Effective-Porosity and Dual-Porosity Approaches to Solute Transport in Fractured Tuff of the Saturated Zone at Yucca Mountain: Implications for Repository Performance Assessment

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Abstract:

The effective-porosity approach and the dual-porosity approach are examined as two alternative conceptual models of radionuclide migration in fractured media of the saturated zone at Yucca Mountain. Numerical simulations of one-dimensional radionuclide transport are performed for the domain relevant to repository performance assessment using the two alternative conceptual approaches. The dual-porosity solute transport modeling produces similar results to the effective-porosity model for fracture spacing of less than approximately 1 m and greater than about 200 m, corresponding to values of effective porosity equal to the matrix porosity and the fracture porosity, respectively. For intermediate values of fracture spacing, the dual-porosity approach results in concentration breakthrough curves that differ significantly from the effective-porosity approach and are characterized by earlier first arrival, greater apparent dispersion, and lower concentrations at later times. The effective-porosity approach, as implemented in recent performance assessment analyses of saturated zone transport at Yucca Mountain, is conservative compared to the dual-porosity approach from the perspective of both radionuclide concentrations and generally for travel times.

1. Introduction

Yucca Mountain, Nevada is being investigated as the potential site for the construction of a high-level radioactive waste repository. The repository system would consist of large, metal waste packages emplaced in drifts excavated within the unsaturated zone beneath the mountain. The potential repository elevation is approximately 300 m to 400

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m below the land surface and about 300 m above the water table.

Radionuclides escaping a radioactive waste repository, following corrosion and breaching of the waste package, are conceptualized to travel downward, transported by groundwater in the unsaturated zone, to the water table where they enter the saturated zone. Ground water flow in the saturated zone below and directly down-gradient of the potential repository at Yucca Mountain occurs in fractured volcanic rocks. The permeability of the rock matrix of this volcanic medium is generally several orders of magnitude lower than the bulk permeability of the fracture network, indicating that groundwater flow occurs predominantly in fractures. The contrasting values of fracture porosity and matrix porosity in the fractured tuffs suggest that the storage of groundwater and the potential storage of contaminants would occur primarily in the rock matrix.

Characterization of solute transport in the fractured medium of the saturated zone has important implications for the performance assessment of a potential repository at the Yucca Mountain site. Efficient solute mass transfer from flowing groundwater in the fractures to the immobile groundwater in the matrix would result in a relatively long delay in the migration of contaminants to a point of likely groundwater withdrawal and release to the biosphere. Slower solute mass transfer from the fractures and into the matrix would result in more rapid migration of contaminants and earlier arrival of radionuclides at the accessible environment. Radiological dose to human beings residing in the biosphere at the location of radionuclide release is the primary measure of repository performance considered in performance assessment calculations. Numerical modeling of these processes and other components of the repository system have recently been formally synthesized in the Total System Performance Assessment – Viability Assessment (TSPA-VA) (CRWMS M&O, 1998).

1.1. Background

Various approaches have been investigated to simulate radionuclide transport in fractured media. One approach is to treat the fractured medium as an equivalent effective continuum at the scale of interest (Berkowitz et al., 1988; Schwartz and Smith, 1988). Work by Robinson (1994) indicates that the equivalent continuum approach, using an effective porosity equal to the matrix porosity, would be appropriate for the prediction of radionuclide migration in the saturated zone from Yucca Mountain. The equivalent continuum approach, assuming a range of uncertainty in the value of effective porosity, was utilized in saturated-zone flow and transport simulations in the TSPA-VA (CRWMS M&O, 1998). Alternatively, the physical process of solute diffusion into the matrix may be explicitly considered using the dual-porosity approach. A number of dual-porosity analytical solutions for contaminant transport in fractured media that assume idealized homogeneous geometries for the fracture network have been developed, including Grisak and Pickens (1981) and Sudicky and Frind (1982). More recently, multiple rates of diffusion in heterogeneous, dual-porosity media have also been considered (Haggerty and Gorelick, 1995).

1.2. Objectives

The objectives of this study include numerical evaluation and comparison of the effective-porosity and the dual-porosity approaches to radionuclide transport in that portion of the flowpath in the fractured tuff in the saturated zone at Yucca Mountain. In addition, the implications of these alternative approaches for matrix diffusion in the saturated zone to repository performance assessment are analyzed. These objectives are addressed using numerical simulations of one-dimensional groundwater flow and transport, from the repository to a distance of 20 km.

