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Model Administrative Change Notice

QA: QA
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Complete only applicable items.

1. Document Number:	MDL-NBS-HS-000010	2. Revision:	02	3. ACN:	013 ^{ENT} 3/28/05
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6. Approvals:	
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Checker:	<div style="display: flex; justify-content: space-between;"> <div>Kenneth Rehfeldt, Kenneth Rehfeldt Print name and sign</div> <div style="text-align: right;">3/24/2005 Date</div> </div>
QER:	<div style="display: flex; justify-content: space-between;"> <div>Judy Gebhart Print name and sign</div> <div style="text-align: right;">3/25/05 Date</div> </div>
Independent Technical Reviewer:	<div style="display: flex; justify-content: space-between;"> <div>Jean L Younker Jean L Younker Print name and sign</div> <div style="text-align: right;">3-24-05 Date</div> </div>
Responsible Manager:	<div style="display: flex; justify-content: space-between;"> <div>Ming Zhu Print name and sign</div> <div style="text-align: right;">3/25/05 Date</div> </div>
7. Affected Pages	8. Description of Change:
4-6	Update citations and generate a <u>single direct</u> ACN DIRs entry. Table 4-2 – Add Section # to all citations to DIRS 170042 in Table 4-2: BSC 2004 (DIRS 170042, <u>Section 6.5.2</u>) Related to TBV 6667
6-6	Update citation and generate indirect ACN DIRs entry Paragraph numbered “#2”, Sentence 4: In the SZ flow model, such lithologic members are represented as single zones, <u>each represented by homogenous hydrologic properties with its equivalent permeability</u> (BSC 2004 [DIRS 170037], <u>Table 6-22-Table 5-1</u>) Related to TBV 6669
6-10	Update citation and generate indirect ACN DIRs entry Paragraph numbered “#6”, Second to last sentence: The largest heterogeneities are represented explicitly in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], <u>Section 6- Section 6.3.2.9</u>). Related to TBV 6669
6-40	Update citations and generate a <u>single indirect</u> ACN DIRs entry. Table 6.4-3 – Add Section # to first citation to DIRS reference 170042 in Table 6.4-3 as follows: BSC 2004 (DIRS 170042, <u>Section 6.5.2.1</u>) Related to TBV 6667

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1. Document Number:	MDL-NBS-HS-000010	2. Revision:	02	3. ACN:	01B / <i>encl</i>
4. Title:	SITE-SCALE SATURATED ZONE TRANSPORT <i>3/28/05</i>				
6-41	<p>Update text to reflect change in referenced source document. Generate a <u>single</u> indirect ACN DIRs entry.</p> <p>Paragraph 3, sentence 2</p> <p>Particle source locations were distributed over <u>under and east of</u> the anticipated repository footprint at the water table (BSC 2004 [DIRS 170042], Section 6.5.2.13).</p> <p>Related to TBV 6667</p>				
6-41	<p>Update citation and generate indirect ACN DIRs entry</p> <p>Last paragraph, last sentence:</p> <p>The flow paths in Figure 6.5-2 appear to converge toward the southern portion of the model due to the large-scale heterogeneities that are explicitly included in the hydrologic framework model shown in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Table 6-17 <u>Section 6.3.2.9</u>).</p> <p>Related to TBV 6669</p>				
6-44	<p>Update citation and generate indirect ACN DIRs entry</p> <p>Table 6.6-1a, Column "Basis", First Row, third sentence:</p> <p>In the second case, considering the steady-state nature of the flow system as presented in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Sections 5 and Section 6), if some flow is occurring out of the matrix into the fractures, then equivalent flow must also occur from fractures into the matrix blocks.</p> <p>Related to TBV 6669</p>				
7-17	<p>Correct citation in text of <i>Site-Scale Saturated Zone Transport</i>. MDL-NBS-HS-000010 to match source report. Generate indirect ACN DIRs entry</p> <p>7.1.2.6.1 Alluvial Tests at NC-EWDP-19D1 (fifth sentence from end). Correct citation as shown:</p> <p>Values ranging from 1.2 to 9.4 m/y, depending on conceptual model and parameter uncertainties, were obtained from <i>Saturated Zone In-Situ Testing</i> (BSC 2004 [DIRS 170010], Table G-7 <u>Table G-8</u>).</p> <p>Related to TBV 6668</p>				

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4. Title:	SITE-SCALE SATURATED ZONE TRANSPORT <i>3/28/05</i>				
7-22	<p>Update several citations related to flow paths deduced from hydrochemistry data and generate a single ACN DIRs entry, if possible, to match existing DIRS "input description"</p> <p>7.2.1 Comparison of Flow Paths Against Those Deduced from Hydrochemistry Data</p> <p>Paragraph 1, Sentence 4:</p> <p>Flow paths deduced from the hydrochemistry data are shown in Figure 7-9 (a and b) are given in Saturated Zone Site-Scale Flow Model (BSC 2004 [DIRS 170037], Section <u>A6.3.11</u> and Figure A6-62 A6-6.14).</p> <p>Paragraph 1, Sentence 6:</p> <p>As explained in detail in Saturated Zone Site-Scale Flow Model (BSC 2004 [DIRS 170037], Section <u>A6.3.11</u> A6-6.14), graphical analysis was done of the variations in the hydrochemical concentrations and isotopic ratios to estimate plausible flow lines.</p> <p>Paragraph 2, Sentence 3:</p> <p>This pathway is drawn on the basis of similar anion and cation concentrations along the flow path and dissimilarities to regions to the east and west. Further details are presented in Saturated Zone Site-Scale Flow Model (BSC 2004 [DIRS 170037], Section <u>A6.3.11</u> A6-6.14).</p> <p>Paragraph 3, Sentence 1 and 3:</p> <p>Flow path 7 traces the movement of groundwater from northern Yucca Mountain southeastward toward wells in the Dune Wash area and then southwestward along the western edge of the Fortymile Wash shown in Saturated Zone Site-Scale Flow Model (BSC 2004 [DIRS 170037], Section <u>A6.3.11</u> A6-6.14)..... A detailed discussion is presented in Saturated Zone Site-Scale Flow Model (BSC 2004 [DIRS 170037], Section <u>A6.3.11</u> A6-6.14).</p> <p>Related to TBV 6669</p>				
7-25	<p>Update citation and generate a single indirect ACN DIRs entry grouped accordingly.</p> <p>Paragraph 2, Sentences 2 and 3</p> <p>¹⁴C is rapidly incorporated into the atmospheric CO₂ and becomes available for terrestrial processes including that of dissolution into atmospheric precipitation as presented in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section <u>A6.3.1.2.2</u> A6-6.1.2.2). ¹⁴C enters the SZ groundwater through recharge and is transported principally as bicarbonate as given in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section <u>A6.3.1.2.2</u> A6-6.1.2.2) as a nonsorbing species.</p> <p>Related to TBV 6669</p>				
7-25	<p>Update citation and generate indirect ACN DIRs entry</p> <p>Paragraph 2, Sentence 4:</p> <p>Estimates of groundwater age are obtained from the measured ¹⁴C activity, corrected for possible water/rock interactions are given in Saturated Zone Site-Scale Flow Model (BSC 2004 [DIRS 170037], Section A6.3.6.6.2 A6-6.1.2.2).</p> <p>Related to TBV 6669</p>				

