	9.205E - 02
1.840E + 02	9.265E - 02	9.280E - 02	9.265E - 02
1.880E + 02	9.321E - 02	9.336E - 02	9.321E - 02
1.920E + 02	9.372E - 02	9.387E - 02	9.372E - 02
1.960E + 02	9.419E - 02	9.434E - 02	9.419E - 02
2.000E + 02	9.462E - 02	9.477E - 02	9.462E - 02
2.040E + 02	9.503E - 02	9.518E - 02	9.502E - 02
2.080E + 02	9.540E - 02	9.555E - 02	9.540E - 02
2.120E + 02	9.574E - 02	9.589E - 02	9.574E - 02
2.160E + 02	9.605E - 02	9.621E - 02	9.605E - 02
2.200E + 02	9.635E - 02	9.650E - 02	9.635E - 02
2.240E + 02	9.662E - 02	9.677E - 02	9.662E - 02
2.280E + 02	9.686E - 02	9.701E - 02	9.686E - 02
2.320E + 02	9.709E - 02	9.724E - 02	9.709E - 02
2.360E + 02	9.731E - 02	9.746E - 02	9.731E - 02
2.400E + 02	9.750E - 02	9.765E - 02	9.750E - 02
2.440E + 02	9.768E - 02	9.783E - 02	9.768E - 02
2.480E + 02	9.785E - 02	9.800E - 02	9.785E - 02
2.520E + 02	9.800E - 02	9.815E - 02	9.800E - 02
2.560E + 02	9.814E - 02	9.829E - 02	9.814E - 02
2.600E + 02	9.828E - 02	9.843E - 02	9.828E - 02
2.640E + 02	9.840E - 02	9.855E - 02	9.840E - 02
2.680E + 02	9.851E - 02	9.866E - 02	9.851E - 02
2.720E + 02	9.861E - 02	9.876E - 02	9.861E - 02
2.760E + 02	9.871E - 02	9.886E - 02	9.871E - 02
2.800E + 02	9.879E - 02	9.894E - 02	9.879E - 02

Table 2-7. Continued.

Distance x (m)	FRACVAL	EXACT*	STEFH**
2.840E+02	9.888E-02	9.903E-02	9.888E-02
2.880E+02	9.895E-02	9.910E-02	9.895E-02
2.920E+02	9.902E-02	9.917E-02	9.902E-02
2.960E+02	9.908E-02	9.923E-02	9.908E-02
3.000E+02	9.914E-02	9.929E-02	9.914E-02
3.040E+02	9.920E-02	9.935E-02	9.920E-02
3.080E+02	9.925E-02	9.940E-02	9.925E-02
3.120E+02	9.929E-02	9.944E-02	9.929E-02
3.160E+02	9.934E-02	9.949E-02	9.934E-02
3.200E+02	9.938E-02	9.953E-02	9.938E-02
3.240E+02	9.941E-02	9.956E-02	9.941E-02
3.280E+02	9.945E-02	9.960E-02	9.945E-02
3.320E+02	9.948E-02	9.963E-02	9.948E-02
3.360E+02	9.951E-02	9.966E-02	9.951E-02
3.400E+02	9.953E-02	9.968E-02	9.953E-02
3.440E+02	9.956E-02	9.971E-02	9.956E-02
3.480E+02	9.958E-02	9.973E-02	9.958E-02
3.520E+02	9.960E-02	9.975E-02	9.960E-02
3.560E+02	9.962E-02	9.977E-02	9.962E-02
3.600E+02	9.964E-02	9.979E-02	9.964E-02
3.640E+02	9.965E-02	9.980E-02	9.965E-02
3.680E+02	9.967E-02	9.982E-02	9.967E-02
3.720E+02	9.968E-02	9.983E-02	9.968E-02
3.760E+02	9.969E-02	9.985E-02	9.969E-02
3.800E+02	9.971E-02	9.986E-02	9.971E-02
3.840E+02	9.972E-02	9.987E-02	9.972E-02
3.880E+02	9.973E-02	9.988E-02	9.973E-02
3.920E+02	9.974E-02	9.989E-02	9.974E-02
3.960E+02	9.975E-02	9.990E-02	9.975E-02
4.000E+02	9.975E-02	9.990E-02	9.975E-02

* EXACT is the name of the mathematical model
(van Genuchten and Alves, 1982)

** Based on Stefhest, 1970

Figure 2-1. Relative Concentration of Cs-135 Versus Distance x , at Time $t = 3,000$ Years, Zero Matrix Diffusion, for Different Retardation Factors ($R = 50, 100, 200$) (Case 1A: Step Release Mode)

Dashed line indicates residual concentration.

Figure 2-2. Relative Concentration of Cs-135 Versus Distance x , at Time $t = 3,000$ Years, Zero Matrix Diffusion, for Different Retardation Factors ($R = 50, 100, 200$) (Case 1B: Band Release Mode)

Dashed line indicates residual concentration.

Table 2-8. Input Parameters for Case 2

Species	Np-237
Type of Release Mode	Step
$T_{1/2}$	2.14×10^6 yr
Λ_0^*	1.0
a_1^*	0.0
a_2^*	0.0
α	0.0
b_1^*	0.0
D_p	$0.01 \text{ m}^2/\text{yr}$
u	10.0 m/yr
D_x	$1.0 \text{ m}^2/\text{yr}$
b	0.005 m
R	1.0
R'	50, 100, 200

*(arbitrary units of activity/L³)

Table 2-9. Case 2 Results: Concentration of Np-237 in the Fracture, at Time $t = 10,000$ Years, Step Release Mode, Retardation Factor $R = 1$

Distance x (m)	FRACVAL	STEFH*	FRACFLO
1.000E+01	9.956E-01	9.956E-01	9.956E-01
1.500E+01	9.951E-01	9.951E-01	9.951E-01
2.000E+01	9.945E-01	9.945E-01	9.945E-01
3.000E+01	9.934E-01	9.934E-01	9.934E-01
4.000E+01	9.923E-01	9.923E-01	9.923E-01
5.000E+01	9.911E-01	9.911E-01	9.911E-01
6.000E+01	9.900E-01	9.900E-01	9.900E-01
7.000E+01	9.889E-01	9.889E-01	9.889E-01
8.000E+01	9.878E-01	9.878E-01	9.878E-01
9.000E+01	9.866E-01	9.866E-01	9.866E-01
1.000E+02	9.855E-01	9.855E-01	9.855E-01
1.500E+02	9.799E-01	9.799E-01	9.799E-01
2.000E+02	9.743E-01	9.743E-01	9.743E-01
3.000E+02	9.630E-01	9.630E-01	9.630E-01
4.000E+02	9.517E-01	9.517E-01	9.517E-01
5.000E+02	9.404E-01	9.404E-01	9.404E-01
6.000E+02	9.292E-01	9.292E-01	9.292E-01
7.000E+02	9.179E-01	9.179E-01	9.179E-01
8.000E+02	9.066E-01	9.066E-01	9.066E-01
9.000E+02	8.954E-01	8.954E-01	8.954E-01
1.000E+03	8.841E-01	8.841E-01	8.841E-01
1.500E+03	8.281E-01	8.281E-01	8.281E-01
2.000E+03	7.726E-01	7.726E-01	7.726E-01
3.000E+03	6.645E-01	6.645E-01	6.645E-01
4.000E+03	5.619E-01	5.619E-01	5.619E-01
5.000E+03	4.667E-01	4.667E-01	4.667E-01
6.000E+03	3.802E-01	3.802E-01	3.802E-01
7.000E+03	3.037E-01	3.037E-01	3.037E-01
8.000E+03	2.374E-01	2.374E-01	2.374E-01
9.000E+03	1.815E-01	1.815E-01	1.815E-01
1.000E+04	1.356E-01	1.356E-01	1.356E-01
1.500E+04	2.133E-02	2.133E-02	2.133E-02
2.000E+04	1.561E-03	1.561E-03	1.561E-03
3.000E+04	3.959E-07	3.963E-07	3.959E-07
4.000E+04	2.842E-13	-1.130E-11	2.842E-13

* Based on Stefhest, 1970

Table 2-10. Case 2 Results: Concentration of Np-237 in the Fracture, at Time $t = 10,000$ Years, Step Release Mode, Retardation Factor $R = 100$

Distance x (m)	FRACVAL	STEFH*	FRACFLO
1.000E+01	9.855E-01	9.855E-01	9.855E-01
1.500E+01	9.799E-01	9.799E-01	9.799E-01
2.000E+01	9.743E-01	9.743E-01	9.743E-01
3.000E+01	9.630E-01	9.630E-01	9.630E-01
4.000E+01	9.518E-01	9.518E-01	9.518E-01
5.000E+01	9.406E-01	9.406E-01	9.406E-01
6.000E+01	9.293E-01	9.293E-01	9.293E-01
7.000E+01	9.181E-01	9.181E-01	9.181E-01
8.000E+01	9.069E-01	9.069E-01	9.069E-01
9.000E+01	8.958E-01	8.958E-01	8.958E-01
1.000E+02	8.846E-01	8.846E-01	8.846E-01
1.500E+02	8.292E-01	8.292E-01	8.292E-01
2.000E+02	7.746E-01	7.746E-01	7.746E-01
3.000E+02	6.688E-01	6.688E-01	6.688E-01
4.000E+02	5.690E-01	5.690E-01	5.690E-01
5.000E+02	4.769E-01	4.769E-01	4.769E-01
6.000E+02	3.935E-01	3.935E-01	3.935E-01
7.000E+02	3.195E-01	3.195E-01	3.195E-01
8.000E+02	2.552E-01	2.552E-01	2.552E-01
9.000E+02	2.005E-01	2.005E-01	2.005E-01
1.000E+03	1.548E-01	1.548E-01	1.548E-01
1.500E+03	3.251E-02	3.251E-02	3.251E-02
2.000E+03	4.277E-03	4.277E-03	4.277E-03
3.000E+03	1.664E-05	1.664E-05	1.664E-05
4.000E+03	7.972E-09	7.972E-09	7.972E-09
5.000E+03	4.255E-13	3.524E-13	4.255E-13
6.000E+03	2.322E-18	-2.249E-14	2.322E-18
7.000E+03	1.195E-24	6.985E-16	1.195E-24
8.000E+03	5.349E-32	1.831E-17	5.349E-32
9.000E+03	1.922E-40	-2.212E-18	1.922E-40
1.000E+04	5.102E-50	-7.266E-20	5.102E-50

* Based on Stefhest, 1970

Table 2-11. Case 2 Results: Concentration of Np-237 in the Fracture, at Time $t = 10,000$ Years, Step Release Mode, Retardation Factor $R = 10,000$