2. Yucca Mountain Saturated-Zone System

The saturated-zone system at Yucca Mountain is important to repository performance because it is an important component of the natural system that constitutes a barrier between radionuclide releases from the unsaturated zone below the potential repository and the biosphere. Regulatory guidance (NRC, 1999) suggests that a significant mechanism for release of radionuclides to the biosphere would be by groundwater discharge from hypothetical well(s) at a distance of approximately 20 km from the repository. Transport of radionuclides in the saturated zone would tend to dilute radionuclide concentrations (e.g., through dispersive processes) and delay the release (e.g., by matrix diffusion and/or sorption) of radionuclides to the biosphere.

2.1. Geology and Regional Flow System

The bedrock underlying Yucca Mountain consists of a stratified sequence of Miocene age ash-flow and ash-fall tuffs. Fractured carbonate rocks and clastic units of Paleozoic age occur deeper in the saturated zone flow system in the area of Yucca Mountain. At distances greater than about 10 to 20 km down-gradient from the repository, groundwater flows through interfingered alluvial and volcanic units.

The geological structures observed at Yucca Mountain are consistent with extensional tectonics of the Basin and Range Province. The geometry of the normal faults and strike-slip faults controls much of the topography at Yucca Mountain (Luckey et al., 1996). The normal faults generally are oriented north-south, dip steeply to the west, and typically have a component of oblique slip displacement. Displacements on the faults range from less than 1 m to more than 300 m.

Yucca Mountain is part of the Death Valley regional groundwater flow system. On the regional scale, groundwater flow occurs from areas of recharge in upland regions and mountain ranges to areas of discharge at wells, springs and playas. Most of the regional-scale groundwater flow occurs in the Paleozoic carbonate rocks (Winograd and Thordarson, 1975).

2.2. Inferred Flow Pathways

Water level measurements in wells indicate that the general direction of groundwater flow in the saturated zone is from the north to the south in the area downgradient of the potential repository. A relatively shallow hydraulic gradient extends from beneath the repository to the southeast for a distance of approximately 7 km, turning to the south and south-southwest for a distance up to 20 km (Figure 1). A significant upward hydraulic gradient from the deeper volcanic units and the Paleozoic carbonate aquifer (Luckey et al., 1996) suggests that groundwater flow pathways from Yucca Mountain would remain relatively near the water table. Recharge to the saturated zone along Fortymile Wash (Savard, 1998) may result in deepening of the flow pathway toward the south.

The flow pathway in the saturated zone occurs in fractured tuffs for 10 to 20 km from the potential repository. Flow in the shallow saturated zone occurs in alluvium or valley-fill units further downgradient. Uncertainty in subsurface geology and in the horizontal location of the flowpath precludes exact determination of the point along the flowpath at which groundwater flow transits from fractured volcanic units to alluvium.

2.3. Previous Modeling Work

Previous modeling of radionuclide transport in the saturated zone for total system performance assessment analyses has employed dimensional and conceptual simplifications of saturated-zone transport processes. For TSPA-91 (Barnard et al., 1992), one-dimensional transport of radionuclides in the saturated zone was based on two-dimensional flow modeling of the system (Czarnecki and Waddell, 1984). For TSPA-93 (Wilson et al., 1994), radionuclide transport simulations using a three-dimensional saturated-zone model were used to derive a distribution of travel times through the system. Saturated-zone transport simulations for TSPA-95 (CRWMS M&O, 1995) used the saturated-zone groundwater flow fields developed for TSPA-93. In all cases, the values of porosity used to simulate radionuclide migration were approximately equal to the matrix porosity of the fractured volcanic aquifer. This approach implicitly assumes equilibrium of solute concentrations in the fractures with the groundwater in the rock matrix.

2.4. Conceptual Model of Radionuclide Transport Processes

Transport of solutes in fractured volcanic media of the saturated zone at Yucca Mountain is governed by complex interactions among processes, including advection in fractures (and potentially in the matrix), dispersion in the fractures, sorption in fractures and matrix blocks, and diffusive transfer between groundwater in the fractures and in the matrix (Figure 2). Solute mass transfer between groundwater in fractures and rock matrix by molecular diffusion primarily influences the distribution of radionuclide travel times through the system. If radionuclide travel times are long relative to the half-life of a radionuclide, this diffusive process also reduces the concentration at the downstream end of the saturated zone system.