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4. Title:	SITE-SCALE SATURATED ZONE TRANSPORT				
7-25	<p>Update citation and generate a <u>single</u> indirect ACN DIRs entry <u>grouped accordingly</u>.</p> <p>Paragraph 3, Sentence 4:</p> <p>Data from water samples taken from 7 wells in the vicinity of Yucca Mountain were analyzed for ^{14}C activity as shown in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section A6.3.6.6.2 A6.6.6.6.2) and the resulting ages are reported to lie in the range of 11,430 years to 16,390 years as presented in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Table A6-7 A6-9).</p> <p>Related to TBV 6669</p>				
7-25	<p>Update citation and correct citation and generate a <u>single</u> indirect ACN DIRs entry:</p> <p>Paragraph 4, Sentence 1:</p> <p>Groundwater transit times can also be inferred from measured ^{14}C activity from water samples taken from wells that are inferred to lie along a flow path and where the geochemical compositions of waters suggests that flow paths exist between the two wells as given in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section A6.3.9A6.3.6.6.2 A6.6.8.10).</p> <p>Related to TBV 6669</p>				
7-25	<p>Update citation and generate <u>single</u> indirect ACN DIRs entry:</p> <p>Paragraph 4, Sentence 3:</p> <p>The approximate distance between the two wells is 15 km as shown in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section A6.3.9.1A6.3.6.6.2 A6.6.9.1).</p> <p>Related to TBV 6669</p>				
7-26	<p>Update citations and generate <u>separate</u> Indirect ACN DIRs entries</p> <p>First paragraph, first sentence carried over from page 7-25:</p> <p>The ^{14}C transport times lie in the range of 0 (or negative values) years to 3,110 years over the sampled depths shown in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section A6.3.9.1, Table A6-11A6.3.6.6.2 A6.6.9, Table A6-13).</p> <p>First paragraph, second sentence, page 7-26:</p> <p>The zero or negative values, as discussed in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section A6.3.9.1A6.3.6.6.2 A6.6.9.1), likely result from experimental uncertainties, and are not considered in this analysis.</p> <p>Second paragraph, first sentence page 7-26:</p> <p>There are two simplifications built into the above estimates (in addition to the ^{14}C data interpretation as discussed in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Sections A6.3.9, A6.3.1.2.2, and A6.3.6.6.26.6.2.4, 7.2.2.6 Sections A6.6.8 and A6.6.9): one is that in calculating velocities from the transport time estimates, a nominal travel distance is used equal to the well separation, and the second is that a constant velocity is used along the entire flow path.</p> <p>Related to TBV 6669</p>				

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A-5	<p>Update citation and generate <u>single</u> indirect ACN DIRs entry:</p> <p>Paragraph 4, Sentence 1:</p> <p>The chemistry of water in the SZ along potential flow paths to the accessible environment is discussed in Saturated Zone Site-Scale Flow Model (BSC 2004 [DIRS 170037] Table <u>A6-1</u> A6-3)</p> <p>Related to TBV 6669</p>				
C-6 and C-7	<p>Corrected typographical error in report (identified in CR 4451)</p> <p>Pages C-6 and C-7, Appendix C "Derivation of Composite Upscaled K_d Distributions"</p> <p>Section C1.2.1 Stochastic Realizations of K_d</p> <p>CR 4451 identified an error K_d distribution series equation on pages C-6 and C-7. This error, shown below as an example in the equation in the last bullet on Page C-6, is highlighted below:</p> <ul style="list-style-type: none"> K_d distribution for rock-type '1': $K_{d1}^1, K_{d2}^1, K_{d3}^1, K_{d4}^1, K_{d5}^1, K_{d6}^1, K_{d7}^1, \mathbf{K}, K_{dn}^1$ <p>The character K (above) is a typographical error. K should be the mathematical symbol "... " (an ellipsis).</p> <p>This correction above should also be applied to the first and third bulleted equations on Page C-7, named:</p> <ul style="list-style-type: none"> K_d distribution for rock-type '0': Replace K with symbol "... " <p>Combined K_d distribution: Replace K with symbol "... "</p>				
C-11	<p>Added justification to address CR 4615, justification for use of DTN from cancelled AMR</p> <p>Insert as paragraph following table C-10, page C-11 or as a footnote to the "Source DTN", a Table C-10 footnote.</p> <p>DTN LA0003JC831362.001 [DIRS 149557] is related to a cancelled analysis and model report (BSC 2001 [DIRS 160828, Section 6.6). Nevertheless, the reported results of laboratory diffusion transport studies remain valid and suitable for intended use. Primarily, this is because the diffusion coefficient values in Table C-10 overlap with values used in the base-case model (Table 4-2), and are therefore corroborated by the alternative sources used to justify that data in Section 4.1.2.10. Consequently, diffusion coefficient values in Table C-10 are suitable for use in upscaling the composite sorption distributions to the site-scale SZ transport computational grid.</p>				
D-3	<p>Update text to reflect change in referenced source document.</p> <p>Paragraph numbered "# 4", sentence 1</p> <p>Time to first breakthrough for N_p reported in <i>Saturated Zone Flow and Transport Model Abstraction</i> (BSC 2004 [DIRS 170042]), Figure 6-32) is <u>less than about</u> 100 years.</p> <p>Related to TBV 6667</p>				

4.1.2 Parameters and Parameter Uncertainty

The range of values for each input parameter is presented in Table 4-2 and discussed in Sections 4.1.2.1 through 4.1.2.18 and in Appendix A. The ranges of sorption coefficient values presented in Table 4-2 encompass all the radionuclides of interest since the intent of this report is to present a site-scale SZ transport model that can be used by the TSPA-LA with any of these radionuclides. The distributions for individual radionuclides are presented in Table C-14. Base-case values for most parameters were chosen to be the median values for the distributions except for sorption coefficients, which were taken to be 0 to represent a nonsorbing radionuclide such as ^{14}C .

