QA: QA

Model Administrative Change Notice

Complete only applicable items.

1. Document Number:	MDL-NBS-HS-000020	**2. Revision:**	02/AD01	**3. ACN:**	01
4. Title:	Particle Tracking Model and Abstraction of Transport Processes				
5. No. of Pages Attached	6				

6. Approvals:		
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7. Affected Pages	8. Description of Change:
Page 4-10, 4th paragraph, 2nd line	Section 4.1.6 Inserted "the" before "Yucca Mountain site"
Page 4-10, last paragraph, 1st line	Section 4.1.6 Replaced "tracer test" with "tracer tests"
Page 6-46, Figure 6.8.2-5	Section 6.8.2.1 Change made in the text above the plots: changed "dual-k" to "DFM"
Page 6-53, 2nd paragraph, 4th line	Section 6.8.2.2 Changed "90%" to "approximately 99.3%" in the document
Page 6-67, 1st and 2nd line:	Section 6.8.2.2 changed "(left)" to "(top)", and changed "(right)" to "(bottom)"
Page 7-15, Figure 7-12	Section 7.2.3.2 Inserted "of" after "Role" in the figure caption
Page 8-20, 2nd paragraph, 5th line:	Section 8.2.2 Inserted "a" before "very minimal barrier"

The remaining inputs used for matrix diffusion coefficients are for the free-water diffusion coefficients. These inputs are (1) the molar ionic conductivities presented by Lide (1992 [DIRS 166224]), which are considered established fact; (2) speciation results from *Dissolved Concentration Limits of Elements with Radioactive Isotopes* (SNL 2007 [DIRS 177418]), which are qualified; (3) *The Hydrolysis of Cations* (Baes and Mesmer 1986 [DIRS 100702]) for aqueous speciation of cesium, tin, and technetium; (4) *Fresh Water Systems* (Cutter 1989 [DIRS 178861]) for the aqueous speciation of selenium, which are considered established fact; (5) parameters used in the Nernst-Einstein equation (Equation (A-7)) and Stokes-Einstein equation (Equation (A-8)) from Lide (1992 [DIRS 166224]), which are considered established fact; and (6) atomic radii given by Slater (1965 [DIRS 179613]), which are considered established fact.

The free-water diffusion coefficient for TcO_4^- is from Sato et al. (1996 [DIRS 163213] Table 2). This datum may be justified by comparison with diffusion coefficients for the aqueous species analogues MnO_4^- and ReO_4^-. Based on information from Lide (1992 [DIRS 166224]), the free-water diffusion coefficients for MnO_4^- and ReO_4^- are 1.63×10^{-9} m^2/s and 1.46×10^{-9} m^2/s, respectively. The positions of manganese and rhenium in the periodic table of elements suggests that the diffusion coefficient for TcO_4^- should be approximately the average of these values. The average of the diffusion coefficients for MnO_4^- and ReO_4^- is 1.55×10^{-9} m^2/s. The diffusion coefficient reported by Sato et al. (1996 [DIRS 163213], Table 2) for TcO_4^- is 1.95×10^{-9} m^2/s. Therefore, the analogue diffusion coefficient values lie within 21% of the value reported by Sato et al. (1996 [DIRS 163213], Table 2) and all analogue values are well within the uncertainty of the measurement, 0.56×10^{-9} m^2/s, reported by Sato et al. (1996 [DIRS 163213], Table 2).