These radionuclide transport processes in the saturated zone influence repository performance by affecting the travel time of radionuclides to a location where they are likely to be pumped from a well and by changing their concentrations in groundwater. The radionuclide travel times in the saturated zone may be long relative to the 10,000 year time period of regulatory concern (NRC, 1999). Therefore, we must evaluate which methods may provide more realistic and defensible representations of migration velocities.

3. Alternative Conceptual Approaches

Two alternative conceptual approaches to the prediction of radionuclide transport in the fractured media of the saturated zone at Yucca Mountain are considered in this study. These approaches constitute conceptual simplifications of the groundwater flow and solute transport system that are dictated, in part, by lack of detailed knowledge of the physical system and by computational limitations in the numerical representation of the system. Primary uncertainties in the physical system include the geometry of the fracture network, the distribution of groundwater flow within the fracture network, and heterogeneities in the rock matrix. Explicit representation of these complexities is precluded at the scale of interest in performance assessment calculations (i.e., 20 km) and by our inability to characterize the system to this level of detail.

3.1. Effective-Porosity Approach

The effective-porosity approach assumes that some portion of the available matrix porosity in the fractured medium is immediately accessible to solutes in the fractures (Figure 3). If it is assumed that matrix diffusion will completely saturate matrix blocks in the groundwater flow system over the time of transport from the repository to the accessible environment, then a value of effective porosity equal to the matrix porosity would be used. If it is assumed that matrix diffusion will be extremely limited in the system of interest, then a value of effective porosity equal to the fracture porosity would be used. Intermediate values of effective porosity approximate the situation in which some fraction of the total solute storage capacity of the fractured medium has been filled by diffusion. The effective-porosity approach thus implicitly considers the effects of diffusion from fractures into the matrix; however, it must be applied in an ad hoc manner. In reality, the portion of the matrix porosity available for solute storage changes as a function of time. The effective porosity is thus a "lumped" parameter that incorporates uncertainty in underlying processes and results in an approximate solution for solute transport. The accuracy of the effective-porosity approximation, particularly for values of effective porosity intermediate between fracture porosity and matrix porosity, is dependent on several characteristics of the flow system including groundwater velocity, travel distance, and fracture spacing.

3.2. Dual-Porosity Approach

The dual-porosity approach explicitly considers the physical process of matrix diffusion of solutes from groundwater flowing in fractures. In this alternative simplification of the system, the fractured medium is conceptualized to consist of two continua. One continuum represents mobile groundwater in the fractures and the other continuum corresponds to immobile groundwater in the matrix. Advective transport is conceptualized to occur only in the fractures and the matrix is available for the storage of solute mass through the process of molecular diffusion.

Implementation of the dual-porosity conceptual model typically requires idealization of the fracture network geometry and groundwater flow within it, due to the continuum assumption. The dual-porosity approach used in this study conceptualizes groundwater flow to occur through uniformly spaced, parallel fractures in the fractured medium (Figure 3). In this approach, the matrix blocks are homogeneous and uniformly occupy the volume between the parallel fractures. The primary limitation of this approach is the extent to which it misrepresents the geometry of the system. Realistic fracture networks vary considerably in fracture spacing, orientation, and aperture; and divide the rock matrix into blocks of varying size. Consequently, there is significant uncertainty in the representative size of the matrix blocks (i.e., fracture spacing) in fractured media.

4. Numerical Approaches

Numerical simulations of groundwater flow and solute transport are performed using a one-dimensional model of the saturated zone downgradient of Yucca Mountain. The one-dimensional model domain corresponds to the inferred groundwater flowpath at the site. Simulations using the effective-porosity approach and the dual-porosity approach are performed using the FEHM computer code (Zyvoloski et al., 1995). The FEHM code is a finite-element/finite-volume groundwater flow and solute transport simulator. Simulations of solute transport are obtained using the finite-element method. All simulations consist of first solving for a steady-state solution for the pressure distribution in the domain, then running transient solute transport simulations to obtain the concentration breakthrough curves at the downstream end of the system.