Distance x (m)	FRACVAL	STEFH*	FRACFLO
1.000E+01	8.847E-01	8.847E-01	8.847E-01
1.500E+01	8.294E-01	8.294E-01	8.294E-01
2.000E+01	7.748E-01	7.748E-01	7.748E-01
3.000E+01	6.693E-01	6.693E-01	6.693E-01
4.000E+01	5.700E-01	5.700E-01	5.700E-01
5.000E+01	4.783E-01	4.783E-01	4.783E-01
6.000E+01	3.953E-01	3.953E-01	3.953E-01
7.000E+01	3.217E-01	3.217E-01	3.217E-01
8.000E+01	2.576E-01	2.576E-01	2.576E-01
9.000E+01	2.030E-01	2.030E-01	2.030E-01
1.000E+02	1.574E-01	1.574E-01	1.574E-01
1.500E+02	3.418E-02	3.418E-02	3.418E-02
2.000E+02	4.786E-03	4.786E-03	4.786E-03
3.000E+02	2.393E-05	2.393E-05	2.393E-05
4.000E+02	1.863E-08	1.863E-08	1.863E-08
5.000E+02	2.218E-12	2.090E-12	2.218E-12
6.000E+02	4.031E-17	-1.528E-14	4.031E-17
7.000E+02	1.124E-22	1.062E-15	1.124E-22
8.000E+02	4.854E-29	-3.246E-17	4.854E-29
9.000E+02	3.277E-36	1.737E-18	3.277E-36
1.000E+03	3.499E-44	-3.555E-19	3.499E-44

* Based on Stefhest, 1970

Table 2-12. Case 2 Results: Concentration of Np-237 in the Rock Matrix, at Time $t = 10,000$ Years, Step Release Mode, Retardation Factor $R' = 1$

Distance x (m)	FRACVAL	STEFH*	FRACFLO
1.000E-02	9.852E-01	9.852E-01	9.852E-01
1.500E-02	9.850E-01	9.850E-01	9.850E-01
2.000E-02	9.847E-01	9.847E-01	9.847E-01
3.000E-02	9.841E-01	9.841E-01	9.841E-01
4.000E-02	9.835E-01	9.835E-01	9.835E-01
5.000E-02	9.830E-01	9.830E-01	9.830E-01
6.000E-02	9.824E-01	9.824E-01	9.824E-01
7.000E-02	9.819E-01	9.819E-01	9.819E-01
8.000E-02	9.813E-01	9.813E-01	9.813E-01
9.000E-02	9.807E-01	9.807E-01	9.807E-01
1.000E-01	9.802E-01	9.802E-01	9.802E-01
1.500E-01	9.774E-01	9.774E-01	9.774E-01
2.000E-01	9.745E-01	9.745E-01	9.745E-01
3.000E-01	9.689E-01	9.689E-01	9.689E-01
4.000E-01	9.633E-01	9.633E-01	9.633E-01
5.000E-01	9.577E-01	9.577E-01	9.577E-01
6.000E-01	9.521E-01	9.521E-01	9.521E-01
7.000E-01	9.464E-01	9.464E-01	9.464E-01
8.000E-01	9.408E-01	9.408E-01	9.408E-01
9.000E-01	9.352E-01	9.352E-01	9.352E-01
1.000E+00	9.296E-01	9.296E-01	9.296E-01
1.500E+00	9.016E-01	9.016E-01	9.016E-01
2.000E+00	8.738E-01	8.738E-01	8.738E-01
3.000E+00	8.185E-01	8.185E-01	8.185E-01
4.000E+00	7.642E-01	7.642E-01	7.642E-01
5.000E+00	7.109E-01	7.109E-01	7.109E-01
6.000E+00	6.591E-01	6.591E-01	6.591E-01
7.000E+00	6.088E-01	6.088E-01	6.088E-01
8.000E+00	5.603E-01	5.603E-01	5.603E-01
9.000E+00	5.137E-01	5.137E-01	5.137E-01
1.000E+01	4.692E-01	4.692E-01	4.692E-01
1.500E+01	2.815E-01	2.815E-01	2.815E-01
2.000E+01	1.526E-01	1.526E-01	1.526E-01
3.000E+01	3.256E-02	3.256E-02	3.256E-02
4.000E+01	4.446E-03	4.446E-03	4.446E-03

Table 2-12. Continued.

Distance x (m)	FRACVAL	STEFH*	FRACFLO
5.000E + 01	3.824E - 04	3.824E - 04	3.824E - 04
6.000E + 01	2.051E - 05	2.051E - 05	2.051E - 05
7.000E + 01	6.812E - 07	6.812E - 07	6.812E - 07
8.000E + 01	1.395E - 08	1.395E - 08	1.395E - 08
9.000E + 01	1.754E - 10	1.755E - 10	1.754E - 10
1.000E + 02	1.352E - 12	1.244E - 12	1.352E - 12

* Based on Stefhest, 1970

Table 2-13. Case 2 Results: Concentration of Np-237 in the Rock Matrix, at Time $t = 10,000$ Years, Step Release Mode, Retardation Factor $R' = 100$

Distance x (m)	FRACVAL	STEFH*	FRACFLO
1.000E-02	8.818E-01	8.818E-01	8.818E-01
1.500E-02	8.790E-01	8.790E-01	8.790E-01
2.000E-02	8.763E-01	8.763E-01	8.763E-01
3.000E-02	8.707E-01	8.707E-01	8.707E-01
4.000E-02	8.652E-01	8.652E-01	8.652E-01
5.000E-02	8.596E-01	8.596E-01	8.596E-01
6.000E-02	8.541E-01	8.541E-01	8.541E-01
7.000E-02	8.485E-01	8.485E-01	8.485E-01
8.000E-02	8.430E-01	8.430E-01	8.430E-01
9.000E-02	8.375E-01	8.375E-01	8.375E-01
1.000E-01	8.320E-01	8.320E-01	8.320E-01
1.500E-01	8.046E-01	8.046E-01	8.046E-01
2.000E-01	7.774E-01	7.774E-01	7.774E-01
3.000E-01	7.239E-01	7.239E-01	7.239E-01
4.000E-01	6.716E-01	6.716E-01	6.716E-01
5.000E-01	6.209E-01	6.209E-01	6.209E-01
6.000E-01	5.720E-01	5.720E-01	5.720E-01
7.000E-01	5.249E-01	5.249E-01	5.249E-01
8.000E-01	4.799E-01	4.799E-01	4.799E-01
9.000E-01	4.371E-01	4.371E-01	4.371E-01
1.000E+00	3.966E-01	3.966E-01	3.966E-01
1.500E+00	2.297E-01	2.297E-01	2.297E-01
2.000E+00	1.201E-01	1.201E-01	1.201E-01
3.000E+00	2.373E-02	2.373E-02	2.373E-02
4.000E+00	2.990E-03	2.990E-03	2.990E-03
5.000E+00	2.369E-04	2.369E-04	2.369E-04
6.000E+00	1.169E-05	1.169E-05	1.169E-05
7.000E+00	3.568E-07	3.568E-07	3.568E-07
8.000E+00	6.709E-09	6.710E-09	6.709E-09
9.000E+00	7.746E-11	7.725E-11	7.746E-11
1.000E+01	5.479E-13	5.371E-13	5.479E-13

* Based on Stefhest, 1970

Table 2-14. Case 2 Results: Concentration of Np-237 in the Rock Matrix, at Time $t = 10,000$ Years, Step Release Mode, Retardation Factor $R' = 10,000$

Distance x (m)	FRACVAL	STEFH*	FRACFLO
1.000E-02	1.473E-01	1.473E-01	1.473E-01
1.500E-02	1.377E-01	1.377E-01	1.377E-01
2.000E-02	1.286E-01	1.286E-01	1.286E-01
3.000E-02	1.118E-01	1.118E-01	1.118E-01
4.000E-02	9.676E-02	9.676E-02	9.676E-02
5.000E-02	8.339E-02	8.339E-02	8.339E-02
6.000E-02	7.156E-02	7.156E-02	7.156E-02
7.000E-02	6.114E-02	6.114E-02	6.114E-02
8.000E-02	5.201E-02	5.201E-02	5.201E-02
9.000E-02	4.405E-02	4.405E-02	4.405E-02
1.000E-01	3.714E-02	3.714E-02	3.714E-02
1.500E-01	1.481E-02	1.481E-02	1.481E-02
2.000E-01	5.271E-03	5.271E-03	5.271E-03
3.000E-01	4.726E-04	4.726E-04	4.726E-04
4.000E-01	2.648E-05	2.648E-05	2.648E-05
5.000E-01	9.212E-07	9.212E-07	9.212E-07
6.000E-01	1.980E-08	1.980E-08	1.980E-08
7.000E-01	2.619E-10	2.622E-10	2.619E-10
8.000E-01	2.128E-12	1.973E-12	2.128E-12
9.000E-01	1.060E-14	7.621E-14	1.060E-14
1.000E+00	3.230E-17	-1.697E-14	3.230E-17

* Based on Stefhest, 1970

Figure 2-3. Relative Concentration of Np-237 in the Fracture Versus Distance x , at Time $t = 10,000$ Years, for Different Rock Matrix Retardation Factors ($R' = 1, 10^2, 10^4$) (Case 2: Step Release Mode)

Zero residual concentration in both fracture and rock matrix.

Figure 2-4. Relative Concentration of Np-237 in the Rock Matrix Versus Distance z , at Time $t = 10,000$ Years, for Different Rock Matrix Retardation Factors ($R' = 1, 10^2, 10^4$) (Case 2: Step Release Mode)

Zero residual concentration in both fracture and rock matrix.

2.2.3 Case 3 Results

Case 3 examines the concentration of Np-237 for a non-zero residual concentration distribution in both fracture and rock matrix. This test case is meant to verify the mathematical features describing the transport of Np-237 in both fracture and rock matrix where their respective residual concentration distribution is greater than zero. The residual concentration distribution in the fracture and rock matrix at time equals zero is assumed to be non-uniform in the case of the first medium (see Equation 2-7) and uniform (see Equation 2-8) in the case of the second medium. Solute released at the source is made subject to a band release mode, where the leaching time corresponds to 5,000 years. In the simulations reported here, three values of the rock matrix retardation factor were investigated. Based on the data presented in Table 2-15, the numerical results reported in Tables 2-16 through 2-18 (fracture) and Tables 2-19 through 2-21 (rock matrix) show that both solutions FRACVAL and STEFH are in excellent agreement.

Figures 2-5 and 2-6 show the temporal relative concentration of Np-237 observed in the fracture at a distance of 100 m downstream from the source and the spatial distribution in the rock matrix observed at time corresponding to 10,000 years. Three simulations were performed corresponding to three values of the rock retardation factor ($R' = 1, 100, \text{ and } 10,000$).