Table 4-2. Input Parameters and Range of Values for the Site-Scale SZ Transport Model

Parameter	Base-Case Value(s)	Uncertainty Range	Units	Variable Type	Source/DTN
Specific discharge multiplier ^a	1 ^b	1/30–10	-	Stochastic	BSC 2004 (DIRS 170042, Section 6.5.2) SN0306T0502103.009 (DIRS 168763)
Permeability horizontal anisotropy ratio	4.2 ^c	0.05–20	-	Stochastic	SN0310T0502103.009 (DIRS 168763)
Bulk density in alluvium	1,910 ^c	1,669–2,151 ^d	kg/m ³	Stochastic	BSC 2004 (DIRS 170042, Section 6.5.2) SN0310T0502103.009 (DIRS 168763)
Sorption coefficient in alluvium	0.0 ^e	0–10,000	mL/g	Stochastic	Appendices A and C
Effective porosity in the alluvium, fraction	0.18 ^b	0.02 ^k –0.3	-	Stochastic	BSC 2004 (DIRS 170042, Section 6.5.2) SN0310T0502103.009 (DIRS 168763)
Colloid retardation factor in alluvium for irreversible colloids	N/A ^j	8–5,188	-	Stochastic	BSC 2004 (DIRS 170006) LA0303HV831352.004 (DIRS 163559)
Colloid retardation factor in alluvium for nonsorbing radionuclides	1 ^g	-	-	-	-
Flowing interval porosity, fraction ⁱ	0.01 ^f	0.00001–0.1	-	Stochastic	BSC 2004 (DIRS 170042, Section 6.5.2) SN0310T0502103.009 (DIRS 168763)
Flowing interval spacing	20 ^b	1.22–417	m	Stochastic	SN0310T0502103.009 (DIRS 168763)
Matrix porosity in volcanics, fraction	0.15–0.25 ^h	N/A	-	Assigned value for each unit; not a stochastic parameter	BSC 2004 (DIRS 170042, Section 6.5.2) SN0310T0502103.009 (DIRS 168763)
Effective diffusion coefficient in volcanics	5.0×10^{-11} ^b	5.0×10^{-12} – 5.0×10^{-10}	m ² /s	Stochastic	BSC 2004 (DIRS 170042, Section 6.5.2) SN0310T0502103.009 (DIRS 168763)

Table 4-2. Input Parameters and Range of Values for the Site-Scale SZ Transport Model (Continued)

Parameter	Base-Case Value(s)	Uncertainty Range	Units	Variable Type	Source/DTN
Matrix sorption coefficient in volcanics	0.0 ^e	0–10,000	mL/g	Stochastic	Appendices A and C
Colloid retardation factor in volcanics for irreversible colloids	N/A ^j	6.0–794 ^l	-	Stochastic	BSC 2004 (DIRS 170006) LA0303HV831352.002 (DIRS 163558)

Section 6.3.3), this approach leads to results that are generally conservative with respect to radionuclide concentrations and transport times.

As shown in Section 6.6.2.3 of the *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037]), the general flow direction starting at the repository footprint is to the south. The flow lines remain shallow and subhorizontal within the SZ. Thus, fluid flow occurs within the fractured volcanics immediately below and downstream of the repository footprint, entering the alluvium further downstream, and continuing through the alluvium to the boundary of the accessible environment at 18 km.

2. *The radionuclides advect and disperse with the groundwater through the fractured portions of the tuffs near the water table.* Flow occurs within the fractured portions of the tuffs near the water table. Flow intervals identified in well tests correlate with fracture locations (Erickson and Waddell 1985 [DIRS 105279], p. 18), the extent of fracturing correlates reasonably well with the degree of welding (Waddell et al. 1984 [DIRS 101064], p. 26), and the degree of welding is one of the criteria used to define the submembers within a lithologic unit. In the SZ flow model, such lithologic members are represented as single zones, each represented by homogeneous hydrologic properties (BSC 2004 [DIRS 170037], Table 5-1). This representation is also used in the transport model; however, the influence of heterogeneities within a permeability zone is incorporated into the model via dispersion and matrix diffusion as discussed below.

A distinction must be made between fracture zones and individual fractures. Fracture zones are typically spaced tens of meters apart, with thicknesses on the order of meters, and contain broken-up matrix blocks and many intersecting fractures that are conduits to flow and to diffusion and retardation. Individual fractures, on the other hand, tend to be spaced as close as a meter or less, have thicknesses on the order of fractions of millimeters, and may or may not contribute to the flow of groundwater.

The conceptual model is that high-permeability regions are offset by low-permeability regions due to the extensive faulting and fracturing observed in the volcanics (Luckey et al. 1996 [DIRS 100465], pp. 8 to 12) in the model domain. These low-permeability regions effectively will act as large-scale heterogeneities that give rise to large-scale macroscopic dispersion due to the tortuous nature of flow over the scale of hundreds of meters to kilometers. Field studies of transport and dispersion at a variety of length scales (from meters to kilometers) presented in *Saturated Zone In-Situ Testing* (BSC 2004 [DIRS 170010], Figures E-39 and E-40) and Neuman (1990 [DIRS 101464], Figure 1) show a trend toward larger apparent dispersion coefficients for transport over longer distances. The estimates of dispersivities from the C-wells tracer tests presented in *Saturated Zone In-Situ Testing* (BSC 2004 [DIRS 170010], Section E.4.1) fall within the range of values from other sites, suggesting that transport in the fractured tuffs exhibits similar dispersive characteristics.

In an equivalent-continuum dispersion model, hydrogeologic features that may be present at scales smaller than the size of a typical grid cell are simulated as averages.

The equivalent-continuum model averages the concentration variations within a grid block into a single value for the block. Concentration differences at scales smaller

the aqueous phase and the colloidal phase with the distribution coefficient (Appendix B, Equations B-2 through B-7). Based on the estimated rate constants and the range of transport times being considered for transport through saturated fractured tuffs, it is shown in *Saturated Zone Colloid Transport* (BSC 2004 [DIRS 170006], Section 6.7) that the equilibrium partitioning is valid for all but the shortest transport times and overestimates transport mobility of radionuclides for the shortest transport times. The distribution coefficient K_c is modeled as a function of radionuclide sorption properties, colloid substrate properties, aqueous chemistry, and colloid concentration, but independent of the properties of the immobile media through which transport occurs (Appendix B). The radionuclides that are irreversibly absorbed onto the colloids are modeled to transport in a manner identical to the colloids onto which they are sorbed. The transport of the colloids is simulated using the advection-dispersion equation.

Colloid-facilitated transport is not included in the base-case site-scale SZ transport model because it represents the extreme case of nonsorbing radionuclides.

