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Radionuclide Transport Simulation Using Particle Tracking With Rock Matrix Diffusion

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Introduction

Migration of radionuclides in the unsaturated zone and saturated zone may be a significant factor in the release of these contaminants to the biosphere from the potential radioactive waste repository at Yucca Mountain, Nevada. Processes that influence the groundwater transport of radionuclides in the fractured volcanic rocks of the saturated zone include advection, dispersion, sorption, and diffusive transfer of radionuclide mass between the fractures and rock matrix. Modeling of radionuclide transport in the saturated zone requires a method of numerical simulation that is accurate for the ranges of parameter values used and that is numerically efficient. Also, transport simulation methods should not introduce spurious dilution of radionuclide concentrations by numerical dispersion. This paper describes a groundwater transport modeling approach that employs classical particle tracking coupled with an analytical solution for matrix diffusion in fractured media. Results from radionuclide transport simulations in the saturated zone at Yucca Mountain are also presented.

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Modeling Approach

Numerical methods for radionuclide transport with the streamline particle-tracking approach have been developed in the FEHM computer program[1]. This approach assumes that steady-state groundwater flow occurs in a single continuum representing the fracture network and requires an orthogonal numerical grid. Particles associated with a defined radionuclide mass are moved along advective streamlines in the simulated flow field at the appropriate local groundwater velocity. Hydrodynamic dispersion is simulated by a random walk technique in which the particles are displaced in the longitudinal and transverse directions at the end of each advective time step.

Simulated solute mass transfer between groundwater in the fractures and immobile groundwater in the rock matrix is governed by an analytical solution[2] that assumes an idealized fracture network consisting of uniformly spaced parallel fractures. To facilitate coupling with the particle-tracking method, the analytical solution has been rewritten in terms of two dimensionless variables, as given in the following equations[3]:

$$\frac{c}{c_0} = \frac{1}{\pi} \int_0^\infty \frac{2}{\varepsilon_1} \exp(\varepsilon_R{}^0) \left[\sin(\varepsilon_I{}^0) + \sin(\Omega_I{}^0)\right] d\varepsilon_1 \qquad (1)$$

where:

$$T_1^0 = \frac{t}{\tau_0} - R \qquad (2)$$

$$\tau_0 = \frac{z}{v} \qquad (3)$$

$$\varepsilon_R{}^0 = -\frac{\omega_1 \varepsilon_1}{2} \left(\frac{\sinh(\sigma_1 \varepsilon_1) - \sin(\sigma_1 \varepsilon_1)}{\cosh(\sigma_1 \varepsilon_1) + \cos(\sigma_1 \varepsilon_1)} \right) \qquad (4)$$

$$\varepsilon_I{}^0 = \frac{\varepsilon_1^2 T_1^0}{2} - \frac{\omega_1 \varepsilon_1}{2}\left(\frac{\sinh(\sigma_1\varepsilon_1) + \sin(\sigma_1\varepsilon_1)}{\cosh(\sigma_1\varepsilon_1) + \cos(\sigma_1\varepsilon_1)}\right) \tag{5}$$

$$\Omega_I{}^0 = \frac{\omega_1 \varepsilon_1}{2}\left(\frac{\sinh(\sigma_1\varepsilon_1) + \sin(\sigma_1\varepsilon_1)}{\cosh(\sigma_1\varepsilon_1) + \cos(\sigma_1\varepsilon_1)}\right) \tag{6}$$

with

$$\omega_1 = \frac{\theta(R' D' \tau_0)^{1/2}}{b} \tag{7}$$

$$\sigma_1 = (\frac{R'}{D' \tau_0})^{1/2}(B - b) \tag{8}$$

where c is solute concentration at the outlet of the fracture, c_0 is the inlet concentration, z is the distance along the fracture, v is the groundwater velocity in the fracture, R is the retardation factor in the fracture, θ is the matrix porosity, R' is the retardation factor in the matrix, D' is the diffusion coefficient in the matrix, b is the half-fracture aperture, and B is the half-fracture spacing. ω_1 and σ_1 are the dimensionless variables.