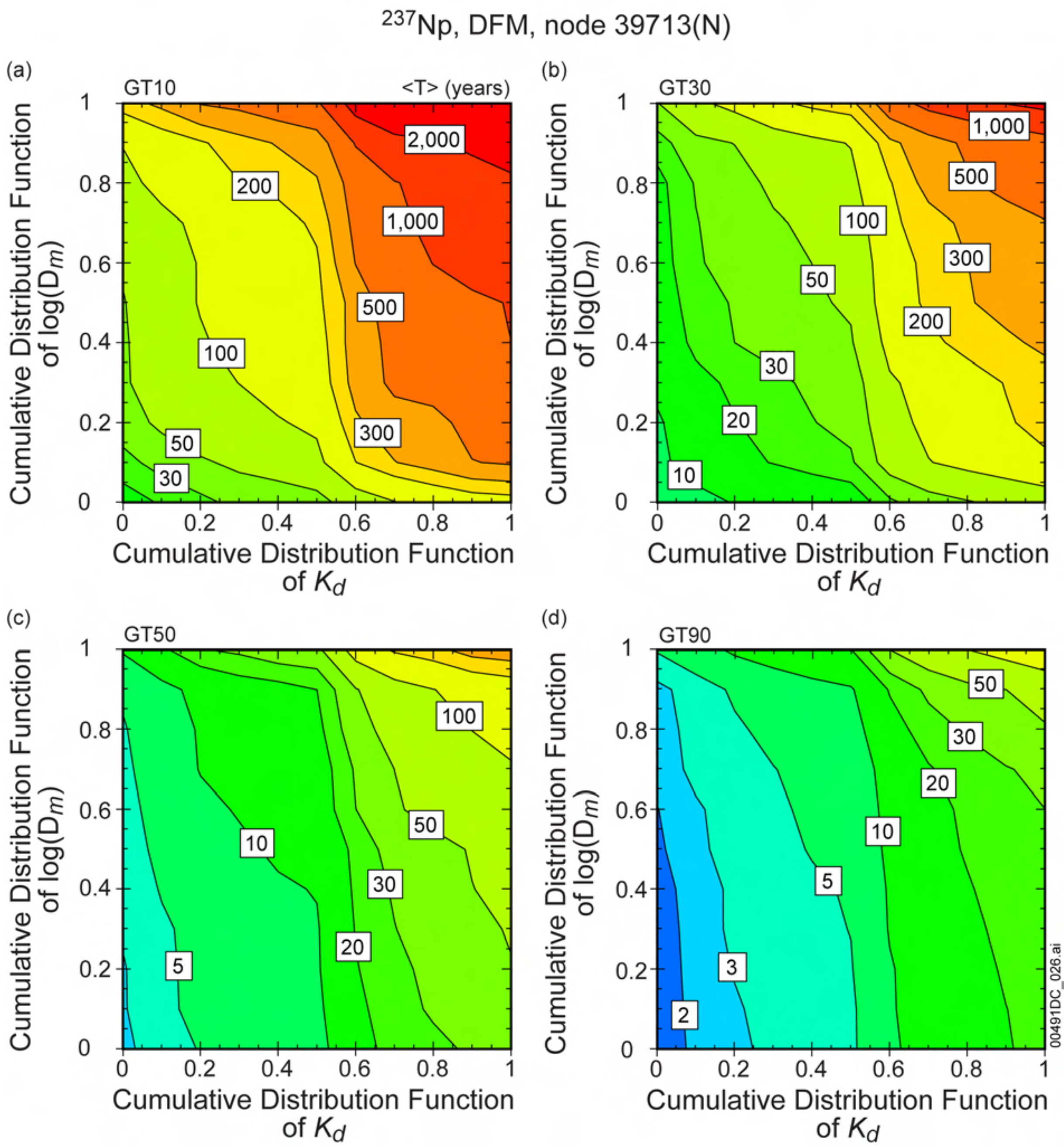
4.1.5 Matrix Sorption Coefficient

The sorption coefficients for radionuclides onto the matrix rock are developed in *Radionuclide Transport Models Under Ambient Conditions* (SNL 2007 [DIRS 177396]). These sorption coefficient distributions, obtained from DTNs: LA0408AM831341.001 [DIRS 171584] and LB0701PAKDSESN.001 [DIRS 179299], are used in this addendum to assign values for use in the representative case simulations and the sensitivity calculations presented in Section 6. The justifications for the uncertainty distributions themselves can be found in *Radionuclide Transport Models Under Ambient Conditions* (SNL 2007 [DIRS 177396]) and the referenced DTNs.

4.1.6 Fracture Dispersivity

The fracture dispersivity is set at a fixed value of 10 m. There are few data available on dispersivity distributions at the Yucca Mountain site. Neuman (1990 [DIRS 101464]) showed that field dispersivity varied with the scale of study. Field tracer tests at the C-holes at Yucca Mountain also showed that, on a 100-m scale, field dispersivity had a range of approximately 3 m to 63 m (SNL 2007 [DIRS 177394], Table 6.3-3). The 10-m value is toward the lower end of the values from field studies available in DTN: LA0303PR831231.005 [DIRS 166259].

With respect to tracer tests under unsaturated conditions, none of the field tests conducted either at the Busted Butte or Alcove 8/Niche 3 site provided definitive information on either the longitudinal or transverse dispersion. For example, *Radionuclide Transport Models Under*



Output DTN: MO0705TRANSTAT.000.