6. *The radionuclides advect and disperse with the groundwater through the alluvium.* Alluvium is valley-fill material consisting of heterogeneous deposits of sand and gravel interbedded with mud and clay-sized materials (Waddell et al. 1984 [DIRS 101064], p. 27). This material is not well consolidated and tends to exhibit a more porous, less-fractured nature. Because of the heterogeneous nature of the medium, flow occurs through the more permeable regions within the alluvium, and the lower-permeability regions act as flow barriers. This characteristic tends to reduce the amount of porosity actually available to flow and transport as compared to the total large-scale porosity of the alluvium. To account for this, the effective flow porosity of the alluvium is considered to be a stochastic variable with a range of input values presented in *Saturated Zone Flow and Transport Model Abstraction* (BSC 2004 [DIRS 170042], Section 6.5.2.3). Dispersion is caused by heterogeneities at all scales, from the scale of individual pore spaces to the scale of the thickness of individual strata and the length of structural features such as faults. The spreading and dilution of radionuclides that result from these heterogeneities could be important to the performance of the repository. The largest heterogeneities are represented explicitly in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section 6.3.2.9). For dispersion at smaller scales, the advective-dispersion model is used with dispersion characterized using a dispersion coefficient tensor.
7. *Sorption reactions occur in alluvium between the solid surfaces and some of the radionuclides, tending to retard the transport of these radionuclides.* In contrast to the fractured tuffs, there are no cross-hole, field-scale tracer transport tests in the alluvium south of Yucca Mountain to confirm the in situ sorption characteristics. However, the transport of sorbing solutes in porous media that is not controlled by fractures has been well studied (e.g., Freeze and Cherry 1979 [DIRS 101173], Chapter 9, pp. 385 to 457). Sorption coefficients onto alluvium from the Nye County wells have been measured for a few key radionuclides. For the remaining radionuclides, sorption coefficients have been estimated based on the corresponding values measured for crushed tuff (Appendix A). Radionuclides could also precipitate in the SZ, forming solid phases on

Table 6.4-3. Additional Parameters Needed for Abstraction Analysis

Input Name (Variable Name and the Control Statement where it Appears in the FEHM V 2.20 Code)	Input Description	Base- Case Value(s)	Units	Type of Uncertainty	Source/DTN
Multiplying factor ^a for SKD in control statement "flow"	Specific discharge multiplication factor	1	-	Stochastic	<i>Saturated Zone Flow and Transport Model Abstraction</i> (BSC 2004 [DIRS 170042, Section 6.5.2.1]) SN0310T0502103.009 [DIRS 168763]
SCALEX, SCALEY in control statement "fper," ratio	Permeability horizontal anisotropy	4.2	-	Stochastic	SN0310T0502103.009 [DIRS 168763]
RD_FRAC in the control statement "sptr," ratio	Colloid retardation factor in volcanics for irreversible colloids	1	-	Epistemic	Table 4-2
Needed in Equations 79 and 80 for calculating the relative concentration of radionuclide on colloids, needed for colloid- facilitated reversible transport	Groundwater concentration of colloids	0	g/mL	Epistemic	Table 4-2
Needed in Equations 79 and 80 for calculating the relative concentration of radionuclide on colloids, needed for colloid- facilitated reversible transport	Sorption coefficient onto colloids	0	mL/g	Epistemic	Table 4-2
In TSPA calculations, used for post processing the breakthrough curves generated by the transport model, fraction	Fraction of colloids transported unretarded	0.0005 ^b	-	Epistemic	<i>Saturated Zone Colloid Transport</i> (BSC 2004 [DIRS 170006], Section 6.6)
Used for calculating colloid sorption coefficient using Equation 57, which is in turn input as the variable K_d in the control statement "sptr," ratio	Colloid retardation factor in alluvium for irreversible colloids	1	-	Epistemic	Table 4-2

^a Base-case permeabilities and recharge and boundary fluxes are multiplied by this factor to vary specific discharge without affecting the flow calibration.

^b This value is different from the base-case value given in Table 4-2. This parameter does not enter the base-case transport model directly. It is used in TSPA calculations for postprocessing the breakthrough curves output from this report.

6.5 BASE-CASE MODEL RESULTS

The base-case model results (output DTN: LA0306SK831231.001) are discussed in this section.

The conceptual and mathematical model described in Sections 6.3 and 6.4 was implemented in the numerical code FEHM V 2.20, a finite-volume/finite-element heat- and mass-transfer code that simulates nonisothermal, multiphase, multicomponent flow and solute transport in porous

media. The details of this code, its usage and verification example are given in the *Validation Test Plan (VTP) for the FEHM Application Version 2.20* (LANL 2003 [DIRS 164150]). The

calibrated base-case site-scale SZ flow model (DTN: LA0304TM831231.002 [DIRS 163788]), which is described in detail in the SZ flow model report, *Site-Scale Saturated Zone Flow Model*, (BSC 2004 [DIRS 170037]), was used as the starting input.

The purpose of this model report is to provide a site-scale SZ transport model to be used as the starting point for the SZ abstractions model presented in *Saturated Zone Flow and Transport Model Abstraction* (BSC 2004 [DIRS 170042], Section 6.3) for use in the TSPA-LA calculations. For this purpose, a single base-case transport model is presented here along with its outputs. The propagations of uncertainties in the input parameters to the output breakthrough curves are presented in Section 6.7 by documenting the breakthrough curves at the boundary of the accessible environment at 18 km (10 CFR 63.302 [DIRS 156605]) for minimum and maximum values of the various parameters. The barrier capabilities of the SZ transport are presented in Section 6.8 of this report, where the influence of key parameters on the radionuclide breakthrough is discussed.

The input transport parameter values and the sources for these values for the base-case model are given in Table 6.4-2. Particle source locations were distributed under and east of the anticipated repository footprint at the water table (BSC 2004 [DIRS 170042], Section 6.5.2.13). Calculations were performed for an instantaneous release of particles at the source location. The breakthrough curve at the boundary of the accessible environment at 18 km was calculated by starting 1,000 particles distributed over the repository footprint and by outputting the cumulative number of particles crossing an east-west vertical plane across the entire width and depth of the model. Output of this model is shown in Figure 6.5-1 where normalized cumulative mass is plotted on the y-axis and the time in years on the log scale on the x-axis.

The base case serves as a reference point for exploring the role of processes and features of the system in subsequent simulations. The solid black curve in Figure 6.5-1a shows the breakthrough curve at the 18 km boundary, which can also be thought of as an arrival time distribution for transport through the SZ. This is the breakthrough curve for a conservative, nonsorbing radionuclide in the absence of radioactive decay. Breakthrough times on the order of hundreds of years are predicted for the bulk of the mass arriving at the water table, with transport times extending into the thousands of years for the slowest moving 20 percent of the mass. This breakthrough curve in Figure 6.5-1 corresponds to a breakthrough time at 50 percent concentration of 705 years.

A similar model calculation was performed where the number of input tracer particles was changed (from 1,000 in the base case) to nine particles spread over the repository footprint, and the output option was changed to produce detailed particle tracks as they moved from the source location to the boundary of the accessible environment at 18 km. These are plotted against a shaded relief map of the SZ site scale model area in Figure 6.5-2. Note that there is very minimal transverse spreading of the flow paths due to the small value of transverse dispersivities (Table 6.4-2). The flow paths in Figure 6.5-2 appear to converge toward the southern portion of the model due to the large-scale heterogeneities that are explicitly included in the hydrologic framework model shown in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section 6.3.2.9).

