



Model Administrative Change Notice

QA: QA

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Complete only applicable items.

1. Document Number:	MDL-NBS-HS-000008	2. Revision:	02/AD 01	3. ACN:	02
4. Title:	Radionuclide Transport Models Under Ambient Conditions				
5. No. of Pages Attached	13				

6. Approvals:	
Preparer:	James Houseworth <i>James E Houseworth</i> 8/22/07 Print name and sign Date
Checker:	Schon Levy <i>Schon A Levy</i> 08/23/07 Print name and sign Date
QCS/Lead Lab QA Reviewer:	Peter Persoff <i>Peter Persoff</i> 08/23/2007 Print name and sign Date
Independent Technical Reviewer:	Ming Zhu <i>Ming Zhu</i> 8/23/07 Print name and sign Date
Responsible Manager:	Stephanie Kuzio <i>Stephanie Kuzio</i> 8/23/07 Print name and sign Date
7. Affected Pages	8. Description of Change:
5 and 6	<p>Section 7[a]</p> <p>Original text: Alcove 8 -- Niche 3.</p> <p>Revised text: Alcove 8 -- Niche 3 (BSC 2004 [DIRS 170004], Section 6.12.2.4; Section 7.3.3 of the parent report)).</p>
6	<p>Section 7[a]</p> <p>Original text: tends to yield</p> <p>Revised text: yields</p>
6	<p>Section 7[a]</p> <p>Original text: matrix-only single continuum (SNL 2007 [DIRS 175177]).</p> <p>Revised text: matrix-only single continuum (SNL 2007 [DIRS 175177], Section 6.1.5).</p>



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6	<p>Section 7[a]</p> <p>Original text: the repository and the water table.</p> <p>Revised text: the repository and the water table (compare BSC 2004 [DIRS 169861], Figure 6.7-1 with SNL 2007 [DIRS 175177], Figures 6.7-1 and 6.7-2).</p>				
7, 7a	<p>Section 9.1[a]</p> <p>Added references:</p> <p>170004 BSC 2004. <i>In Situ Field Testing of Processes</i>. ANL-NBS-HS-000005 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041109.0001; DOC.20051010.0001.</p> <p>169861 BSC 2004. <i>UZ Flow Models and Submodels</i>. MDL-NBS-HS-000006 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041101.0004; DOC.20050629.0003.</p>				
8	<p>Section 9.1[a]</p> <p>Added references:</p> <p>177392 SNL 2007. <i>Site-Scale Saturated Zone Transport</i>. MDL-NBS-HS-000010 REV 03. Las Vegas, Nevada: Sandia National Laboratories.</p>				
9, A-6, A-7, A-10, B-4	<p>Updated DTN reference from</p> <p>DIRS 179829 - LA0702AM150304.001. Probability Distribution Functions and Cross-Radionuclide Correlations for Sampling of Sorption Coefficient Probability Distributions in the SZ at the YM. Submittal date: 02/22/2007.</p> <p>To</p> <p>DIRS 182480 - LA0702AM150304.001. Probability Distribution Functions and Cross-Radionuclide Correlations for Sampling of Sorption Coefficient Probability Distributions in the SZ at the YM. Submittal date: 08/16/2007.</p>				