4.1. Model Domain

The model domain for the one-dimensional SZ flow and transport model consists of four hydrogeologic units corresponding to the approximate flowpath through the system. The respective lengths of these units within the one-dimensional model are taken from the results of three-dimensional saturated zone flow modeling (CRWMS M&O, 1998; TSPA-VA). The three volcanic units are assumed to be fractured media and the alluvium is assumed to be a porous medium. Because of lack of subsurface data, there is significant uncertainty in the location of the contact between the middle volcanic confining unit and the alluvium along the flowpath represented in the one-dimensional flow and transport model. This uncertainty in the subsurface geology of the saturated zone is incorporated into the effective-porosity simulations by varying the fraction of the flowpath through the alluvium. The length of the flowpath through alluvium is held constant at 2 km in the sensitivity studies of the dual-porosity approach to facilitate comparison between the conceptual approaches.

Simulations for the effective-porosity approach are performed using a one-dimensional grid with a 5 m nodal spacing. Simulations for the dual-porosity approach are performed using a quasi-two-dimensional grid in which the second dimension represents length into the matrix continuum. The first column of nodes in the dual-porosity grid corresponds to the fracture. A high-resolution, exponentially-spaced grid consisting of 50 nodes in the transverse direction is employed to accurately simulate diffusive movement of solute in the matrix. The fracture aperture (2b) is defined as the product of fracture porosity and fracture spacing.

4.2. Boundary Conditions

The groundwater boundary conditions applied to the effective-porosity and the dual-porosity transport models consist of specified-pressure at the downstream boundary and specified-flux at the upstream boundary. In the dual-porosity model, the specified flux is applied at the node representing the fracture. A specific-discharge value of 0.6 m/year is used in all cases. As a consequence, the volumetric groundwater flow rate applied at the upstream boundary is a function of the fracture spacing (2B in Figure 3). The lateral boundaries of the quasi-two-dimensional dual-porosity model are no-flow boundaries. A constant, unit mass flux of a conservative radionuclide (^{99}Tc) solute is applied at the upstream boundary of the effective-porosity and dual-porosity transport models.

4.3. Input Parameters

The values of effective porosity applied to the four hydrogeologic units in the effective-porosity modeling approach are varied stochastically. Values ranging from those representative of fracture porosity to the matrix porosity are drawn independently for the units in multiple realizations of the flow and transport system (CRWMS M&O, 1998). The uncertainty distribution for effective porosity is log-triangular, with a mode value of 0.02. The length of the flowpath through the alluvium unit is randomly varied from 0 to 6 km in the effective-porosity realizations. The length of the middle volcanic confining unit is correspondingly varied to maintain the total length of 20 km. The values of longitudinal dispersivity, with a mean of 100 m, are also stochastically varied in the effective-porosity simulations.

The parameter values used in the dual-porosity modeling are summarized in Table 1. The values of matrix porosity are held constant at the estimated value for each of the hydrogeologic units. Fracture porosity is held constant at a value of 1×10^{-4} for the fractured units. The value of fracture spacing (2B in Figure 3) is varied in sensitivity studies from 0.2 m to 200 m. The fracture aperture (2b) varies from 2.0×10^{-5} m to 2.0×10^{-2} m for the range of fracture spacing considered. Longitudinal dispersivity is held constant at 100 m in the dual-porosity simulations. The length of the flowpath in the alluvium unit is specified as a constant of 2 km in the dual-porosity simulations. A value of 3.2×10^{-11} m^2/s is assumed for the effective molecular diffusion coefficient of ^{99}Tc. In the dual-porosity simulations, groundwater flow is restricted to the fracture nodes by the large contrast in permeability (10 orders of magnitude) between the fracture nodes and the matrix nodes.

5. Results

The results of the effective-porosity approach simulations are shown as concentration breakthrough curves in Figure 4. These are the results of 100 realizations for ^{99}Tc transport in the SZ system, as used in performance assessment analyses (CRWMS M&O, 1998). The median travel times for ^{99}Tc vary from less than 200 years to greater than 4000 years for the ranges of uncertainty assessed in these realizations. Variation in the value of longitudinal dispersivity results in significant variation in the apparent dispersion among the breakthrough curves.

The results of the sensitivity analysis for the dual-porosity approach are shown as the dashed concentration breakthrough curves in Figure 5. For comparison, the breakthrough curves for differing values of effective porosity are shown as the solid curves in the same figure. The longitudinal dispersivity and the length of the flowpath in alluvium are held constant in the dual-porosity and effective-porosity simulations for the comparisons shown in Figure 5.