2.2.4 Case 4 Results

Case 4 examines the influence of the hydrodynamic dispersion coefficients on the spatial behavior of Np-237 in both fracture and rock matrix. In the course of these investigations, the dispersion-free solution as reported in Section 2.1 was also verified. As in the former test case, a non-zero residual concentration is assumed, with a non-uniform distribution in the fracture and uniform in the rock matrix. Solute release from the source is subject to a band release mode, where the leaching time corresponds to 1,000 years. In these simulations five values of the hydrodynamic dispersion were investigated. Based on the data presented in Table 2-22, the numerical results reported in Tables 2-23 through 2-27 (fracture) and Tables 2-28 through 2-32 (rock matrix) show that both solutions FRACVAL and STEFH are in excellent agreement.

Figures 2-7 and 2-8 show the spatial relative concentration of Np-237 observed in the fracture and in the rock matrix at a distance of 100 m downstream from the source for a simulation time corresponding to 5,000 years. The influence of the hydrodynamic dispersion coefficient becomes noticeable when it exceeds the value of $100 \text{ m}^2/\text{yr}$. The concentration in the fracture far downstream from the source registers a drop from its original value of approximately 1.5×10^{-4} down to a value of 1.051×10^{-5} (see Figure 2-7). This confirms theory, which for the choice of selected parameter values related to the residual concentration distribution in both media, suggests that in the absence of solute released

Table 2-15. Input Parameters for Case 3

Species	Np-237
Type of Release Mode	Band
Leaching Time T	5×10^3 yr
$T_{1/2}$	2.14×10^6 yr
Λ^0*	1.0
a_1^*	1.5×10^{-3}
a_2^*	5.0×10^{-4}
α	0.2 1/m
b_1^*	1.0×10^{-3}
D_p	0.01 m ² /yr
u	10.0 m/yr
D_x	1.0 m ² /yr
b	0.005 m
R	1.0
R'	1.0, 100, 10,000
ϕ	10^{-2}

*(arbitrary units of activity/L³)

Table 2-16, Case 3 Results: Concentration of Np-237 in the Fracture, at $x = 100$ m, Band Release Mode, and Retardation Factor $R' = 1$

Time t (yr)	FRACVAL	STEFH*	Time t (yr)	FRACVAL	STEFH*
1.000E+00	1.405E-03	1.405E-03	5.000E+03	9.824E-01	9.825E-01
1.500E+00	1.387E-03	1.387E-03	6.000E+03	2.124E-02	2.125E-02
2.000E+00	1.373E-03	1.373E-03	7.000E+03	1.178E-02	1.178E-02
3.000E+00	1.352E-03	1.356E-03	8.000E+03	8.001E-03	8.002E-03
4.000E+00	1.335E-03	1.403E-03	9.000E+03	5.955E-03	5.956E-03
5.000E+00	1.322E-03	1.057E-03	1.000E+04	4.679E-03	4.680E-03
6.000E+00	1.310E-03	1.450E-03	1.500E+04	2.071E-03	2.072E-03
7.000E+00	1.301E-03	7.417E-04	2.000E+04	1.235E-03	1.235E-03
8.000E+00	1.293E-03	4.895E-03	3.000E+04	6.220E-04	6.226E-04
9.000E+00	1.369E-03	-8.316E-03	4.000E+04	3.898E-04	3.902E-04
1.000E+01	2.109E-02	3.294E-02	5.000E+04	2.732E-04	2.736E-04
1.500E+01	5.262E-01	5.276E-01	6.000E+04	2.051E-04	2.055E-04
2.000E+01	6.546E-01	6.555E-01	7.000E+04	1.612E-04	1.616E-04
3.000E+01	7.519E-01	7.519E-01	8.000E+04	1.311E-04	1.314E-04
4.000E+01	7.964E-01	7.964E-01	9.000E+04	1.093E-04	1.096E-04
5.000E+01	8.232E-01	8.232E-01	1.000E+05	9.291E-05	9.321E-05
6.000E+01	8.416E-01	8.416E-01	1.500E+05	4.998E-05	5.022E-05
7.000E+01	8.552E-01	8.552E-01	2.000E+05	3.229E-05	3.249E-05
8.000E+01	8.659E-01	8.659E-01	3.000E+05	1.748E-05	1.765E-05
9.000E+01	8.744E-01	8.745E-01	4.000E+05	1.132E-05	1.146E-05
1.000E+02	8.816E-01	8.816E-01	5.000E+05	8.076E-06	8.194E-06
1.500E+02	9.049E-01	9.049E-01	6.000E+05	6.124E-06	6.228E-06
2.000E+02	9.183E-01	9.183E-01	7.000E+05	4.842E-06	4.935E-06
3.000E+02	9.338E-01	9.338E-01	8.000E+05	3.945E-06	4.031E-06
4.000E+02	9.428E-01	9.428E-01	9.000E+05	3.290E-06	3.368E-06
5.000E+02	9.490E-01	9.490E-01	1.000E+06	2.793E-06	2.864E-06
6.000E+02	9.534E-01	9.534E-01			
7.000E+02	9.569E-01	9.569E-01			
8.000E+02	9.597E-01	9.597E-01			
9.000E+02	9.619E-01	9.619E-01			
1.000E+03	9.639E-01	9.639E-01			
1.500E+03	9.703E-01	9.703E-01			
2.000E+03	9.741E-01	9.741E-01			
3.000E+03	9.784E-01	9.784E-01			
4.000E+03	9.809E-01	9.809E-01			

* Based on Stefhest, 1970

Table 2-17. Case 3 Results: Concentration of Np-237 in the Fracture, at $x = 100$ m, Band Release Mode, and Retardation Factor $R' = 100$

Time t (yr)	FRACVAL	STEFH*	Time t (yr)	FRACVAL	STEFH*
1.000E+00	1.128E-03	1.128E-03	5.000E+03	8.401E-01	8.401E-01
1.500E+00	1.107E-03	1.107E-03	6.000E+03	2.016E-01	2.016E-01
2.000E+00	1.094E-03	1.094E-03	7.000E+03	1.143E-01	1.143E-01
3.000E+00	1.078E-03	1.078E-03	8.000E+03	7.828E-02	7.828E-02
4.000E+00	1.068E-03	1.068E-03	9.000E+03	5.853E-02	5.853E-02
5.000E+00	1.062E-03	1.062E-03	1.000E+04	4.612E-02	4.612E-02
6.000E+00	1.056E-03	1.056E-03	1.500E+04	2.055E-02	2.055E-02
7.000E+00	1.052E-03	1.052E-03	2.000E+04	1.228E-02	1.228E-02
8.000E+00	1.049E-03	1.049E-03	3.000E+04	6.203E-03	6.203E-03
9.000E+00	1.046E-03	1.046E-03	4.000E+04	3.892E-03	3.892E-03
1.000E+01	1.044E-03	1.044E-03	5.000E+04	2.730E-03	2.731E-03
1.500E+01	1.036E-03	1.036E-03	6.000E+04	2.051E-03	2.051E-03
2.000E+01	1.048E-03	1.048E-03	7.000E+04	1.613E-03	1.614E-03
3.000E+01	2.848E-03	2.848E-03	8.000E+04	1.312E-03	1.312E-03
4.000E+01	1.147E-02	1.147E-02	9.000E+04	1.094E-03	1.095E-03
5.000E+01	2.722E-02	2.722E-02	1.000E+05	9.309E-04	9.312E-04
6.000E+01	4.746E-02	4.746E-02	1.500E+05	5.017E-04	5.019E-04
7.000E+01	6.985E-02	6.985E-02	2.000E+05	3.246E-04	3.248E-04
8.000E+01	9.289E-02	9.289E-02	3.000E+05	1.763E-04	1.764E-04
9.000E+01	1.157E-01	1.157E-01	4.000E+05	1.144E-04	1.145E-04
1.000E+02	1.378E-01	1.378E-01	5.000E+05	8.183E-05	8.193E-05
1.500E+02	2.334E-01	2.334E-01	6.000E+05	6.219E-05	6.228E-05
2.000E+02	3.061E-01	3.061E-01	7.000E+05	4.927E-05	4.935E-05
3.000E+02	4.072E-01	4.072E-01	8.000E+05	4.023E-05	4.030E-05
4.000E+02	4.746E-01	4.746E-01	9.000E+05	3.361E-05	3.367E-05
5.000E+02	5.235E-01	5.235E-01	1.000E+06	2.858E-05	2.864E-05
6.000E+02	5.609E-01	5.609E-01			
7.000E+02	5.907E-01	5.907E-01			
8.000E+02	6.152E-01	6.152E-01			
9.000E+02	6.357E-01	6.357E-01			
1.000E+03	6.533E-01	6.533E-01			
1.500E+03	7.141E-01	7.141E-01			
2.000E+03	7.510E-01	7.510E-01			
3.000E+03	7.954E-01	7.954E-01			
4.000E+03	8.220E-01	8.220E-01			

* Based on Stefhest, 1970

Table 2-18. Case 3 Results: Concentration of Np-237 in the Fracture, at $x = 100$ m, Band Release Mode, and Retardation Factor $R' = 10,000$