6.6 ALTERNATIVE CONCEPTUAL MODELS

Credible alternatives to the conceptual model of SZ transport presented in Section 6.3 were evaluated in regards to their impact on the radionuclide transit times from the repository footprint to the boundary of the accessible environment at 18 km. The alternative conceptual models fall into two classes. One class consists of the alternative conceptual models that are excluded from further consideration because they lead to transit times greater than those calculated by the site-scale SZ transport model. The key components of each of these alternative conceptual models, and the basis for the disposition are presented in Table 6.6-1a. The other class consists of alternative conceptual models that are implicitly included in the site-scale SZ transport model through the range of uncertainty in parameter values. The key components of each of these alternative conceptual models, the disposition of each alternative conceptual model and the basis for the disposition are presented in Table 6.6-1b.

Table 6.6-1a. Key Components and Basis for the Alternative Conceptual Models Excluded from Further Consideration Because They Lead to Transit Times Greater than the Base-Case Results

Alternative Conceptual Model	Key Components	Basis
Fluid flow in matrix blocks	The matrix material in the intervening space between the flowing intervals in the volcanics has significant permeability and transmits significant amounts of fluid by advection for the flow conditions in the SZ.	There are three situations possible: (1) flow occurs from the fractures into the matrix, (2) flow occurs from the matrix into the fractures, and (3) flow occurs independently within matrix blocks. In the first case, flow out of the fractures into the matrix would enhance the effects of the matrix diffusion, leading to transit times greater than those calculated by this model. In the second case, considering the steady-state nature of the flow system as presented in <i>Saturated Zone Site-Scale Flow Model</i> (BSC 2004 [DIRS 170037], Section 6), if some flow is occurring out of the matrix into the fractures, then equivalent flow must also occur from fractures into the matrix blocks. Thus, the matrix diffusion effects will be negated in some areas and enhanced in others, and the overall effect on the effective diffusion coefficient will be small. In the third case, an effective porosity would have to be used that is larger than that being used for the fractured flowing intervals, thus leading to transit times greater than those calculated by this model.
Irreversible sorption	Rate of desorption of radionuclides from the rock surfaces is slower than the rate of absorption.	Sorption reactions that are not fully reversible result in rates of transport that are slower than would be the case for fully reversible reactions. Therefore, for radionuclides that sorb irreversibly, using a sorption coefficient would result in diminished total radionuclide mass breakthrough from the SZ. A potential scenario for which this simplification could lead to longer transit times is when deposition of radionuclides takes place under the ambient geochemical conditions, and later, because of geochemical changes, the deposited radionuclides re-enter the aqueous phase and are transported downstream as a pulse. On the basis of available geochemical and mineralogical data, this situation is not considered likely. It is being addressed as a FEP in <i>Features, Events, and Processes in SZ Flow and Transport</i> (BSC 2004 [DIRS 170013]).

7.1.2.6 Advection in the Alluvium

7.1.2.6.1 Alluvial Tests at NC-EWDP-19D1

Three single-well injection-withdrawal tracer tests were conducted in the saturated alluvium at NC-EWDP-19D1 between December 2000 and April 2001. In each of the three tracer tests, two nonsorbing solute tracers with different diffusion coefficients were simultaneously injected (a halide and a fluorinated benzoic acid dissolved in the same solution). The three tests were conducted in essentially the same manner except for the time that was allowed to elapse between the cessation of tracer and chase-water injection and the initiation of pumping—that is, the so-called “rest” or “shut-in” period. The rest period was systematically varied from approximately 0.5 hour to approximately 2 days and to approximately 30 days in the tests to vary the time allowed for tracers to diffuse into stagnant water in the flow system and for the tracers to migrate with the natural groundwater flow. Test interpretations were based on comparing the responses of the different tracers in the same test as well as the responses of similar tracers in the different tests. Differences in the responses of the two tracers injected in the same test provided information on diffusion into stagnant water in the system, whereas differences in the responses of tracers injected in different tests (after correcting for the effects of diffusion) provided information on tracer drift during the rest periods of the tests. Because the three tracer tests used different drift durations, a comparison of the results, combined with an idealized model of the groundwater flow behavior near the well, could be used to estimate the specific discharge. Values ranging from 1.2 to 9.4 m/y, depending on conceptual model and parameter uncertainties, were obtained from *Saturated Zone In-Situ Testing* (BSC 2004 [DIRS 170010], Table G-7). This range is in agreement with the values calculated in the calibrated site-scale SZ flow model as presented in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section 6.6.2.4) and the range of input values used in this report (Table 4-2). The site-scale SZ transport model is intended for use in making TSPA-LA predictions using a wide range of parameter input values that reflect uncertainty in the input. Hence, a comparison of the range of values is considered sufficient. This result lends strong support to the process of advection in the alluvium.

7.1.2.6.2 CAMBRIC (NTS)

Velocities of movement under forced-gradient conditions used in the CAMBRIC experiment are not directly relevant to natural-gradient flow and transport at Yucca Mountain. However, modeling analyses performed by Thompson et al. (1999 [DIRS 162686], Chapter 10) for the NTS Environmental Restoration (ER) Project provide information on relevant hydrologic and transport parameter estimates for alluvium at the site. Using a heterogeneous distribution of permeability and constant porosities ranging from 0.1 to 0.38 (Thompson et al. 1999 [DIRS 162686], Table 20), Thompson showed that a continuum model, after calibration, was able to match the tritium breakthrough curve well (Thompson et al. 1999 [DIRS 162686], Figure 40). Note that this range of porosities compares favorably with the uncertainty range of 0.02 to 0.3 for the effective alluvium porosity in Table 4-2 of this report. In a simulation of tracer migration in which the fluid extraction rate is specified, the key parameters controlling the breakthrough curve are the effective porosity, which controls the mean arrival time, and the correlation length of the heterogeneity, which controls the macrodispersive spreading of the breakthrough curve. In the site-scale SZ transport model, porosity and permeability are taken to be uniform within hydrogeologic units, and a macrodispersion model governs the dispersion. The NTS and

7.2 POST-DEVELOPMENT VALIDATION TO SUPPORT THE SCIENTIFIC BASIS OF THE MODEL

Numerical results from the site-scale SZ transport model have been compared both to data and to independent models to provide confidence that, when combining the submodels with appropriate geologic-, hydrologic-, and boundary-condition information, the overall model is consistent with available observational data. Specifically, the flow pathways from the model are compared to hydrochemistry data (Section 7.2.1), and the transit times computed from the site-scale SZ transport model are compared to ^{14}C data at the field scale (Section 7.2.2).