For a fracture spacing of 0.2 m with the dual-porosity approach, the concentration breakthrough curve corresponds to the breakthrough curve for the effective-porosity approach in which the values of matrix porosity are assigned to all hydrogeologic units. For a fracture spacing of 200 m with the dual-porosity approach, the mid-point of the concentration breakthrough curve corresponds approximately to the results of the effective-porosity approach in which the value of effective porosity in the fractured units is 0.005 or less. The breakthrough time for the mid-point of the curve (about 1200 years) in this case indicates very rapid transport through the fractured units. Note that for the case of fracture spacing of 200 m with the dual-porosity approach there is some attenuation of the maximum concentration at later times. For intermediate values of fracture spacing (2 m to 20 m) with the dual-porosity approach, there are significant differences in the shapes of the concentration breakthrough curves between the dual-porosity simulations and the effective-porosity simulations. The dual-porosity simulations exhibit earlier ^{99}Tc breakthrough, greater apparent dispersion, and long tails for intermediate values of fracture spacing.

6. Discussion

The results of the dual-porosity simulations of the saturated zone system at Yucca Mountain shown in Figure 5 indicate that for fracture spacing of about 1 m or less there would be nearly complete saturation of the matrix blocks within the fractured units along the flowpath of the contaminant plume. For this case of relatively closely spaced fractures carrying groundwater flow, diffusive solute mass transfer from the fractures to the matrix is dominant relative to the advective movement of solute in the fracture system. Consequently, the solute travel times to the 20 km compliance boundary for the repository are relatively long. In addition, the effective-porosity approach, using values of effective porosity equal to the matrix porosity of the fractured tuffs, would yield a relatively accurate solution for the concentration breakthrough curve and long travel time at these fracture spacings.

The modeling results for fracture spacing of greater than 200 m indicate that there would be minimal interaction between contaminated groundwater flowing in the fractures and the groundwater contained in the matrix of the fractured units. For this case of widely spaced fractures, migration of contaminants in the system is dominated by advective movement in the fracture system relative to the solute mass transfer by diffusion from the fractures to the matrix. Transport of solutes to a distance of 20 km is much more rapid for large fracture spacing. The effective-porosity approach results in a relatively accurate solution for the concentration breakthrough curves, using values of effective porosity representative of fracture porosity at this large fracture spacing.

For intermediate values of spacing between fractures carrying groundwater, the dual-porosity modeling results indicate that the migration of contaminants is dominated by neither advection in the fractures nor diffusive mass transfer between fractures and matrix. The concentration breakthrough curves for these cases are characterized by relatively early first arrival of solute at the 20 km boundary, but significant solute mass loss to the matrix and consequent lower concentrations at later times. The effective-porosity approach is inappropriate for these intermediate values of fracture spacing, in terms of providing an accurate solution for solute transport through the saturated zone system.

It should be noted that the conclusions with regard to the values of fracture spacing stated above are specific to the travel distance and specific discharge assumed in this study. Solute transport in the dual-porosity approach is a function of distance through the system and the groundwater velocity.

Comparison of Figure 4 and Figure 5 indicates that the effective-porosity approach, as implemented in TSPA-VA analyses (CRWMS M&O, 1998), has potentially significant differences from the dual-porosity approach, but these inaccuracies produce generally conservative, and thus more easily defended, results from the perspective of regulatory assessments of repository performance. Conservatism is defined here as computational results that underestimate radionuclide travel times or overestimate radionuclide concentrations relative to other computational methods. The shortest median travel times among the TSPA-VA realizations using the effective-porosity approach shown in Figure 4 are shorter than the median travel times for the fastest breakthrough curves from the dual-porosity model shown in Figure 5. This is because the effective porosity in the alluvium was stochastically varied to include lower values in the TSPA-VA analyses and was held constant at a higher value (0.25) in the dual-porosity simulations shown in Figure 5. The longest median travel times among the effective-porosity realizations are shorter than the longest median travel times shown in Figure 5. This result occurs because none of the 100 TSPA-VA realizations shown in Figure 4 simultaneously sampled values of effective porosity near the matrix porosity values for all three fractured hydrogeologic units.