Time t (yr)	FRACVAL	STEFH*	Time t (yr)	FRACVAL	STEFH*
1.000E+00	1.014E-03	1.014E-03	5.000E+03	4.702E-02	4.702E-02
1.500E+00	1.012E-03	1.012E-03	6.000E+03	6.936E-02	6.936E-02
2.000E+00	1.010E-03	1.010E-03	7.000E+03	9.067E-02	9.067E-02
3.000E+00	1.008E-03	1.008E-03	8.000E+03	1.049E-01	1.049E-01
4.000E+00	1.007E-03	1.007E-03	9.000E+03	1.113E-01	1.113E-01
5.000E+00	1.006E-03	1.006E-03	1.000E+04	1.123E-01	1.123E-01
6.000E+00	1.006E-03	1.006E-03	1.500E+04	9.107E-02	9.107E-02
7.000E+00	1.005E-03	1.005E-03	2.000E+04	6.922E-02	6.922E-02
8.000E+00	1.005E-03	1.005E-03	3.000E+04	4.323E-02	4.323E-02
9.000E+00	1.005E-03	1.005E-03	4.000E+04	2.991E-02	2.991E-02
1.000E+01	1.004E-03	1.004E-03	5.000E+04	2.220E-02	2.220E-02
1.500E+01	1.004E-03	1.004E-03	6.000E+04	1.729E-02	1.729E-02
2.000E+01	1.003E-03	1.003E-03	7.000E+04	1.396E-02	1.396E-02
3.000E+01	1.003E-03	1.003E-03	8.000E+04	1.157E-02	1.157E-02
4.000E+01	1.002E-03	1.002E-03	9.000E+04	9.794E-03	9.794E-03
5.000E+01	1.002E-03	1.002E-03	1.000E+05	8.430E-03	8.430E-03
6.000E+01	1.002E-03	1.002E-03	1.500E+05	4.704E-03	4.704E-03
7.000E+01	1.002E-03	1.002E-03	2.000E+05	3.096E-03	3.096E-03
8.000E+01	1.002E-03	1.002E-03	3.000E+05	1.710E-03	1.710E-03
9.000E+01	1.001E-03	1.001E-03	4.000E+05	1.120E-03	1.120E-03
1.000E+02	1.001E-03	1.001E-03	5.000E+05	8.049E-04	8.049E-04
1.500E+02	1.001E-03	1.001E-03	6.000E+05	6.138E-04	6.138E-04
2.000E+02	1.001E-03	1.001E-03	7.000E+05	4.875E-04	4.875E-04
3.000E+02	1.001E-03	1.001E-03	8.000E+05	3.988E-04	3.988E-04
4.000E+02	1.001E-03	1.001E-03	9.000E+05	3.336E-04	3.337E-04
5.000E+02	1.000E-03	1.000E-03	1.000E+06	2.841E-04	2.841E-04
6.000E+02	1.000E-03	1.000E-03	1.500E+06	1.506E-04	1.506E-04
7.000E+02	1.000E-03	1.000E-03	2.000E+06	9.369E-05	9.369E-05
8.000E+02	1.001E-03	1.001E-03	3.000E+06	4.513E-05	4.513E-05
9.000E+02	1.004E-03	1.004E-03	4.000E+06	2.507E-05	2.507E-05
1.000E+03	1.011E-03	1.011E-03	5.000E+06	1.497E-05	1.497E-05
1.500E+03	1.298E-03	1.298E-03	6.000E+06	9.339E-06	9.340E-06
2.000E+03	2.691E-03	2.691E-03	7.000E+06	5.992E-06	5.993E-06
3.000E+03	1.117E-02	1.117E-02	8.000E+06	3.921E-06	3.921E-06
4.000E+03	2.683E-02	2.683E-02	9.000E+06	2.603E-06	2.604E-06
			1.000E+07	1.748E-06	1.748E-06

* Based on Stefhest, 1970

Table 2-19. Case 3 Results: Concentration of Np-237 in the Rock Matrix, at $x = 100$ m, Time $t = 10,000$ Years, Band Release Mode, Retardation Factor $R' = 1$

Distance x (m)	FRACVAL	STEFH*	Distance x (m)	FRACVAL	STEFH*
1.000E-02	4.796E-03	4.796E-03	5.000E+00	1.101E-01	1.101E-01
1.500E-02	4.913E-03	4.913E-03	6.000E+00	1.259E-01	1.259E-01
2.000E-02	5.030E-03	5.030E-03	7.000E+00	1.393E-01	1.393E-01
3.000E-02	5.263E-03	5.263E-03	8.000E+00	1.500E-01	1.500E-01
4.000E-02	5.497E-03	5.497E-03	9.000E+00	1.580E-01	1.580E-01
5.000E-02	5.731E-03	5.731E-03	1.000E+01	1.633E-01	1.633E-01
6.000E-02	5.965E-03	5.965E-03	1.500E+01	1.543E-01	1.543E-01
7.000E-02	6.199E-03	6.199E-03	2.000E+01	1.103E-01	1.103E-01
8.000E-02	6.433E-03	6.433E-03	3.000E+01	3.102E-02	3.102E-02
9.000E-02	6.667E-03	6.667E-03	4.000E+01	5.381E-03	5.381E-03
1.000E-01	6.900E-03	6.900E-03	5.000E+01	1.378E-03	1.378E-03
1.500E-01	8.069E-03	8.069E-03	6.000E+01	1.017E-03	1.017E-03
2.000E-01	9.237E-03	9.237E-03	7.000E+01	9.974E-04	9.974E-04
3.000E-01	1.157E-02	1.157E-02	8.000E+01	9.968E-04	9.968E-04
4.000E-01	1.390E-02	1.390E-02	9.000E+01	9.968E-04	9.968E-04
5.000E-01	1.623E-02	1.623E-02	1.000E+02	9.968E-04	9.968E-04
6.000E-01	1.856E-02	1.856E-02			
7.000E-01	2.088E-02	2.088E-02			
8.000E-01	2.320E-02	2.320E-02			
9.000E-01	2.551E-02	2.551E-02			
1.000E+00	2.782E-02	2.782E-02			
1.500E+00	3.925E-02	3.925E-02			
2.000E+00	5.046E-02	5.046E-02			
3.000E+00	7.201E-02	7.201E-02			
4.000E+00	9.202E-02	9.202E-02			

* Based on Stefhest, 1970

Table 2-20. Case 3 Results: Concentration of Np-237 in the Rock Matrix, at $x = 100$ m, Time $t = 10,000$ Years, Band Release Mode, Retardation Factor $R' = 100$

Distance x (m)	FRACVAL	STEFH*	Distance x (m)	FRACVAL	STEFH*
1.000E-02	4.723E-02	4.723E-02	1.000E+00	1.663E-01	1.663E-01
1.500E-02	4.835E-02	4.835E-02	1.500E+00	1.410E-01	1.410E-01
2.000E-02	4.946E-02	4.946E-02	2.000E+00	9.303E-02	9.303E-02
3.000E-02	5.168E-02	5.168E-02	3.000E+00	2.332E-02	2.332E-02
4.000E-02	5.388E-02	5.388E-02	4.000E+00	3.957E-03	3.957E-03
5.000E-02	5.608E-02	5.608E-02	5.000E+00	1.233E-03	1.233E-03
6.000E-02	5.826E-02	5.826E-02	6.000E+00	1.008E-03	1.008E-03
7.000E-02	6.043E-02	6.043E-02	7.000E+00	9.971E-04	9.971E-04
8.000E-02	6.258E-02	6.258E-02	8.000E+00	9.968E-04	9.968E-04
9.000E-02	6.473E-02	6.473E-02	9.000E+00	9.968E-04	9.968E-04
1.000E-01	6.686E-02	6.686E-02	1.000E+01	9.968E-04	9.968E-04
1.500E-01	7.727E-02	7.727E-02			
2.000E-01	8.728E-02	8.728E-02			
3.000E-01	1.059E-01	1.059E-01			
4.000E-01	1.223E-01	1.223E-01			
5.000E-01	1.362E-01	1.362E-01			
6.000E-01	1.476E-01	1.476E-01			
7.000E-01	1.563E-01	1.563E-01			
8.000E-01	1.622E-01	1.622E-01			
9.000E-01	1.655E-01	1.655E-01			

* Based on Stefhest, 1970

Table 2-21. Case 3 Results: Concentration of Np-237 in the Rock Matrix, at $x = 100$ m, Time $t = 10,000$ Years, Band Release Mode, Retardation Factor $R' = 10,000$

Distance x (m)	FRACVAL	STEFH*	Distance x (m)	FRACVAL	STEFH*
1.000E-02	1.073E-01	1.073E-01	1.000E-01	3.485E-02	3.485E-02
1.500E-02	1.024E-01	1.024E-01	1.500E-01	1.521E-02	1.521E-02
2.000E-02	9.750E-02	9.750E-02	2.000E-01	6.181E-03	6.181E-03
3.000E-02	8.787E-02	8.787E-02	3.000E-01	1.468E-03	1.468E-03
4.000E-02	7.859E-02	7.859E-02	4.000E-01	1.023E-03	1.023E-03
5.000E-02	6.978E-02	6.978E-02	5.000E-01	9.977E-04	9.977E-04
6.000E-02	6.151E-02	6.151E-02	6.000E-01	9.968E-04	9.968E-04
7.000E-02	5.387E-02	5.387E-02	7.000E-01	9.968E-04	9.968E-04
8.000E-02	4.687E-02	4.687E-02	8.000E-01	9.968E-04	9.968E-04
9.000E-02	4.053E-02	4.053E-02	9.000E-01	9.968E-04	9.968E-04
			1.000E+00	9.968E-04	9.968E-04

* Based on Stefhest, 1970

Figure 2-5. Breakthrough Curves Showing the Relative Concentration of Np-237 in the Fracture Versus Time at $x = 100$ m for Different Rock Matrix Retardation Factors ($R' = 1, 100, 10,000$) (Case 3: Band Release Mode)

Zero residual concentration in both fracture and rock matrix.

Figure 2-6. Relative Concentration of Np-237 in the Rock Matrix Versus Distance z , at Time $t = 10,000$ Years, for Different Rock Matrix Retardation Factors ($R' = 1, 100, 10,000$) (Case 3: Band Release Mode)

Dashed line indicates residual concentration.

Table 2-22. Input Parameters for Case 4

Species	Np-237
Type of Release Mode	Band
Leaching Time T	10^3 yr
$T_{1/2}$	2.14×10^6 yr
A_0^*	1.0
a_1^*	1.5×10^{-4}
a_2^*	$-(0.5 \times 10^{-4})^{**}$
α	0.2 1/m
b_1^*	1.0×10^{-5}
D_p	0.01 m ² /yr
u	10.0 m/yr
D_x	0, 10, 100, 1,000, 10,000 m ² /yr
b	0.005 m
R	3.0
R'	1,000
t	5,000 yr
ϕ	10^{-2}

*(arbitrary units of activity/L³)

**This indicates that in Equation 2-7 the constant
+ a_2 becomes - a_2 .

at the source, the concentration gradient is such that transfer of Np-237 must proceed from fracture to rock matrix until the concentration equalizes on each side of the fracture rock interface.