Numerical integration is used to evaluate the solution of relative concentration (equation 1) as a function of time over a range of values for ω_1 and σ_1 (equations 7 and 8). The resulting solutions constitute a set of type curves that cover the range of expected conditions in the saturated zone at Yucca Mountain. The type curves are stored as arrays of tabulated values for access by the FEHM code during particle tracking. This computationally efficient method avoids repetitive numerical evaluation of the analytical solution for matrix diffusion during the execution of FEHM. An example set of type curves for a single value of σ_1 is shown in Figure 1.

The analytical solutions contained in the type curves are coupled to the particle-tracking algorithm in the following manner. After each time step the particle is advanced to a position along the streamline by groundwater advection in the fracture continuum. Based on the local groundwater velocity, the advective time-step size, and the other parameters controlling the matrix diffusion process, the appropriate type curve is chosen. The type curve represents a cumulative distribution function (cdf) of possible travel times through the fractured media. A random number from a uniform distribution between 0 and 1 is drawn and used to determine the actual travel time for the particle for that advective time step, based on this cdf of possible travel times. The particle is moved forward in time based on the actual travel time, which includes the impact of matrix diffusion. The particle is then displaced by the random walk method to account for hydrodynamic dispersion. Implementation of the algorithm in the FEHM computer code has been validated by comparison to the analytical solution[4].

Saturated-Zone Transport Simulations

The particle-tracking algorithm in the FEHM computer program is used with the SZ site-scale flow and transport model to simulate the migration of radionuclides from the water table beneath the potential repository at Yucca Mountain to the accessible environment at 20 km distance[5]. The simulated groundwater flow paths in the three-dimensional SZ model include migration through fractured volcanic units and through porous alluvium. Monte Carlo simulations of radionuclide transport for ranges of multiple uncertain parameters in the SZ are performed with the model. Results are used in analyses of potential radiological dose to future residents of the site in the Total-System Performance Assessment for Site Recommendation (TSPA-SR).

Example results of radionuclide transport simulations with the SZ site-scale flow and transport model, assuming a constant source are shown in Figure 2. Sensitivity to the flowing interval spacing parameter (effective fracture spacing) is shown for two cases, a nonreactive tracer and

^{237}Np (without radioactive decay). Flowing interval spacing is one of the important parameters controlling the matrix diffusion process[6].

The results shown in Figure 2 are consistent with the conceptual and numerical models of matrix diffusion implemented with the particle-tracking algorithm. The first graph indicates longer travel times for smaller flowing interval spacing (1 m and 2 m), indicating nearly complete diffusive equilibrium of solute concentration between mobile groundwater in the fractures and immobile groundwater in the rock matrix of the volcanic units. Greater flowing interval spacing (50 m and 100 m) results in relatively little solute mass transfer from the fractures to the matrix and consequently shorter travel times through the SZ system. Note that the several hundred years of travel time for the larger values of flowing interval spacing shown in the first graph are due to migration in the porous medium of the alluvium. The breathrough curves for intermediate values of flowing interval spacing shown in the first graph show the shapes that are characteristic of dual-porosity solute transport. The simulated breakthrough curves for ^{237}Np in the second graph of Figure 2 show a similar pattern of sensitivity to effective fracture spacing. ^{237}Np is subject to minor sorption in the matrix of the fractured volcanic units and significant sorption in the alluvium. Access to the sorptive capacity of the rock matrix in the volcanic units via diffusion can have a significant impact on ^{237}Np travel times in the SZ (about 20,000 year delay), as indicated by the differences in the breakthrough curves for large and small flowing interval spacing.

Conclusions

An innovative, numerically efficient algorithm for the simulation of radionuclide mass transport in saturated, fractured media has been developed and implemented in the FEHM computer program. The algorithm employs particle tracking coupled with an analytical solution for matrix diffusion in dual-porosity, fractured media. The analytical solutions of matrix diffusion are stored as a set of type curves for a wide range of input parameters that are accessed by the particle tracking algorithm during execution of the FEHM code. The transport methodology is applied in the SZ site-scale model to simulate radionuclide migration in the SZ at Yucca Mountain, Nevada for use in TSPA-SR analyses of potential repository performance. Radionuclide transport simulation results are consistent with the conceptual model of contaminant transport in dual-porosity media. Sensitivity analysis indicates the importance of the flowing interval spacing in the matrix diffusion process and on the resulting radionuclide travel times through the SZ system. Sensitivity analysis for transport of ^{237}Np indicates the potentially important role of matrix diffusion in providing access to the sorptive capacity of the rock matrix during transport in the fractured volcanic rocks of the SZ.