The simulated concentrations using the dual-porosity model shown in Figure 5 are significantly lower for intermediate values of fracture spacing at later times (e.g., 8000 years) than the simulated concentrations from the effective-porosity approach. This result also indicates that the effective-porosity approach is conservative from the perspective of repository performance. Results from the dual-porosity modeling for intermediate values of fracture spacing indicate significantly greater spreading of the breakthrough curves (greater apparent dispersion) and earlier first arrival of solute than the effective-porosity approach as shown in Figure 5. The lower apparent dispersion from the effective-porosity approach is conservative in the context of TSPA calculations because longitudinal dispersion leads to attenuation of peak concentrations resulting from pulses of radionuclide mass at the source. The earlier first arrival of solute mass exhibited by the dual-porosity approach indicates that the effective-porosity approach is potentially non-conservative in terms of travel time. However, comparison of the first-arrival times shown for various fracture spacings in Figure 5 and the first-arrival times shown in Figure 4 indicates that the potential for early radionuclide arrival was represented in the TSPA-VA realizations. This result is a consequence of the uncertainty analysis in the effective-porosity modeling for TSPA-VA and is not inherent in the effective-porosity approach.

The effective-porosity approach as implemented in the TSPA-VA analyses of saturated zone transport is conservative compared to the dual-porosity approach from the perspective of both radionuclide concentrations and generally for travel times. Future TSPA analyses of potential repository performance at Yucca Mountain may utilize more explicit modeling of matrix diffusion, which will have the effect of providing more realistic results than does the effective-porosity approach.

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Table 1. Parameter Values Used in Dual-Porosity Transport Model (CRWMS M&O, 1998).

Hydrogeological Units	**Matrix porosity**	**Fracture porosity**	**Fracture Spacing (m)**	**Fracture Aperture (m)**
upper volcanic aquifer	0.163	1.0×10^{-4}	0.2 - 200	2.0×10^{-5} – 2.0×10^{-2}
middle volcanic aquifer	0.227	1.0×10^{-4}	0.2 - 200	2.0×10^{-5} – 2.0×10^{-2}
middle volcanic confining unit	0.183	1.0×10^{-4}	0.2 - 200	2.0×10^{-5} – 2.0×10^{-2}
alluvium / undifferentiated valley fill	0.25	N/A	N/A	N/A

Figures:

Figure 1. Region near the potential waste repository at Yucca Mountain, Nevada. The base map is a false-color infrared satellite image. The outline of the potential repository is shown with the light bold line. The inferred flow pathway in the saturated zone from beneath the repository to a hypothetical receptor at a distance of 20 km is shown by the dashed line. The locations of wells at which water level measurements have been made are shown by the + symbols. The outlined area is 30 km by 45 km, with the axes labeled in UTM coordinates (meters).