Table 2-23. Case 4 Results: Concentration of Np-237 in the Fracture, at
Time $t = 5,000$ Years, Band Release Mode, Zero Dispersion,
 $D_x = 0 \text{ m}^2/\text{yr}$

Distance x (m)	FRACVAL	STEFH*
1.000E+00	5.948E-04	5.948E-04
1.500E+00	8.922E-04	8.922E-04
2.000E+00	1.190E-03	1.190E-03
3.000E+00	1.784E-03	1.784E-03
4.000E+00	2.379E-03	2.379E-03
5.000E+00	2.973E-03	2.973E-03
6.000E+00	3.568E-03	3.568E-03
7.000E+00	4.161E-03	4.161E-03
8.000E+00	4.755E-03	4.755E-03
9.000E+00	5.348E-03	5.348E-03
1.000E+01	5.940E-03	5.940E-03
1.500E+01	8.889E-03	8.889E-03
2.000E+01	1.181E-02	1.181E-02
3.000E+01	1.754E-02	1.754E-02
4.000E+01	2.304E-02	2.304E-02
5.000E+01	2.825E-02	2.825E-02
6.000E+01	3.310E-02	3.310E-02
7.000E+01	3.754E-02	3.754E-02
8.000E+01	4.151E-02	4.151E-02
9.000E+01	4.499E-02	4.499E-02
1.000E+02	4.793E-02	4.793E-02
1.500E+02	5.440E-02	5.440E-02
2.000E+02	4.893E-02	4.893E-02
3.000E+02	2.360E-02	2.360E-02
4.000E+02	6.364E-03	6.364E-03
5.000E+02	1.019E-03	1.019E-03
6.000E+02	1.073E-04	1.073E-04
7.000E+02	1.623E-05	1.623E-05
8.000E+02	1.072E-05	1.072E-05
9.000E+02	1.052E-05	1.052E-05
1.000E+03	1.051E-05	1.051E-05
1.500E+03	1.051E-05	1.051E-05
2.000E+03	1.051E-05	1.051E-05

* Based on Stefhest, 1970

Table 2-24. Case 4 Results: Concentration of Np-237 in the Fracture, at Time $t = 5,000$ Years, Band Release Mode, $D_x = 10 \text{ m}^2/\text{yr}$

Distance x (m)	FRACVAL	STEFH*
1.000E+00	5.946E-04	5.946E-04
1.500E+00	8.919E-04	8.919E-04
2.000E+00	1.189E-03	1.189E-03
3.000E+00	1.783E-03	1.783E-03
4.000E+00	2.378E-03	2.378E-03
5.000E+00	2.971E-03	2.971E-03
6.000E+00	3.564E-03	3.564E-03
7.000E+00	4.157E-03	4.157E-03
8.000E+00	4.749E-03	4.749E-03
9.000E+00	5.341E-03	5.341E-03
1.000E+01	5.931E-03	5.931E-03
1.500E+01	8.871E-03	8.871E-03
2.000E+01	1.178E-02	1.178E-02
3.000E+01	1.747E-02	1.747E-02
4.000E+01	2.292E-02	2.292E-02
5.000E+01	2.807E-02	2.807E-02
6.000E+01	3.285E-02	3.285E-02
7.000E+01	3.721E-02	3.721E-02
8.000E+01	4.111E-02	4.111E-02
9.000E+01	4.451E-02	4.451E-02
1.000E+02	4.738E-02	4.738E-02
1.500E+02	5.368E-02	5.368E-02
2.000E+02	4.841E-02	4.841E-02
3.000E+02	2.394E-02	2.394E-02
4.000E+02	6.854E-03	6.854E-03
5.000E+02	1.217E-03	1.217E-03
6.000E+02	1.463E-04	1.463E-04
7.000E+02	2.051E-05	2.051E-05
8.000E+02	1.100E-05	1.100E-05
9.000E+02	1.053E-05	1.053E-05
1.000E+03	1.051E-05	1.051E-05
1.500E+03	1.051E-05	1.051E-05
2.000E+03	1.051E-05	1.051E-05
3.000E+03	1.051E-05	1.051E-05

* Based on Stefhest, 1970

Table 2-25. Case 4 Results: Concentration of Np-237 in the Fracture, at
Time $t = 5,000$ Years, Band Release Mode, $D_x = 100 \text{ m}^2/\text{yr}$

Distance x (m)	FRACVAL	STEFH*
1.000E+00	5.810E-04	5.810E-04
1.500E+00	8.710E-04	8.710E-04
2.000E+00	1.161E-03	1.161E-03
3.000E+00	1.739E-03	1.739E-03
4.000E+00	2.316E-03	2.316E-03
5.000E+00	2.891E-03	2.891E-03
6.000E+00	3.464E-03	3.464E-03
7.000E+00	4.036E-03	4.036E-03
8.000E+00	4.606E-03	4.606E-03
9.000E+00	5.174E-03	5.174E-03
1.000E+01	5.741E-03	5.741E-03
1.500E+01	8.541E-03	8.541E-03
2.000E+01	1.129E-02	1.129E-02
3.000E+01	1.657E-02	1.657E-02
4.000E+01	2.156E-02	2.156E-02
5.000E+01	2.618E-02	2.618E-02
6.000E+01	3.042E-02	3.042E-02
7.000E+01	3.423E-02	3.423E-02
8.000E+01	3.760E-02	3.760E-02
9.000E+01	4.051E-02	4.051E-02
1.000E+02	4.296E-02	4.296E-02
1.500E+02	4.855E-02	4.855E-02
2.000E+02	4.504E-02	4.504E-02
3.000E+02	2.627E-02	2.627E-02
4.000E+02	1.045E-02	1.045E-02
5.000E+02	3.068E-03	3.068E-03
6.000E+02	7.001E-04	7.001E-04
7.000E+02	1.339E-04	1.339E-04
8.000E+02	2.840E-05	2.840E-05
9.000E+02	1.265E-05	1.265E-05
1.000E+03	1.073E-05	1.073E-05
1.500E+03	1.051E-05	1.051E-05
2.000E+03	1.051E-05	1.051E-05
3.000E+03	1.051E-05	1.051E-05
4.000E+03	1.051E-05	1.051E-05

* Based on Stefhest, 1970

Table 2-26. Case 4 Results: Concentration of Np-237 in the Fracture, at Time $t = 5,000$ Years, Band Release Mode, $D_x = 1,000 \text{ m}^2/\text{yr}$

Distance x (m)	FRACVAL	STEFH*	Distance x (m)	FRACVAL	STEFH*
1.000E+00	3.764E-04	3.765E-04	1.000E+02	2.684E-02	2.684E-02
1.500E+00	5.639E-04	5.639E-04	1.500E+02	3.273E-02	3.273E-02
2.000E+00	7.508E-04	7.508E-04	2.000E+02	3.473E-02	3.473E-02
3.000E+00	1.123E-03	1.123E-03	3.000E+02	3.111E-02	3.111E-02
4.000E+00	1.493E-03	1.493E-03	4.000E+02	2.310E-02	2.310E-02
5.000E+00	1.861E-03	1.861E-03	5.000E+02	1.511E-02	1.511E-02
6.000E+00	2.226E-03	2.226E-03	6.000E+02	8.973E-03	8.973E-03
7.000E+00	2.589E-03	2.589E-03	7.000E+02	4.920E-03	4.920E-03
8.000E+00	2.951E-03	2.951E-03	8.000E+02	2.522E-03	2.522E-03
9.000E+00	3.310E-03	3.310E-03	9.000E+02	1.220E-03	1.220E-03
1.000E+01	3.666E-03	3.666E-03	1.000E+03	5.620E-04	5.620E-04
1.500E+01	5.417E-03	5.417E-03	1.500E+03	1.604E-05	1.604E-05
2.000E+01	7.113E-03	7.113E-03	2.000E+03	1.054E-05	1.054E-05
3.000E+01	1.034E-02	1.034E-02	3.000E+03	1.051E-05	1.051E-05
4.000E+01	1.334E-02	1.334E-02	4.000E+03	1.051E-05	1.051E-05
5.000E+01	1.612E-02	1.612E-02	5.000E+03	1.051E-05	1.051E-05
6.000E+01	1.869E-02	1.869E-02	6.000E+03	1.051E-05	1.051E-05
7.000E+01	2.104E-02	2.104E-02	7.000E+03	1.051E-05	1.051E-05
8.000E+01	2.318E-02	2.318E-02	8.000E+03	1.051E-05	1.051E-05
9.000E+01	2.511E-02	2.511E-02	9.000E+03	1.051E-05	1.051E-05
			1.000E+04	1.051E-05	1.051E-05

* Based on Stefhest, 1970

Table 2-27. Case 4 Results: Concentration of Np-237 in the Fracture, at Time $t = 5,000$ Years, Band Release Mode, $D_x = 10,000 \text{ m}^2/\text{yr}$

Distance x (m)	FRACVAL	STEFH*	Distance x (m)	FRACVAL	STEFH*
1.000E+00	1.372E-04	1.376E-04	1.000E+02	1.161E-02	1.161E-02
1.500E+00	2.058E-04	2.063E-04	1.500E+02	1.590E-02	1.590E-02
2.000E+00	2.743E-04	2.748E-04	2.000E+02	1.930E-02	1.930E-02
3.000E+00	4.111E-04	4.115E-04	3.000E+02	2.381E-02	2.381E-02
4.000E+00	5.474E-04	5.478E-04	4.000E+02	2.583E-02	2.583E-02
5.000E+00	6.832E-04	6.836E-04	5.000E+02	2.601E-02	2.601E-02
6.000E+00	8.186E-04	8.190E-04	6.000E+02	2.491E-02	2.491E-02
7.000E+00	9.536E-04	9.539E-04	7.000E+02	2.299E-02	2.299E-02
8.000E+00	1.088E-03	1.088E-03	8.000E+02	2.061E-02	2.061E-02
9.000E+00	1.222E-03	1.222E-03	9.000E+02	1.804E-02	1.804E-02
1.000E+01	1.356E-03	1.356E-03	1.000E+03	1.548E-02	1.548E-02
1.500E+01	2.017E-03	2.017E-03	1.500E+03	5.742E-03	5.742E-03
2.000E+01	2.667E-03	2.667E-03	2.000E+03	1.628E-03	1.628E-03
3.000E+01	3.933E-03	3.933E-03	3.000E+03	8.447E-05	8.447E-05
4.000E+01	5.155E-03	5.155E-03	4.000E+03	1.247E-05	1.247E-05
5.000E+01	6.335E-03	6.335E-03	5.000E+03	1.055E-05	1.055E-05
6.000E+01	7.471E-03	7.471E-03	6.000E+03	1.051E-05	1.051E-05
7.000E+01	8.566E-03	8.566E-03	7.000E+03	1.051E-05	1.051E-05
8.000E+01	9.620E-03	9.620E-03	8.000E+03	1.051E-05	1.051E-05
9.000E+01	1.063E-02	1.063E-02	9.000E+03	1.051E-05	1.051E-05
			1.000E+04	1.051E-05	1.051E-05

* Based on Stefhest, 1970

Table 2-28. Case 4 Results: Concentration of Np-237 in the Rock Matrix, at $x = 100$ m, Time $t = 5,000$ Years, Band Release Mode, Zero Dispersion, $D = 0$ m²/yr