7.2.1 Comparison of Flow Paths Against Those Deduced from Hydrochemistry Data

Flow paths of tracer particles were calculated for the base-case transport model. The particles were started in the vicinity of the repository footprint and allowed to transport downstream to the boundary of the accessible environment at 18 km. The transport parameter values used in this model calculation are given in Table 6.4-2 of this report. The results are shown in Figure 7-9b. Flow paths deduced from the hydrochemistry data are shown in Figure 7-9 (a and b) and are given in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.11 and Figure A6-62). Chemical and isotopic compositions were measured for groundwater samples taken from a number of wells in the area of the site-scale SZ flow model. As explained in detail in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.11), graphical analysis was done of the variations in the hydrochemical concentrations and isotopic ratios to estimate plausible flow lines. Of particular interest are the flow paths labeled # 2 and #7 in Figure 7-9 (a and b) from this analysis. Flow path 7, which is derived from hydrochemistry data, originates in the vicinity of the repository footprint and generally overlaps the model-calculated flow paths as seen in Figure 7-9b. Flow path 2 is also of interest here, although it originates northeast of the repository, because it closely bounds flow path #7 to the east. Note that the flow path 9 (shown by broad dashed line in Figure 7-9a going from east to west), which appears to cut across the flow paths 2 and 7 in the two-dimensional figure, actually represents regional underflow in the deep carbonate aquifer that underlies the volcanics and the alluvium in the SZ model area, and thus does not interfere with the flow paths 2 and 7.

Flow path 2 traces the movement of groundwater from the Fortymile Canyon area southward along the axis of Fortymile Wash into the Amargosa Desert. This pathway is drawn on the basis of similar anion and cation concentrations along the flow path and dissimilarities to regions to the east and west. Further details are presented in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.11).

Flow path 7 traces the movement of groundwater from northern Yucca Mountain southeastward toward wells in the Dune Wash area and then southwestward along the western edge of the Fortymile Wash shown in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.11). High $^{234}\text{U}/^{238}\text{U}$ activity ratios and low Cl^- , SO_4^{2-} , δD and $\delta^{18}\text{O}$ values characterize this flow path. A detailed discussion is presented in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.11).

The flow paths deduced from the geochemistry data are qualitative in nature and denote broad areas of flow continuity inferred from available data, rather than specific streamlines. They are meant to represent broad flow directions and not the detailed variations that can be seen in a streamline computed from the model. It is seen in Figure 7-9b that the model streamlines originating at the repository footprint follow the general orientation and remain within the flow regions defined by the Flow paths 7 and 2 deduced from the geochemistry data. Hence, this validation is considered acceptable as defined in the technical work plan (BSC 2003 [DIRS 163965], Section 2.3, second validation criteria)

7.2.2 Comparison of Transit Times Against Those Deduced from ^{14}C Data

The radioactive isotope of carbon, ^{14}C , is produced in the atmosphere primarily by the interaction of cosmic rays with the atmospheric ^{14}N . ^{14}C decays with a half-life of 5,730 years. ^{14}C is rapidly incorporated into the atmospheric CO_2 and becomes available for terrestrial processes including that of dissolution into atmospheric precipitation as presented in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.1.2.2). ^{14}C enters the SZ groundwater through recharge and is transported principally as bicarbonate as given in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.1.2.2) as a nonsorbing species. Estimates of groundwater age are obtained from the measured ^{14}C activity, corrected for possible water/rock interactions are given in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.6.6.2). In interpreting these age estimates, it must be noted that the possibility of a fraction of younger water mixing with older water leading to the apparent age as determined from the ^{14}C activity cannot be ruled out with complete certainty. Radiometric dates in geochemically open systems are mixed dates that can be used for estimating upper and lower bounds of the groundwater ages. Hence, the values obtained from ^{14}C activity data should be interpreted as representing the likely range of groundwater ages, without excluding some probability of groundwater ages having values outside the indicated range.

Data from water samples taken from 7 wells in the vicinity of Yucca Mountain were analyzed for ^{14}C activity as shown in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.6.6.2) and the resulting ages are reported to lie in the range of 11,430 years to 16,390 years as presented in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Table A6-7). These ages reflect the time from atmospheric precipitation to the present and thus include transport time through the UZ as well as the SZ, along with the residence time within SZ. Thus, they are not direct indicators of transit times in the SZ, but they do provide a plausible upper bound on the SZ transit time.

Groundwater transit times can also be inferred from measured ^{14}C activity from water samples taken from wells that are inferred to lie along a flow path and where the geochemical compositions of waters suggests that flow paths exist between the two wells as given in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.9). Data from two wells were used: UE-25 WT#3 and NC-EWDP-19D, both of which are downstream of the repository footprint, and lie on the interpreted flow path 7 that starts at Yucca Mountain and moves downstream in an overall southwardly direction (Figure 7-9a). The approximate distance between the two wells is 15 km as shown in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.9.1). The ^{14}C transport times lie in the range of 0 (or negative values) years to 3,110 years over the sampled depths shown in *Saturated Zone Site-Scale Flow*

Model (BSC 2004 [DIRS 170037], Section A6.3.9.1, Table A6-11). The zero or negative values, as discussed in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section A6.3.9.1), likely result from experimental uncertainties, and are not considered in this analysis. The data are clustered around two ranges corresponding to different sampling intervals: one in the interval of 188 to 535 years and the other in the interval of 1,601 to 3,110 years. Using the interwell distance of 15 km as stated above, these ranges translate into groundwater velocity ranges of 80 to 28 m/year and 9.4 to 4.8 m/year. Using a nominal distance of 18 km from the repository footprint to the boundary of the accessible environment at 18 km and taking constant velocities along the flow path, these velocities lead to transit time ranges of 226 to 643 years and 1,915 to 3,750 years. As discussed in the previous paragraph, in interpreting these transit time estimates, it must be noted that the possibility of a fraction of younger water mixing with older water leading to the apparent age as determined from the ^{14}C activity cannot be ruled out with complete certainty. Hence, the values obtained from ^{14}C activity data should be interpreted as representing the likely range of groundwater transport times, without excluding a small probability of groundwater ages having values outside the indicated range.

There are two simplifications built into the above estimates (in addition to the ^{14}C data interpretation as discussed in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Sections A6.3.9, A6.3.1.2.2, and A6.3.6.6.2): one is that in calculating velocities from the transport time estimates, a nominal travel distance is used equal to the well separation, and the second is that a constant velocity is used along the entire flow path. Regarding the first simplification, using a nominal distance instead of the distance along the actual flow path, details of the tortuousness of the flow path are neglected. In actuality, the distance along the flow path will be somewhat greater than the interwell spacing, and thus the calculated velocity will be somewhat less than the actual velocity. However, the influence of this simplification on the estimated transport time to the 18-km boundary is somewhat offset by the fact that the actual travel distance along the flow path (including the segment beyond the well UE-25 WT#3) is also replaced by the somewhat lower value of 18 km, thus a ratio is taken of two numbers that are both somewhat lower than the actual values in the field. Secondly, in using a constant velocity along the flow path from the well UE-25 WT#3 to the boundary of the accessible environment at 18 km, an average of velocities in the volcanics and the alluvium is applied to the additional distance of 3 km that is traveled within the alluvium from the well NC-EWDP-19D to the boundary of the accessible environment. Considering that the porosity in alluvium is many orders of magnitude greater than the volcanic rocks, the effect of this simplification could be quite large. This would result in the estimated upper limit of 3,750 years being an underestimation of the actual transport time.