Figure 6.8.2-5. Mean Travel Time of ^{237}Np as a Function of Matrix Diffusion Coefficient and Sorption Coefficient for the Glacial-Transition Climate Condition, DFM Model, Northern Release Location released either at the northern or southern release points under the four glacial-transition flow fields, simulated using both the dual-k model DFM models. For nonsorbing species, simple line plots are used, whereas for cases in which both D_m and K_d are varied (sorbing species ^{237}Np and ^{240}Pu), the matrix of 11 D_m values and 11 K_d values are used, and the results are displayed as contour plots.

Figures 6.8.2-11 and 6.8.2-12 plot C/C_0 for species ^{99}Tc for the northern and southern nodes. Due to the long half life and relatively short travel times for ^{99}Tc, this species essentially all reaches the water table without decay, yielding C/C_0 values close to unity. These results indicate that in all cases examined here more than approximately 99.3% of ^{99}Tc reaches the water table. Different models have a slight impact on C/C_0 for the northern release, but they do not have a noticeable effect on C/C_0 for the southern release.

a function of R_{coll} for the four glacial-transition flow fields, for the northern (top) and southern (bottom) release locations. Similar plots for the decay fraction C/C_0 are shown in Figure 6.8.2-24. For the northern release location, travel times are larger for either lower fluid flow rates or larger values of R_{coll}. The southern release location, with its interval of matrix-dominated transport, has generally larger travel times and a smaller impact of fracture retardation of colloids, since this effect "competes with" the matrix transport time for importance. For either release location, the decay fraction is close to unity for this species of ^{240}Pu except for the highest values of R_{coll} in the uncertainty distribution. For other Ic species with shorter half lives, a larger effect of R_{coll} uncertainty on the decay fraction would be expected.

to the abstraction model, these comparisons have reasonable qualitative explanations. This result illustrates that the abstraction model can propagate conceptual model uncertainties for f/m interactions through the TSPA-LA model.