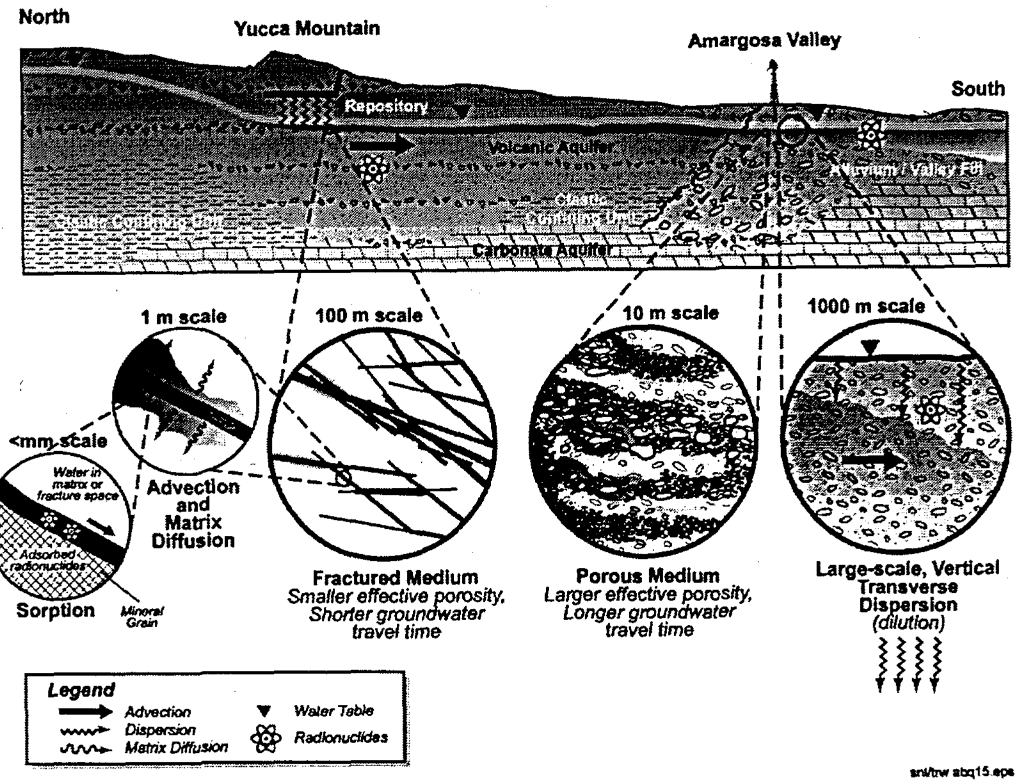

Figure 2. Conceptual model of radionuclide transport processes in the saturated zone. The cross section is a diagramatic representation of the system along the inferred flow pathway in the saturated zone (as shown by the dashed line in Figure 1). Processes that are relevant to the transport of radionuclides at various scales are illustrated in the circular diagrams.

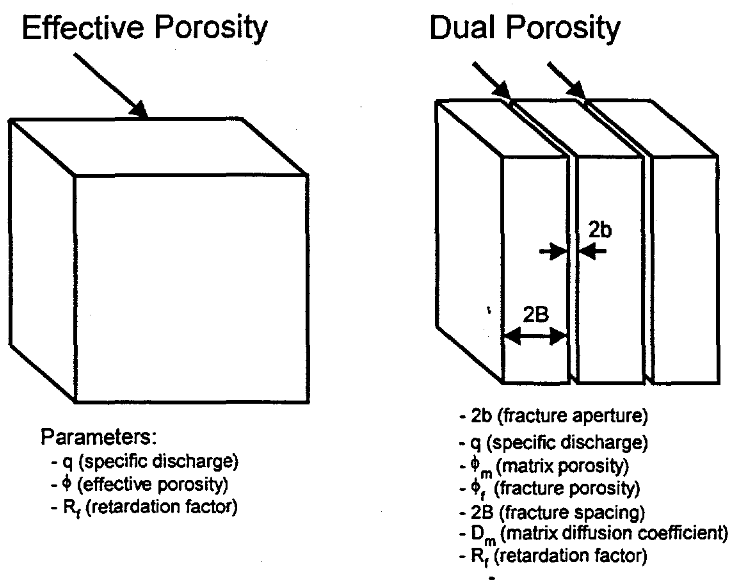

Figure 3. Diagramatic representation of the effective-porosity and dual-porosity approaches to solute transport in fractured media. The bold arrows at the top indicate volumetric groundwater flow rate. In the effective porosity approach, the flow occurs in a single continuum in which the fraction of the total volume available to flow and solute transport is represented by the value of effective porosity. In the dual-porosity approach, flow occurs only within the volume represented by the fracture porosity and the porosity within the matrix is available to solutes by diffusion.