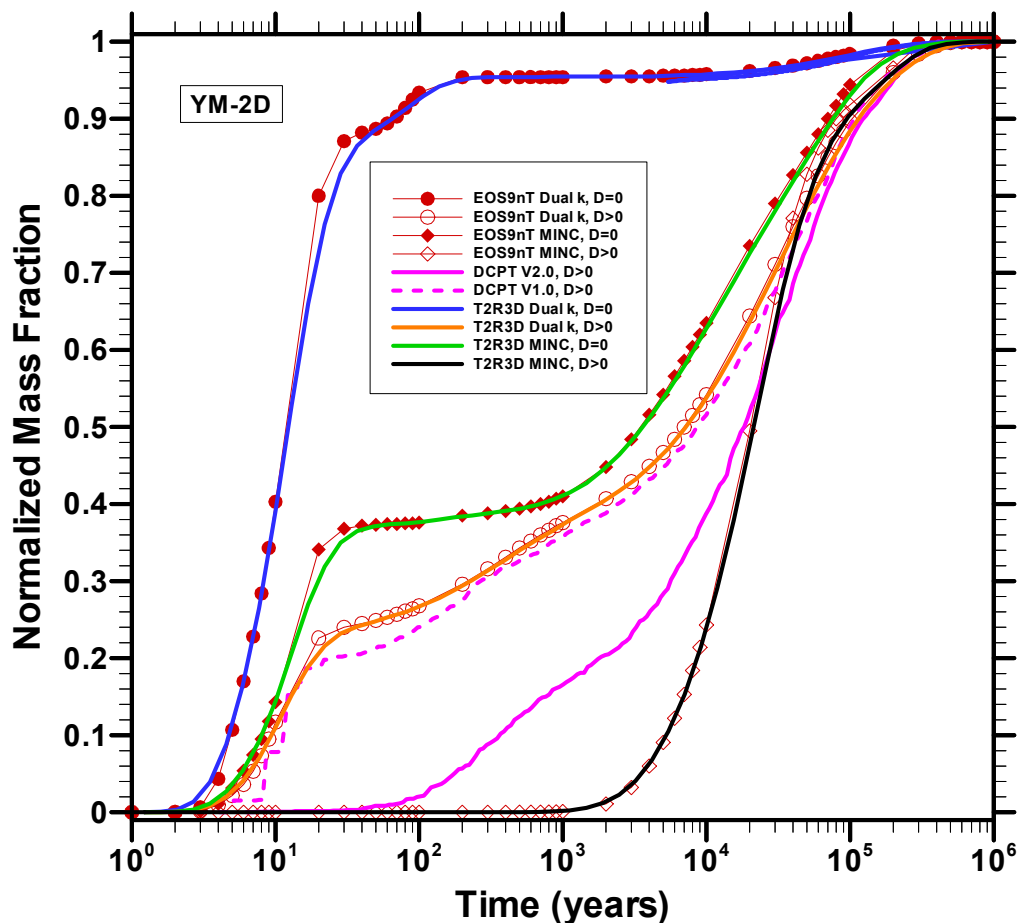
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A-9	<p>Added to Section A2.6.1[a]:</p> <p>This distribution goes to a higher upper bound than reported in DTN: LA0702AM150304.001 [DIRS 182480], Table 4 for SZ transport. This is because the SZ distribution treats the combination of devitrified and zeolitic rock as a composite volcanic rock type. The SZ transport simulations use the sorption distribution on devitrified rock as representative of the composite volcanic rock (SNL 2007 [DIRS 177392] Section A7.10.1). As shown in Section A2.6.2[a], the sorption distribution for tin on zeolitic rock is characterized by a log-uniform distribution from 100 to 5,000 mL/g.</p> <p>Deleted from Section A2.6.1[a] and started new paragraph:</p> <p>(DTN: LA0702AM150304.001 [DIRS 179829], Table 4)</p>				
Appendix B[a] title page	<p>Original text: APPENDIX B</p> <p>Revised text: APPENDIX B[a]</p>				
B-3	<p>Section B1[a]</p> <p>Deleted text: Other factors are not well understood.</p>				



Sources: DTNs: LB03093RADTRNS.001 [DIRS 166225]; LB03093RADTRNS.002 [DIRS 166071].