Transport model simulations were conducted to evaluate the propagation of uncertainty in the input parameter values to the output breakthrough curves, as documented in Section 6.7 of this report. Starting with the base-case parameter values (Section 6), scenarios were constructed by considering one parameter at a time, using the upper and lower limit of each parameter value (Table 6.7-1). The parameters considered include specific discharge, horizontal anisotropy ratio in permeability, effective porosity in the alluvium, flowing interval aperture in the volcanics, effective diffusion coefficient in the volcanics, and the longitudinal dispersivity. Reactive transport parameters were also considered in the analysis described in Section 6.7 but are not considered here, as they are not relevant to ^{14}C transport. The time at which 50 percent of the

injected particles broke through the boundary of the accessible environment at 18 km downstream from the repository footprint is given in Table 6.7-1.

There is another aspect of natural element “background” that is worth mention. That is the fact that those elements-of-interest that have a natural background generally had final solution concentrations in the sorption experiments carried out by the Project that are higher than those calculated only on the basis of the radioactive isotope concentration used in the experiments even in undersaturated solutions. In those cases where the sorption isotherm for the element-of-interest is non-linear, the presence of the natural background concentration in the sorption experiments would generally result in lower sorption coefficients than would be the case in the absence of the natural background concentrations.

Thus, in the derivation of sorption coefficient probability distributions for TSPA, the inclusion of sorption coefficient data from experiments containing natural background concentrations generally results in an underestimation of retardation potential.

Because experiments have been carried out at concentrations up to the solubility limit for most elements of interest, the experimental results reflect this dependency. The only element for which the experimental concentrations did not approach a solubility limit was cesium. The solubility of cesium compounds is very high (Section A7.2). Thus, the sorption-coefficient probability distributions for cesium must be calibrated to the cesium concentrations expected in the SZ.

A3. WATER COMPOSITIONAL RANGES ALONG TRANSPORT PATHWAYS

The chemistry of water in the SZ along potential flow paths to the accessible environment is discussed in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037] Table A6-1). In the SZ, there are two rather distinct water types in the ambient system. One is typified by water from well UE-25 J-13 (J-13), located on the east side of Fortymile Wash. The other is from well UE-25 p#1 (p#1), located near the southern entrance to the Exploratory Shaft Facility.

The J-13 and p#1 waters were used in sorption experiments as end-member compositions intended to bracket the impact of water composition on sorption coefficients. Table A-2a presents these data for a sample from the well UE-25 J-13, a composite water sample from the volcanic portion of the well UE-25 p#1, and a carbonate portion of UE-25 p#1. Comparative information on range of concentrations of the same chemical constituents from other wells in the area is presented in Table A-2b. It can be seen from these tables that for most constituents, these two water compositions approximately bracket the compositions of other wells both in volcanics and alluvium along the potential flow paths to the accessible environment. The pH of the waters from alluvium wells ranges outside that given by J-13 and p#1; however, this is accommodated in the experiments, as seen in Section A7, where water pH ranged up to 8.4.

parameters. Next, the spatial correlation parameters were used to generate multiple realizations of spatial distribution of rock types. The geostatistical approach of sequential indicator simulations (GSLIB V2.0 MSISIM, STN: 10098-2.0MSISIMV2.0-00) (SNL 2000 [DIRS 149114]) was used to generate the spatial distributions. Sequential indicator simulation is a powerful tool that can be used to generate stochastic realizations of parameters. It uses cumulative distribution functions (CDFs) of observed data as input and tries to estimate a discrete, nonparametric true CDF of a simulated parameter. An indicator is a variable used to show the presence or absence of any parameter qualitatively or quantitatively. For example, an indicator can be used to define the presence of a particular rock type at any spatial location. It can also be used to define whether the value of a parameter falls within a certain range of parameter values defined as cutoffs.

After the spatial distributions of rock types were generated, experimental data on K_d values (Appendix A) were used to generate spatial distributions of K_d values. The experimental data were analyzed to derive rock-type specific statistical distributions for K_d . The statistical distributions were used to derive the CDF for each radionuclide. Next, indicators were defined at four CDF cutoffs of 0.2, 0.4, 0.6, and 0.8. These cutoffs, along with the spatial correlation information, were then used to generate spatial distributions. Unlike mineral abundance data, spatial information on K_d observations was not available. As a result, no spatial correlation functions were available for K_d data. In the absence of any spatial correlation functions, the approach used was to generate spatial K_d distributions by varying the correlation length and to understand the impact of varying the correlation length on effective K_d calculations. Four different values were used for correlation length. This range covers the entire spectrum from completely uncorrelated to fully correlated. Four values were used to represent the entire spectrum while not making the number of simulations excessively large:

- Correlation length equal to a single grid block dimension (4 m) that represents spatially random realizations
- Correlation length equal to the correlation length used to generate permeability realizations (60 m)
- Correlation length equal to the large grid block length (500 m)
- Correlation length equal to the correlation length used to generate rock-type data (1,000 m).

All of the above values represent the possible range of correlation lengths that K_d values can be expected to have. The spatial distributions of K_d realizations were generated using the sequential indicator simulation approach. These spatial distributions of K_d values were generated for individual rock types. Distributions for each rock type were generated independent of other rock-type distributions. Finally, the rock-type specific K_d distributions and rock-type distributions were used to generate integrated K_d distributions. The approach used is explained schematically below:

- K_d distribution for rock-type '1': $K_{d1}^1, K_{d2}^1, K_{d3}^1, K_{d4}^1, K_{d5}^1, K_{d6}^1, K_{d7}^1, \dots, K_{dn}^1$

- K_d distribution for rock-type '0': $K_{d1}^0, K_{d2}^0, K_{d3}^0, K_{d4}^0, K_{d5}^0, K_{d6}^0, K_{d7}^0, \dots, K_{dn}^0$
- Rock-type distribution: 1, 0, 1, 1, 1, 0, 0, ..., 1
- Combined K_d distribution: $K_{d1}^1, K_{d2}^0, K_{d3}^1, K_{d4}^1, K_{d5}^1, K_{d6}^0, K_{d7}^0, \dots, K_{dn}^1$, where n is the number of grid points.