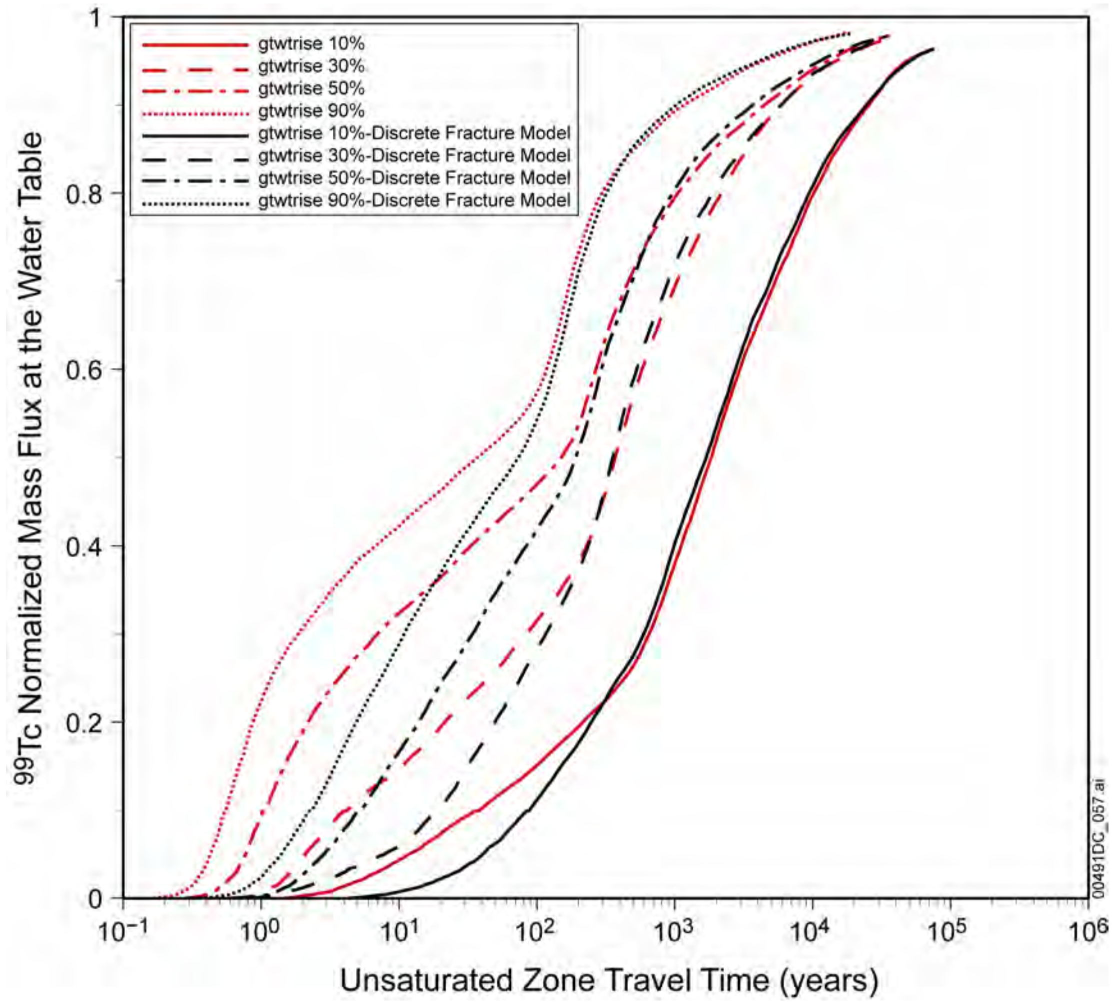


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Figure 7-12. Breakthrough Curves for ^{99}Tc Using the Unsaturated Zone Transport Abstraction Model to Investigate the Role of f/m Interaction Conceptual Model: Simulations for Different Glacial-Transition Infiltration Rate Scenarios (10%, 30%, 50%, and 90%), Representative Parameter Values, and Glacial-Transition Water Table flow field (which varies according to the infiltration scenario chosen) also has an important influence on the calculation of travel times, as illustrated by the travel time contours of Appendix D.1. However, the general flow patterns are independent of infiltration scenario, as illustrated by the similarity of the patterns reflected in the figures of Appendix D.1.

Sensitivity analyses focused on the capability of the unsaturated zone to perform as a barrier to migration of radionuclides to the water table. The mean travel time and the decay fraction C/C_0 are two metrics used for this purpose. For nonsorbing species, diffusion coefficient and flow scenario have an impact on these two metrics, but if these radionuclides have long half lives, such as ^{99}Tc, the unsaturated zone provides a very minimal barrier to radionuclide migration over the ranges of uncertainty in diffusion and flow rate. Similarly, the selection of the diffusion conceptual model (dual-k versus DFM) is also relatively unimportant for ^{99}Tc, as neither model predicts a significant barrier for this radionuclide and others like it (nonsorbing, long-half-life radionuclides). For sorbing species, contour plots of the mean travel time or C/C_0 were constructed spanning the ranges of diffusion coefficient and K_d given by the uncertainty distributions of these parameters. For more strongly sorbed species, the impact of diffusion coefficient and diffusion conceptual model becomes more important. There is interplay between diffusion and sorption for the northern release locations, which exhibit fracture-dominated transport. For the southern release locations, the intervening layer of matrix-dominated transport makes travel times and barrier capability dependent only on the sorption coefficient, and the diffusion model and parameters become relatively unimportant. Lastly, the range of colloid retardation factors for the irreversibly sorbed species (Ic) is such that the resulting transport behavior ranges from minimal barrier to effective barrier, depending on the retardation factor and the half life of the species.

Finally, the relative importance of conceptual and parameter uncertainties must be treated separately for each radionuclide; the analysis techniques applied herein provide insights into the behavior of species in the TSPA model. However, the actual predicted performance of the unsaturated zone barrier system within the repository total system must be examined in the TSPA model itself.

8.3 HOW THE APPLICABLE ACCEPTANCE CRITERIA ARE ADDRESSED

There is no change to the list of acceptance criteria that apply to the parent report or this addendum. The summary below places the work performed in this addendum in the context of the acceptance criteria by identifying which criteria are better satisfied by the specific work element. The nomenclature for identifying the acceptance criterion from the parent report is to identify the criterion number, followed by the item number within that acceptance criterion. For example, Acceptance Criterion 1, Item 4 refers first to the first acceptance criterion "System Description and Model Integration Are Adequate," and then to the fourth item, which is on boundary and initial conditions.

Acceptance Criterion 1, Item 4: The development of repository percolation bins containing the repository nodes (Section 6.5.15) is an updated version of these percolation bins that provides a boundary condition for radionuclide releases that reflects the current unsaturated zone flow models. This work was conducted in part to address CR 7225.