Figure 6-1[a]. Effect of the MINC Concept and Application of Particle-Tracking Approaches on Breakthrough Predictions at a Two-Dimensional Vertical Cross Section of the Unsaturated Zone for an Instantaneous Release under Mean, Present-Day Climate for a Nonsorbing, Non-decaying Tracer

7[a]. VALIDATION

Level II model validation was planned in *Technical Work Plan for: Unsaturated Zone Flow, Drift Seepage and Unsaturated Zone Transport Modeling* (BSC 2006 [DIRS 177465], Section 2.2.1.3). That model validation plan was developed under LP-2.29Q-BSC, *Models*, which was then in effect. The plan also meets the requirements for Level II model validation in SCI-PRO-002, Attachment 3, by addressing all the requirements for confidence building during development as well as two post-development validation activities. Specifically, the model validation plan includes confidence-building steps previously documented for this model in *Radionuclide Transport Models under Ambient Conditions* (BSC 2004 [DIRS 167969]) as well as additional during-development confidence-building and post-development validation activities that are associated with planned model enhancements to the UZ radionuclide transport model (i.e., use of the MINC approach to fracture–matrix interaction and adjustments to the range in matrix diffusion to include the transport behavior as observed in Alcove 8 – Niche 3 (BSC 2004

[DIRS 170004], Section 6.12.2.4; Section 7.3.3 of the parent report)). However, these model enhancements have not been performed, and therefore, the associated model validation activities are not necessary. The existing treatment of the fracture-matrix diffusion using the dual permeability method yields conservative estimates of transport times through the unsaturated zone as shown in sensitivity analyses documented in Section 6.19.1 of the parent report. Similarly, the existing UZ radionuclide transport model without incorporating observations from the Alcove 8 – Niche 3 is also a conservative treatment for matrix diffusion. Also note that Section 7 of the parent report used the model validation methods as planned in *Technical Work Plan for: Unsaturated Zone Flow, Drift Seepage and Unsaturated Zone Transport Modeling* (BSC 2006 [DIRS 177465], Section 2.2.1.3), but the specific model validation activities were different, and actually follow the validation plan described in *Technical Work Plan for: Performance Assessment Unsaturated Zone* (BSC 2004 [DIRS 167969], Section I-2-1-1). Despite this deviation, the model validation presented in Section 7 of the parent report meets the requirements for Level II model validation in SCI-PRO-002, Attachment 3, by addressing all the requirements for confidence building during model development as well as two post-development validation activities.

The unsaturated zone flow model has been revised to reflect changes in infiltration, associated changes in calibration properties, and a change in treatment of the Calico Hills nonwelded vitric (CHnv) rock as a dual continuum instead of a matrix-only single continuum (SNL 2007 [DIRS 175177], Section 6.1.5). However, these changes have not been implemented in the unsaturated zone radionuclide transport process model. The reason for not updating the model is that the primary use of the unsaturated zone radionuclide transport process model is to provide radionuclide transport solutions using a traditional, process-based model to validate the unsaturated zone radionuclide transport abstraction model. Although the changes in the flow model would affect results of both process and abstraction transport models, these changes are not important for performing validation comparisons. The important aspects of validation are that the models are compared on the same problem and that the problem is reasonably representative of the important transport processes and time scales involved. The changes in the unsaturated zone flow model are not sufficiently large to affect the important transport process or time scales involved in radionuclide transport between the repository and the water table (compare BSC 2004 [DIRS 169861], Figure 6.7-1 with SNL 2007 [DIRS 175177], Figures 6.7-1 and 6.7-2). Therefore, the existing calculations using the unsaturated zone radionuclide transport process model calculations are suitable for validation of the unsaturated zone radionuclide transport abstraction model.

8[a]. CONCLUSIONS

No change.

9[a]. REFERENCES

The following is a list of the references cited in this addendum. The unique six digit numerical identifier (the Document Input Reference System number) preceding each reference below is also placed in the text following the reference callout (e.g., BSC 2004 [DIRS 161340]). The purpose of these numbers is to assist in locating a specific reference.