The approach explained above incorporates the effect of spatial heterogeneity and rock mineralogy on the spatial distribution of K_d . Multiple realizations for the spatial distribution of K_d values were generated with this approach.

C1.2.2 Stochastic Realizations of Permeability

Similar to the K_d distributions, spatial distributions of permeability were generated using the stochastic approach. The approach and data used were similar to that in *Modeling Sub Gridblock Scale Dispersion in Three-Dimensional Heterogeneous Fractured Media (S0015)* (CRWMS M&O 2000 [DIRS 152259], Sections 5.2 and 6.1). The computer code GS2FEHM.C (GS2FEHM.C V1.0, STN: 10923-1.0-00) (SNL 2002 [DIRS 163837]) was used to create files for the "perm" macro needed as input to FEHM. These permeability realizations represented continuum distributions of permeability for fractured rocks.

C1.3 RESULTS

C1.3.1 Stochastic Realizations of K_d

Figures C-4 and C-5 show the semivariograms calculated from the rock-type data (converted from available mineral abundance data). The figures also show the correlation functions fit to the semivariograms. There is scatter in the data, but the fits are considered reasonable. The parameters for the model fit are shown in Table C-2.

These correlation parameters were used to generate spatial distributions of rock types. The sequential indicator simulation algorithm SISIM (GSLIB V2.0MSISIM;), which is part of GSLIB, was used to generate these distributions. Five different rock-type realizations were generated using this approach. The proportions of zeolitic and devitrified rocks in the five output realizations are shown in Table C-3.

Spatial realizations for K_d were generated for four different radionuclides: uranium, neptunium, cesium, and plutonium. Neptunium is shown to be an important contributor to dose CRWMS M&O 2000 [DIRS 153246], Section 4.1.1) and neptunium to cesium covers the low to high K_d spectrum. The small-scale uncertainty distributions based on experimentally available data for these radionuclides (discussed in Appendix A) are given in Table C-4 (reproduced from Table A-4 for convenience).

C1.3.2 Results of Breakthrough Curve Calculations Using the Particle-Tracking Algorithm

These multiple K_d realizations were used to compute breakthrough curves and model the sorption behavior of each radionuclide. A two-step approach was used. In the first step, steady-state flow fields were computed for 50 different permeability realizations. The properties used for these calculations are shown in Table C-9.

Table C-9. Values of Properties Used in Flow and Transport Calculations

Property	Value
Matrix porosity	0.22 ^a
Rock bulk density	1,997.5 ^a kg/m ³
Flowing interval porosity	0.001 ^a
Flowing interval spacing	19.49 ^a m
Hydraulic gradient	2.9x10 ⁻⁴ ^b

^a Value chosen to fall within the range given in Table 4-2 of this report.

^b *Modeling Sub Gridblock Scale Dispersion in Three-Dimensional Heterogeneous Fractured Media* (CRWMS M&O 2000 [DIRS 152259], pp. 14, Sec. 5.2).

The steady-state flow fields were used in the particle-tracking calculations. In these calculations, 4,000 particles were released along one face of the model and were allowed to move under the influence of the steady-state flow field. The locations of the particle releases were determined by a flux-weighted placement scheme. As mentioned in Section C2.1, two sets of particle-tracking calculations were performed for each steady-state flow field. In the first set of calculations, the baseline breakthrough curve was calculated for transport with diffusion from fracture to matrix and no matrix sorption. In the second set of calculations, the breakthrough curve was calculated for transport with diffusion followed by sorption on the matrix. For these calculations, the stochastically generated K_d distributions were used. The values of the diffusion coefficient used for these calculations are shown in Table C-10.

Table C-10. Values of Diffusion Coefficients Used for the Particle-Tracking Calculations

Radionuclide	Diffusion Coefficient (m ² /s)
Anion (Uranium)	3.2 x 10 ⁻¹¹
Cation (Plutonium, Cesium, Neptunium)	1.6 x 10 ⁻¹⁰

Source DTN: LA0003JC831362.001 [DIRS 149557].

DTN: LA0003JC831362.001 [DIRS 149557] is related to a cancelled analysis and model report (BSC 2001 [DIRS 160828, Section 6.6). Nevertheless, the reported results of laboratory diffusion transport studies remain valid and suitable for intended use. Primarily, this is because the diffusion coefficient values in Table C-10 overlap with values used in the base-case model (Table 4-2), and are therefore corroborated by the alternative sources used to justify that data in Section 4.1.2.10. Consequently, diffusion coefficient values in Table C-10 are suitable for use in upscaling the composite sorption distributions to the site-scale SZ transport computational grid.

These breakthrough curves were used to calculate the effective K_d values using the procedure described in Section C2.1. The procedure was repeated for 50 realizations of K_d . The statistics of the calculated effective K_d values are provided in Table C-11. These calculations of stochastic realizations of K_d were performed using a correlation length of 500 m. As can be seen from the results, the effective K_d distributions are very narrow compared to the distributions of experimentally observed K_d values.

To calculate the Da number, a reverse kinetic rate is needed. Using a representative value of K_d for Pu in devitrified tuff of 100 mL/g (Section A7.4.1 of this report), $k_{rev} = k_{for}/100 = 0.002 \text{ hr}^{-1}$ is obtained.

4. Estimate a travel time through the system:

Time to first breakthrough for Np reported in *Saturated Zone Flow and Transport Model Abstraction* (BSC 2004 [DIRS 170042]), Figure 6-32) is about 100 years. Hence, a conservative value of 10 years is used for travel time through the fractured volcanics in the SZ.

5. Calculate the Damköhler number:

$$Da = k_{rev}RT = 175 \quad (\text{Eq. D-2})$$

Valocchi found that equilibrium is well estimated for $Da > 100$ (1985 [DIRS 144579], p. 813, Fig. 2).

Based on this analysis, the local equilibrium approach is valid for plutonium transport in the SZ of Yucca Mountain.

It should be noted that colloid-facilitated transport could not be ruled out as an explanation for the early breakthrough of ^{239}Pu in the column experiments used in this analysis. The kinetic interpretation of these column studies is also consistent with a colloid transport interpretation where the sorption and desorption rate constants are equivalent to colloid filtration and detachment rate constants. Another possible explanation for the early ^{239}Pu breakthrough in the column experiments is that microbial growth or other processes in the columns may have resulted in localized reducing conditions that caused some of the injected Pu(V) to be reduced, sorb strongly to microbial colloidal material, and be transported faster than the portion of Pu sorbed onto the rock matrix. However, if the early plutonium breakthroughs in the column experiments were a result of colloid-facilitated transport of a portion of the plutonium, then the sorption of rate constants for the soluble plutonium fraction would have to be greater than those obtained assuming that all the plutonium was soluble. This scenario would only strengthen the conclusion that the equilibrium approximation is valid for soluble plutonium over large time scales.