Distance x (m)	FRACVAL	STEFH*	Distance x (m)	FRACVAL	STEFH*
1.000E-02	4.857E-02	4.857E-02	1.000E+00	1.380E-04	1.380E-04
1.500E-02	4.917E-02	4.917E-02	1.500E+00	1.006E-05	1.006E-05
2.000E-02	4.974E-02	4.974E-02	2.000E+00	9.984E-06	9.984E-06
3.000E-02	5.078E-02	5.078E-02	3.000E+00	9.984E-06	9.984E-06
4.000E-02	5.168E-02	5.168E-02	4.000E+00	9.984E-06	9.984E-06
5.000E-02	5.244E-02	5.244E-02	5.000E+00	9.984E-06	9.984E-06
6.000E-02	5.306E-02	5.306E-02	6.000E+00	9.984E-06	9.984E-06
7.000E-02	5.354E-02	5.354E-02	7.000E+00	9.984E-06	9.984E-06
8.000E-02	5.390E-02	5.390E-02	8.000E+00	9.984E-06	9.984E-06
9.000E-02	5.412E-02	5.412E-02	9.000E+00	9.984E-06	9.984E-06
1.000E-01	5.422E-02	5.422E-02	1.000E+01	9.984E-06	9.984E-06
1.500E-01	5.294E-02	5.294E-02			
2.000E-01	4.921E-02	4.921E-02			
3.000E-01	3.738E-02	3.738E-02			
4.000E-01	2.438E-02	2.438E-02			
5.000E-01	1.384E-02	1.384E-02			
6.000E-01	6.899E-03	6.899E-03			
7.000E-01	3.042E-03	3.042E-03			
8.000E-01	1.194E-03	1.194E-03			
9.000E-01	4.218E-04	4.218E-04			

* Based on Stefhest, 1970

Table 2-29. Case 4 Results: Concentration of Np-237 in the Rock Matrix, at
 $x = 100$ m, Time $t = 5,000$ Years, Band Release Mode, Zero
Dispersion, $D = 10$ m²/yr

Distance x (m)	FRACVAL	STEFH*
1.000E-02	4.802E-02	4.802E-02
1.500E-02	4.862E-02	4.862E-02
2.000E-02	4.919E-02	4.919E-02
3.000E-02	5.023E-02	5.023E-02
4.000E-02	5.113E-02	5.113E-02
5.000E-02	5.189E-02	5.189E-02
6.000E-02	5.252E-02	5.252E-02
7.000E-02	5.302E-02	5.302E-02
8.000E-02	5.338E-02	5.338E-02
9.000E-02	5.362E-02	5.362E-02
1.000E-01	5.373E-02	5.373E-02
1.500E-01	5.255E-02	5.255E-02
2.000E-01	4.894E-02	4.894E-02
3.000E-01	3.734E-02	3.734E-02
4.000E-01	2.448E-02	2.448E-02
5.000E-01	1.399E-02	1.399E-02
6.000E-01	7.023E-03	7.023E-03
7.000E-01	3.121E-03	3.121E-03
8.000E-01	1.236E-03	1.236E-03
9.000E-01	4.405E-04	4.405E-04
1.000E+00	1.451E-04	1.451E-04
1.500E+00	1.007E-05	1.007E-05
2.000E+00	9.984E-06	9.984E-06
3.000E+00	9.984E-06	9.984E-06
4.000E+00	9.984E-06	9.984E-06
5.000E+00	9.984E-06	9.984E-06
6.000E+00	9.984E-06	9.984E-06
7.000E+00	9.984E-06	9.984E-06
8.000E+00	9.984E-06	9.984E-06
9.000E+00	9.984E-06	9.984E-06
1.000E+01	9.984E-06	9.984E-06

* Based on Stefhest, 1970

Table 2-30. Case 4 Results: Concentration of Np-237 in the Rock Matrix, at $x = 100$ m, Time $t = 5,000$ Years, Band Release Mode, Zero Dispersion, $D = 100 \text{ m}^2/\text{yr}$

Distance x (m)	FRACVAL	STEFH*
1.000E-02	4.361E-02	4.361E-02
1.500E-02	4.423E-02	4.423E-02
2.000E-02	4.482E-02	4.482E-02
3.000E-02	4.590E-02	4.590E-02
4.000E-02	4.687E-02	4.687E-02
5.000E-02	4.772E-02	4.772E-02
6.000E-02	4.845E-02	4.845E-02
7.000E-02	4.905E-02	4.905E-02
8.000E-02	4.955E-02	4.955E-02
9.000E-02	4.992E-02	4.992E-02
1.000E-01	5.018E-02	5.018E-02
1.500E-01	4.987E-02	4.987E-02
2.000E-01	4.722E-02	4.722E-02
3.000E-01	3.735E-02	3.735E-02
4.000E-01	2.547E-02	2.547E-02
5.000E-01	1.519E-02	1.519E-02
6.000E-01	7.982E-03	7.982E-03
7.000E-01	3.722E-03	3.722E-03
8.000E-01	1.549E-03	1.549E-03
9.000E-01	5.797E-04	5.797E-04
1.000E+00	1.989E-04	1.989E-04
1.500E+00	1.014E-05	1.014E-05
2.000E+00	9.984E-06	9.984E-06
3.000E+00	9.984E-06	9.984E-06
4.000E+00	9.984E-06	9.984E-06
5.000E+00	9.984E-06	9.984E-06
6.000E+00	9.984E-06	9.984E-06
7.000E+00	9.984E-06	9.984E-06
8.000E+00	9.984E-06	9.984E-06
9.000E+00	9.984E-06	9.984E-06
1.000E+01	9.984E-06	9.984E-06

* Based on Stefhest, 1970

Table 2-31. Case 4 Results: Concentration of Np-237 in the Rock Matrix, at
 $x = 100$ m, Time $t = 5,000$ Years, Band Release Mode, Zero
Dispersion, $D = 1,000 \text{ m}^2/\text{yr}$

Distance x (m)	FRACVAL	STEFH*
1.000E-02	2.772E-02	2.772E-02
1.500E-02	2.858E-02	2.858E-02
2.000E-02	2.943E-02	2.943E-02
3.000E-02	3.105E-02	3.105E-02
4.000E-02	3.260E-02	3.260E-02
5.000E-02	3.406E-02	3.406E-02
6.000E-02	3.544E-02	3.544E-02
7.000E-02	3.673E-02	3.673E-02
8.000E-02	3.792E-02	3.792E-02
9.000E-02	3.901E-02	3.901E-02
1.000E-01	4.001E-02	4.001E-02
1.500E-01	4.351E-02	4.351E-02
2.000E-01	4.457E-02	4.457E-02
3.000E-01	4.043E-02	4.043E-02
4.000E-01	3.116E-02	3.116E-02
5.000E-01	2.081E-02	2.081E-02
6.000E-01	1.218E-02	1.218E-02
7.000E-01	6.297E-03	6.297E-03
8.000E-01	2.890E-03	2.890E-03
9.000E-01	1.185E-03	1.185E-03
1.000E+00	4.379E-04	4.379E-04
1.500E+00	1.053E-05	1.053E-05
2.000E+00	9.984E-06	9.984E-06
3.000E+00	9.984E-06	9.984E-06
4.000E+00	9.984E-06	9.984E-06
5.000E+00	9.984E-06	9.984E-06
6.000E+00	9.984E-06	9.984E-06
7.000E+00	9.984E-06	9.984E-06
8.000E+00	9.984E-06	9.984E-06
9.000E+00	9.984E-06	9.984E-06
1.000E+01	9.984E-06	9.984E-06

* Based on Stefhest, 1970

Table 2-32. Case 4 Results: Concentration of Np-237 in the Rock Matrix, at
 $x = 100$ m, Time $t = 5,000$ Years, Band Release Mode, Zero
Dispersion, $D = 10,000$ m²/yr

Distance x (m)	FRACVAL	STEFH*
1.000E-02	1.282E-02	1.282E-02
1.500E-02	1.402E-02	1.402E-02
2.000E-02	1.521E-02	1.521E-02
3.000E-02	1.756E-02	1.756E-02
4.000E-02	1.986E-02	1.986E-02
5.000E-02	2.210E-02	2.210E-02
6.000E-02	2.428E-02	2.428E-02
7.000E-02	2.639E-02	2.639E-02
8.000E-02	2.842E-02	2.842E-02
9.000E-02	3.037E-02	3.037E-02
1.000E-01	3.223E-02	3.223E-02
1.500E-01	4.005E-02	4.005E-02
2.000E-01	4.514E-02	4.514E-02
3.000E-01	4.699E-02	4.699E-02
4.000E-01	4.009E-02	4.009E-02
5.000E-01	2.910E-02	2.910E-02
6.000E-01	1.830E-02	1.830E-02
7.000E-01	1.008E-02	1.008E-02
8.000E-01	4.902E-03	4.902E-03
9.000E-01	2.115E-03	2.116E-03
1.000E+00	8.168E-04	8.168E-04
1.500E+00	1.126E-05	1.126E-05
2.000E+00	9.984E-06	9.984E-06
3.000E+00	9.984E-06	9.984E-06
4.000E+00	9.984E-06	9.984E-06
5.000E+00	9.984E-06	9.984E-06
6.000E+00	9.984E-06	9.984E-06
7.000E+00	9.984E-06	9.984E-06
8.000E+00	9.984E-06	9.984E-06
9.000E+00	9.984E-06	9.984E-06
1.000E+01	9.984E-06	9.984E-06

* Based on Stefhest, 1970

Figure 2-7. Relative Concentration of Np-237 in the Fracture Versus Distance x , at Time $t = 5,000$ Years for Different Hydrodynamic Dispersion Coefficients ($D_x = 0, 10, 100, 1,000, 10,000 \text{ m}^2/\text{yr}$) (Case 4: Band Release Mode)

Dashed line indicates residual concentration.

Figure 2-8. Relative Concentration of Np-237 in the Rock Matrix Versus Distance z , at Time $t = 5,000$ Years for Different Hydrodynamic Dispersion Coefficients ($D_x = 0, 10, 100, 1,000, 10,000 \text{ m}^2/\text{yr}$) (Case 4: Band Release Mode)

Dashed line indicates residual concentration.

2.3 SUMMARY AND CONCLUSIONS

Analytical solutions based on the Laplace transforms have been derived for predicting the one-dimensional, transient, advective-dispersive transport of a reacting radionuclide in a discrete planar fracture of constant aperture with infinite rock matrix diffusion. The particular features of these solutions reside in their additional analytical capability designed to handle residual concentrations in both fracture and rock matrix. The latter are represented by a constant and/or a spatially dependent function in the case of the fracture and a constant in the case of the rock matrix. The closed-form solutions for the case of zero-dispersion have also been presented.

The reported solutions can handle an exponentially decaying source of solute at the upstream end of the fracture, which may be subject either to a step or band release mode. A convergent integration of the solution for the general case was obtained by means of a composite Gauss-Legendre quadrature scheme.