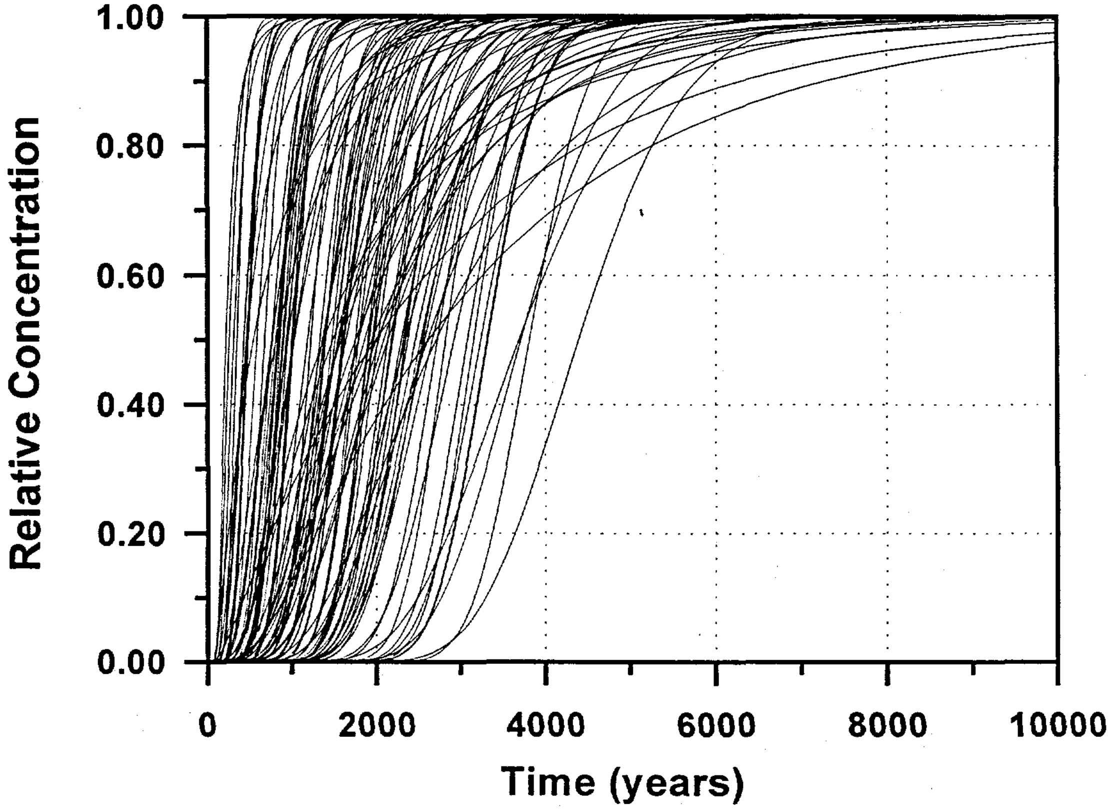

Figure 4. Concentration breakthrough curves for ^{99}Tc from 100 realizations of the one-dimensional transport model using the effective-porosity approach.

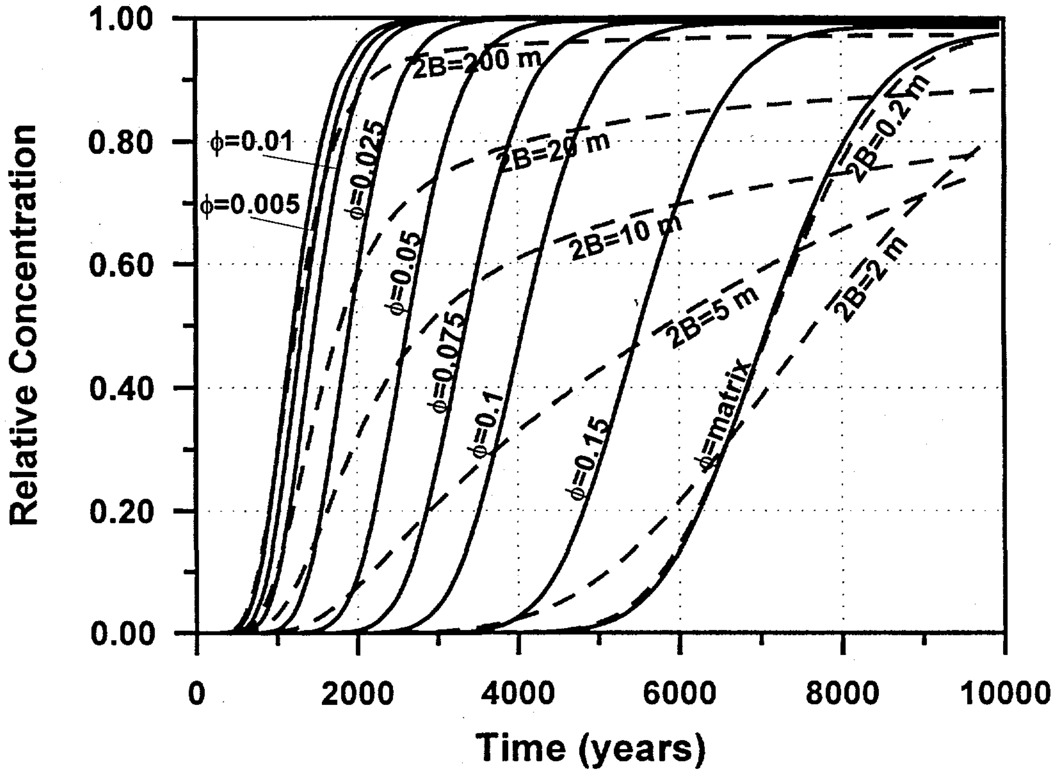

Figure 5. Concentration breakthrough curves for ^{99}Tc from the one-dimensional transport model for several values of fracture spacing with the dual-porosity approach and for several values of effective porosity with the effective-porosity approach. Results for the dual-porosity approach are shown as dashed lines and results for the effective-porosity approach are shown as the solid lines.