Acknowledgments

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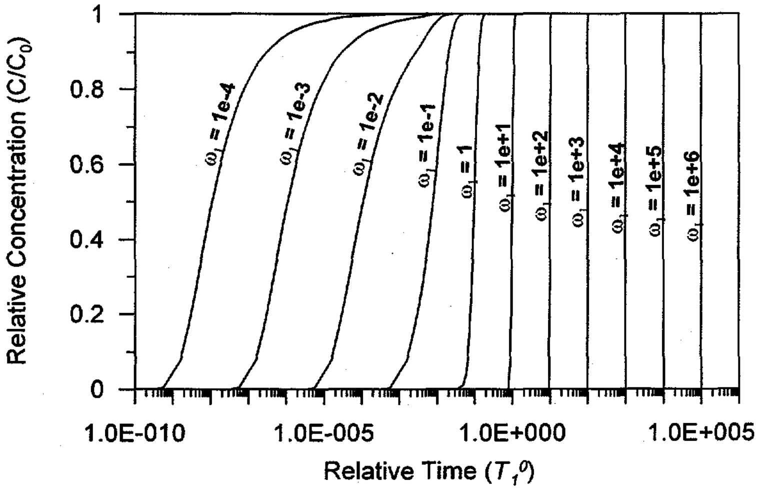

Figure 1. Type curves for the analytical solution for matrix diffusion. Type curves are shown for σ_l equal to 0.1.

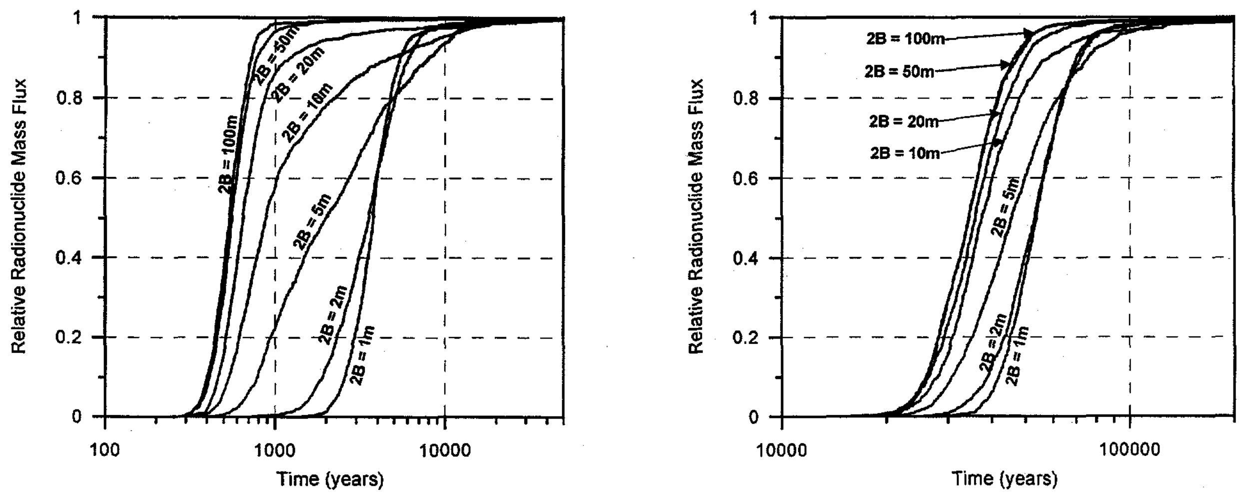

Figure 2. Radioncuclide mass breakthrough curves from the SZ site-scale flow and transport model for a non-sorbing species (left) and for ^{237}Np (right) at 20 km distance from the potential repository, as a function of flowing interval spacing (2B). Transport simulations are conducted using the expected value of other uncertain parameters for a constant source. Note that travel times are for transport in the SZ only.