The module of the computer code FRACVAL which evaluates the analytical solutions presented in this report has been successfully tested on the one hand against works published by Van Genuchten and Alves (1982) and Gureghian (1990) dealing with particular aspects of the problem at hand, and by means of a solution based on a numerical inversion of the Laplace transforms proposed by Stehfest (1970) on the other hand.

The solutions presented in this section of the report are primarily related to performance assessment investigations of potential nuclear waste repository sites restricted to typical scenario analyses associated with long-term migration of radionuclides in an idealized fractured rock system. In addition, these solutions can be conveniently used to simulate the behavior of a decaying species in fractured rock within a laboratory environment and subsequently through a validation process to provide the investigator with site-specific information regarding the magnitude and importance of the various geochemical parameters gearing the transport process through the fractured rock system of interest.

2.4 REFERENCES FOR PART 1

Bear, J., 1972. Dynamics of Fluid in Porous Media, American Elsevier Publishing Co., New York, NY.

Gradshteyn, I. S., and I. M. Ryzhik, 1980. Table of Integrals, Series and Products, Academic Press, New York, NY, p. 1160.

Gureghian, A. B., 1990. FRACFLO: Analytical Solutions for Two-Dimensional Transport of a Decaying Species in a Discrete Planar Fracture and Equidistant Multiple Fractures with Rock Matrix Diffusion, BMI/OWTD-5, Office of Waste Technology Development, Battelle, Willowbrook, IL.

Gureghian, A. B., 1990. "STEFH: A Solution Based on the Numerical Inversion of the Laplace Transform for the One-Dimensional Transport of a Decaying Species in a Single Fracture with Rock Matrix Diffusion," Draft Computer Code. Available from project office.

Gureghian, A.B., and S. Steidl, 1990. FRACVAL User's Guide and XYPI.OT - Version 1.0 for FRACVAL: Validation (Nonlinear Least Squares Method) of the Solution of One-Dimensional Transport of a Decaying Species in a Discrete Planar Fracture With Rock Matrix Diffusion, Battelle Office of Waste Technology Development, Willowbrook, IL.

Neretnieks, I., 1980. "Diffusion in the Rock Matrix: An Important Factor in Radionuclide Retardation?" Journal of Geophysical Research, Vol. 85, pp. 4379-4397.

Neretnieks, I., T. Eriksen, and P. Tahtinen, 1982. "Tracer Movement in a Single Fissure in Granitic Rock: Some Experimental Results and Their Interpretation," Water Resources Research, Vol. 18, No. 4, pp. 849-858.

Stefhest, H., 1970. "Numerical Inversion of Laplace Transforms," Commun. ACM, Vol. 13, No. 1, pp. 47-49.

van Genuchten, M. Th., and W. J. Alves, 1982. Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equations, U.S. Department of Agriculture, Technical Bulletin No. 1661.

APPENDIX A

THEOREMS AND LAPLACE TRANSFORMS

In this appendix, a selected number of theorems, inverse Laplace transforms, and derivatives are reported (Abramowitz and Stegun, 1972).

A.1 THEOREMS

The operations for the Laplace transformation reported in Part 1 require, in some cases, the use of the following theorems.

A.1.1 Translation

$$L^{-1} \left[e^{-bs} f(s) \right] = F(t-b) U(t-b), \quad b > 0 \quad (\text{A.1-1})$$

where $U(t)$ is the Heaviside unit step function defined as

$$U(t) = \begin{cases} 0, & t < 0 \\ 1, & t > 0 \end{cases}$$

A.1.2 Linear Transformation

$$L^{-1} [f(s-a)] = e^{at} F(t) \quad (\text{A.1-2})$$

A.1.3 Differentiation

$$L^{-1} s f(s) - F(+0) = F'(t) \quad (\text{A.1-3a})$$

$$L^{-1} s^n f(s) - L^{-1} s^{n-1} F(+0) - L^{-1} s^{n-2} F'(+0) - \dots - F^{(n-1)}(+0) = F^{(n)}(t) \quad (\text{A.1-3b})$$

A.2 LAPLACE TRANSFORMS

$f(s)$	$F(t)$	
$\frac{e^{-a\sqrt{s}}}{s}$	$= \operatorname{erfc}\left(\frac{a}{2\sqrt{t}}\right)$	(A.2-1)
$\frac{e^{-a\sqrt{s}}}{\sqrt{s}}$	$= \frac{1}{\sqrt{\pi t}} \exp\left(-\frac{a^2}{4t}\right)$	(A.2-2)
$e^{-a\sqrt{s}}$	$= \frac{a}{2\sqrt{\pi t^3}} \exp\left(-\frac{a^2}{4t}\right)$	(A.2-3)
$\frac{1}{\sqrt{s(a+\sqrt{s})}}$	$= e^{a^2 t} \operatorname{erfc} a\sqrt{t}$	(A.2-4)
$\frac{e^{-k\sqrt{s}}}{\sqrt{s(a+\sqrt{s})}} \quad (k \geq 0)$	$= e^{ak} e^{a^2 t} \operatorname{erfc}\left(a\sqrt{t} + \frac{k}{2\sqrt{t}}\right)$	(A.2-5)
$\frac{1}{\sqrt{s} + a}$	$= \frac{1}{\sqrt{\pi t}} - ae^{a^2 t} \operatorname{erfc} a\sqrt{t}$	(A.2-6)
$\frac{e^{-k\sqrt{s}}}{a + \sqrt{s}} \quad (k \geq 0)$	$= \frac{1}{\sqrt{\pi t}} \exp\left(-\frac{k^2}{4t}\right) - ae^{ak} e^{a^2 t} \operatorname{erfc}\left(a\sqrt{t} + \frac{k}{2\sqrt{t}}\right)$	(A.2-7)
$\frac{e^{-k\sqrt{s}}}{s(a + \sqrt{s})}$	$= \frac{1}{a} \left[\operatorname{erfc} \frac{k}{2\sqrt{t}} - e^{ak} e^{a^2 t} \operatorname{erfc}\left(a\sqrt{t} + \frac{k}{2\sqrt{t}}\right) \right]$	(A.2-8)
$\frac{1}{s(a + \sqrt{s})}$	$= \frac{1}{a} \left[1 - e^{a^2 t} \operatorname{erfc}(a\sqrt{t}) \right]$	(A.2-9)

A.3 APPENDIX A REFERENCE

Abramowitz, M., and I. A. Stegun, 1972. Handbook of Mathematical Functions, Dover Publications, Inc., New York, NY.

APPENDIX B

QUADRATURE

The solution presented in this report requires for the most part the evaluation of integrals. An exception is made in the case of the dispersion-free solution. The integrals associated with the general solution of Equations 2-30 and 2-34 with limits $(0, \infty)$ are evaluated by means of the Gauss-Legendre quadrature scheme (see Carnahan et al., 1969; Stroud and Secrest, 1966) after transformation of the original limits to finite ones.

B.1 TRANSFORMATION FOR INFINITE INTEGRALS ASSOCIATED WITH THE PRESENCE OF LONGITUDINAL DISPERSION

The integral of interest has the following form

$$I = \int_0^{\infty} f(x) dx \quad (B-1)$$

when the dependent variable of the integrand corresponds in our case to σ (see Equation 2-15). Hence by virtue of the properties inherent to the Heaviside function (see Equations 2-13), the lower limit, say $\sigma_{\min}$, must meet the following criterion

$$t \geq R\chi \quad (B-2)$$

Substitution for χ given by Equation 2-29b. The potential lower limit may then be written as

$$1^{\sigma_{\min}} = \frac{x}{2} \left(\frac{R}{D_x t} \right)^{1/2} \quad (B-3)$$

The choice of the upper and lower limits of integration are also dictated by the condition that the maximum absolute value of the exponential argument appearing in Equation 2-29a written as

$$\psi(x, \sigma) = \frac{2}{\sqrt{\pi}} \exp \left[- \left(\sigma - \frac{\gamma}{\sigma} \right)^2 \right] \quad (B-4)$$

with

$$\gamma = \frac{ux}{4D_x} \quad (B-5)$$

should always be less than or equal to the one allowed by the computer, say ARG. Hence equating the latter with the argument of the exponential form in Equation B-4, we obtain

$$\sigma^4 - (ARG + 2\gamma)\sigma^2 + \gamma^2 = 0 \quad (B-6)$$

where the roots of the above equation are given by

$$\sigma_{\max}^2 = \frac{(\text{ARG} + 2\gamma) + \left| (\text{ARG} + 2\gamma)^2 - 4\gamma^2 \right|^{1/2}}{2} \quad (\text{B-7})$$

$$2\sigma_{\min}^2 = \frac{(\text{ARG} + 2\gamma) - \left| (\text{ARG} + 2\gamma)^2 - 4\gamma^2 \right|^{1/2}}{2} \quad (\text{B-8})$$

Note that both roots are positive. The potential values for the integration limits given by Equations B-7 and B-8 are now used to extract suitable upper (σ_{UL}) and lower limits (σ_{LL}). The integration domain is split over two finite intervals, i.e., $[\sigma_{LL}, \sigma_{IN}]$ and $[\sigma_{IN}, \sigma_{UL}]$, where σ_{IN} will correspond to the value of σ in Equation B-6 when function $\psi(x, \sigma)$ (see Equation 2-29a) is a maximum:

$$\sigma_{IN} = \gamma^{1/2}, \sigma_{LL} < \gamma^{1/2} < \sigma_{UL} \quad (\text{B-9})$$

If the above condition is not satisfied, then

$$\sigma_{IN} = \frac{1}{2} (\sigma_{LL} + \sigma_{UL}), \gamma^{1/2} < \sigma_{LL} \text{ or } \gamma^{1/2} > \sigma_{UL} \quad (\text{B-10})$$

where

$$\sigma_{LL} = \text{MAX}[\sigma_{\min}, 2\sigma_{\min}] \quad (\text{B-11a})$$

$$\sigma_{UL} = \text{MAX}[\sigma_{\min}, \sigma_{\max}] \quad (\text{B-11b})$$

Results yielded by this method proved to be very satisfactory, however, at the expense of an additional computational effort.

REFERENCES

Carnahan, B., H. A. Luther, and J. O. Wilkes, 1969. Applied Numerical Methods, John Wiley and Sons, Inc., New York, NY.

Stroud, A. H., and D. Secrest, 1966. Gaussian Quadrature Formulas, Prentice-Hall, Inc., Englewood Cliffs, NJ.

APPENDIX C

EVALUATION OF ERROR FUNCTION AND PRODUCT OF EXPONENTIAL AND COMPLEMENTARY ERROR FUNCTION TERMS

The error or probability function is defined as

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi. \quad (\text{C-1})$$

with

$$\operatorname{erf}(-x) = -\operatorname{erf}(x) \quad (\text{C-2})$$

When x is small the integrand may be conveniently expanded in a power series convergent everywhere and integrated term by term to yield

$$\begin{aligned} \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \left[x - \frac{x^3}{3 \cdot 1!} + \frac{x^5}{5 \cdot 2!} - \frac{x^7}{7 \cdot 3!} + \dots \right. \\ \left. + (-1)^{n+1} \frac{x^{2n+1}}{(2n+1) \cdot n!} + \dots \right]. \end{aligned} \quad (\text{C-3})$$

A few terms in the expansion are necessary to determine the value of $\operatorname{erf} x$ to a given number of decimal places. However, as x becomes large the loss in accuracy must be compensated by a large number of terms which renders the calculation tedious and impractical. A rational Chebyshev approximation may be used to alleviate this problem when $x \geq 4$ (see Cody, 1969). Alternatively, the asymptotic expansion reported by Abramowitz and Stegun (1964) expressed in terms of the complementary error function $\operatorname{erfc}(x)$ (Equation C-1) may also be written as

$$\operatorname{erf}(x) = 1 - \operatorname{erfc}(x) \quad (\text{C-4})$$

where

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-\xi^2} d\xi. \quad (\text{C-5})$$

In view of Equations (C-2) and (C-4), we have

$$\operatorname{erfc}(-x) = 2 - \operatorname{erfc}(x). \quad (\text{C-6})$$

Asymptotic Expansion

The asymptotic expansion of $\text{erfc}(x)$ as given by Abramowitz and Stegun (1964) may be written as

$$\text{erfc}(x) = \frac{e^{-x^2}}{x\sqrt{\pi}} \left[1 + \sum_{n=1}^{\infty} (-1)^n \frac{1 \cdot 3 \dots (2n-1)}{(2x^2)^n} \right] + R_n(x) \quad (\text{C-7})$$

If $R_n(x)$ is the remainder after n terms then

$$R_n(x) = (-1)^n \frac{1 \cdot 3 \dots (2n-1)}{(2x^2)^n} \int_0^{\infty} e^{-t} \left(1 + \frac{t}{x^2} \right)^{-n-\frac{1}{2}} dt \quad (\text{C-8})$$

$R_n(x)$ is less in absolute value than the first neglected term and of the same sign.

The solution of Equations (2-30) and (2-34) includes terms involving products of an exponential and complementary error functions, respectively. The evaluation of such terms is performed by means of function `EXP_ERFC` in the `FRACVAL` mathematical model described below, and which uses the properties of the error and complementary error functions outlined above. Letting α or β correspond to the argument of the exponential and complementary error function, respectively, evaluate

$$S = \alpha - \beta^2 \quad (\text{C-9})$$

using Eq. (C-7) and neglecting the remainder term. The product of $\exp(\alpha)$ and $\text{erfc}(\beta)$ is given by

$$Ea = \frac{\exp(\alpha)}{\beta\sqrt{\pi}} \left[1 + \sum_{n=1}^{\infty} (-1)^n \frac{1 \cdot 3 \dots (2n-1)}{(2\beta^2)^n} \right] \quad (\text{C-10})$$

and with

$$Ec = \exp(\alpha) \text{erfc}(\beta) \quad (\text{C-11})$$

where $\text{erfc}(\beta)$ is evaluated based on Cody (1969), the calculation of `EXP_ERFC` proceeds as outlined in Figure C-1. Note that `EXMAX` is the largest positive argument of the exponential function allowed by a particular computer.

Figure C-1. Evaluation of EXP_ERFC

References

Abramowitz, M., and I. A. Stegun, 1964. Handbook of Mathematical Functions, Dover Publications, Inc., New York, NY.

Cody, W. J., 1969. "Rational Chebyshev Approximation for the Error Function," Mathematics of Computation, Vol. 23, No. 107, pp. 631-637.

APPENDIX D

NOTATIONS

a_1, a_2, a	constants in the model for residual concentration in the fracture
a_L	longitudinal dispersivity
A	concentration in the fracture
A^0	concentration of the species at the source at time equals zero
b	half-thickness of the fracture
b_1	residual concentration in the rock matrix
B	concentration in the rock matrix
D_d	molecular diffusion of nuclide in water
D_o	effective diffusion coefficient in the rock matrix
D_p	pore diffusivity
D_x	hydrodynamic dispersion coefficient in the fracture
g_f	geometric factor (δ_d/t'^2)
J	diffusive rate of nuclide at surface of fracture per unit area of fracture surface
K_f	surface distribution coefficient in the fracture
K_r	distribution coefficient in the rock matrix
R	retardation factor in the fracture
R'	retardation factor in the rock matrix
t	time
T	leaching time
$T_{1/2}$	half-life
u	average fluid velocity vector in the fracture
x	position vector in the fracture
z	position vector in the rock matrix
δ_d	constrictivity for diffusion

λ	first-order rate constant for decay
ρ_r	rock density
τ	tortuosity of the fracture
τ'	tortuosity of the rock matrix
ϕ	rock porosity

APPENDIX E

MODEL PARAMETERS

ALFA	Constant alpha in the exponential term in the residual concentration model in the fracture (1/L)
CC0	Concentration of the species at the source at time equals zero (units of activity/L ³)
CINF(1)	Constant in residual concentration model in the fracture (units of activity/L ³)
CINF(2)	Coefficient of exponential term in residual concentration model in the fracture (units of activity/L ³)
CINR	Residual concentration in the rock matrix (units of activity/L ³)
DENSR	Rock matrix bulk density (M/L ³) (used if IDIST(2) = 1)
DIFF	Molecular diffusion of species in water (L ² /T) (used if IDISP = 1)
DIFFR	Pore diffusivity (L ² /T) (IGEOF = 0) or geometric factor (L/L) (IGEOF = 1)
DIMENS(I,J)	Dimensions used in the problem; each must be ≤ 12 characters in length <div style="margin-left: 20px;"> (1,J) = species name (2,J) = time (year) (3,J) = length (meter) (4,J) = L/T (meter/year) (5,J) = L²/T (m²/year) (6,J) = mass/volume (g/cc) (7,J) = volume/mass (cc/g) (8,J) = 1/time (1/year) (9,J) = arbitrary units of activity/volume (UA/L³) (10,J) = 1/length (1/m) </div>
DISPX	Hydrodynamic dispersion coefficient (L ² /T) (IDISP = 0) or Longitudinal dispersivity (L) (IDISP = 1)
DISTRB__F	Fracture surface distribution coefficient (L) [IDIST (1) = 1]
DISTRB__R	Rock matrix distribution coefficient (L ³ /M) [IDIST (2) = 1]
EXMAX*	Largest allowed magnitude for exponential arguments
HALFL	Half-life of species (T)
HALF__THICK	Half-thickness of the fracture (L)

* Computer-dependent.

IAUTO	= 0 User supplies arrays REFX, REFZ, and TIME, including parameters NX, NZ, and NT = 1 Automatic generation of arrays REFX, REFZ, and TIME, including parameters NX, NZ, and NT (see Note)
IBAND	= 0 Step release mode at source = 1 Band release mode at source
ICONCF	= 0 Do not calculate fracture concentrations = 1 Do calculate fracture concentrations
ICONCR	= 0 Do not calculate rock concentrations = 1 Do calculate rock concentrations
IDISP	= 0 DISPX, corresponds to dispersion coefficient in fracture = 1 DISPX, corresponds to dispersivity in fracture
IDIST(1)	= 0 RETARD__F corresponds to retardation factor in fracture = 1 RETARD__F corresponds to surface distribution coefficient in fracture, i.e., DISTRB__F
IDIST(2)	= 0 RETARD__R corresponds to retardation factor in rock matrix = 1 RETARD__R corresponds to distribution coefficient in rock matrix, i.e., DISTRB__R
IGAUSL	= 0 Interval of integration constant = 1 Interval of integration limits divided in INTERV/2 subintervals
IGEOF	= 0 DIFFR corresponds to pore diffusivity = 1 DIFFR corresponds to geometric factor
IGRAPH	= 0 Graphics output disabled = 1 Graphics output enabled; formatted graphics written to logical unit 30
INTERV	Number of subintervals x 2 for Gauss-Legendre integration (i.e., ≤ 4 (used if IGAUSL = 1))
MSG1	≤ 80 characters, first line of graphics output
MSG2	≤ 80 characters, second line of graphics output
NMAX	Number of Gaussian points for Gauss-Legendre quadrature (can have only values of 4, 10, 20, 60, 104, or 256)
NRUNMAX	Number of data sets to be run
NT	≤ 500 , number of time values to be evaluated (skip if IAUTO = 1)
NVAL	Index for selecting solution module = 0 Option for analytical solution = 1 Option for optimization module
NX	≤ 500 , number of positions to be evaluated in x direction (skip if IAUTO = 0)

NZ	≤ 500 , number of positions to be evaluated in z direction (skip if IAUTO = 0)
POROSR	Average porosity in rock matrix (L^3/L^3)
REFX(I)	x-position in space (read if IAUTO = 0)
REFZ(I)	z-position in space (read if IAUTO = 0)
RETARD__F	Retardation factor [IDIST(1) = 0] or surface distribution coefficient in the fracture, i.e., DISTRB__F [IDIST(1) = 1]
RETARD__R	Retardation factor [IDIST(2) = 0] or distribution coefficient in the rock, i.e., DISTRB__R [IDIST(2) = 1]
TIME(I)	t-position in time (T) (read if IAUTO = 0)
TIML	Leaching time (T) (used if IBAND = 1)
TITLE	2 lines, ≤ 80 characters per line, title of data set
TORT	Tortuosity of the fracture (L^n) (used if IDISP = 1)
VELX	Average fluid velocity in the fracture (L/T)
XDISP	Longitudinal dispersivity (L) (IDISP = 1)

Note: The following parameters are read in if IAUTO = 1 in order to generate arrays REFX, REFZ, and TIME, and their associated parameters NX, NZ, and NT:

X0	First value of spatial coordinate x = REFX(1)
DX	Spatial increment (skip if NLOG = 1)
ENDX	End value of spatial coordinate x = REFX(NX)
Z0	First value of spatial coordinate z = REFZ(1)
DZ	Spatial increment (skip if NLOG = 1)
ENDZ	End value of spatial coordinate z = REFZ(NZ)
T0	First value of simulation time t = TIME(1)
DT	Time increment (skip if NLOG = 1)
ENDT	End value of simulation time = TIME(NZ)
NLOG	= 0 Positions in space or time are equally spaced = 1 Log scale used for splitting space or time arrays (i.e., 10 divisions per log cycle)

- END -

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