9.1[a] DOCUMENTS CITED

- 169668 Anderson, T.W. 1984. *An Introduction to Multivariate Statistical Analysis*. 2nd Edition. New York, New York: John Wiley & Sons. TIC: 244809.
- 104902 Benjamin, M.M. 1983. "Adsorption and Surface Precipitation of Metals on Amorphous Iron Oxyhydroxide." *Environmental Science and Technology*, 17, 686-692. Easton, Pennsylvania: American Chemical Society. TIC: 239143.
- 170022 BSC (Bechtel SAIC Company) 2004. *Initial Radionuclide Inventories*. ANL-WIS-MD-000020 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040921.0003; DOC.20050927.0005
- 170004 BSC 2004. *In Situ Field Testing of Processes*. ANL-NBS-HS-000005 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041109.0001; DOC.20051010.0001.
- 167969 BSC 2004. *Technical Work Plan for: Performance Assessment Unsaturated Zone*. TWP-NBS-HS-000003 REV 02 [Errata 001]. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20030102.0108; DOC.20040121.0001.
- 169861 BSC 2004. *UZ Flow Models and Submodels*. MDL-NBS-HS-000006 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041101.0004; DOC.20050629.0003.
- 177465 BSC 2006. *Technical Work Plan for: Unsaturated Zone Flow, Drift Seepage and Unsaturated Zone Transport Modeling*. TWP-MGR-HS-000004 REV 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20060824.0001.
- 178861 Cutter, G.A. 1989. "Freshwater Systems." Chapter 10 of Occurrence and Distribution of Selenium. In: M. M. Ichnat, ed. Boca Raton, Florida: CRC Press. TIC: 259080.
- 172215 EPA (U.S. Environmental Protection Agency) 2004. "Review of Geochemistry and Available K_d Values for Americium, Arsenic, Curium, Iodine, Neptunium, Radium, and Technetium." Volume III of *Understanding the Variation in Partition Coefficient, K_d , Values*. EPA 402-R-04-002C. Washington, D.C.: U.S. Environmental Protection Agency. ACC: MOL.20041102.0060.
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- 179611 Neal, R.H.; Sposito, G.; Holtzclaw, K.M.; and Traina, S.J. 1987. "Selenite Adsorption on Alluvial Soils: II. Solution Composition Effects." *Soil Science Society of America Journal*, 51, 1165-1169. Madison, Wisconsin: Soil Science Society of America. TIC: 259196.
- 103316 Press, W.H.; Teukolsky, S.A.; Vetterling, W.T.; and Flannery, B.P. 1992. *Numerical Recipes in Fortran 77, The Art of Scientific Computing*. Volume 1 of *Fortran Numerical Recipes*. 2nd Edition. Cambridge, United Kingdom: Cambridge University Press. TIC: 243606.

- 179484 SNL (Sandia National Laboratories) 2007. *Data Qualification Report for Selenium and Tin Sorption Data Obtained by Los Alamos National Laboratories 1981 - 1984*. DQP-MGR-HS-000001 REV00. Las Vegas, NV: Sandia National Laboratories.
- 180472 SNL 2007. *Initial Radionuclides Inventory*. ANL-WIS-MD-000020 REV 01 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20040921.0003; DOC.20050927.0005.
- 181006 SNL 2007. *Particle Tracking Model and Abstraction of Transport Processes*. MDL-NBS-HS-000020 REV 02 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050808.0006.
- 179466 SNL 2007. *Total System Performance Assessment Data Input Package for Requirements Analysis for Subsurface Facilities*. TDR-TDIP-PA-000001 REV 00. Las Vegas, Nevada: Sandia National Laboratories.
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- 179394 SNL 2007. *Total System Performance Assessment Data Input Package for Requirements Analysis for TAD Canister and Related Waste Package Overpack Physical Attributes Basis for Performance Assessment*. TDR-TDIP-ES-000006 REV 00. Las Vegas, Nevada: Sandia National Laboratories.
- 175177 SNL 2007. *UZ Flow Models and Submodels*. MDL-NBS-HS-000006 REV 03. Las Vegas, Nevada: Sandia National Laboratories.
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9.2[a] CODES, STANDARDS, REGULATIONS, AND PROCEDURES

IM-PRO-002. *Control of the Electronic Management of Information.*

LP-2.29Q-BSC. *Planning for Science Activities.*

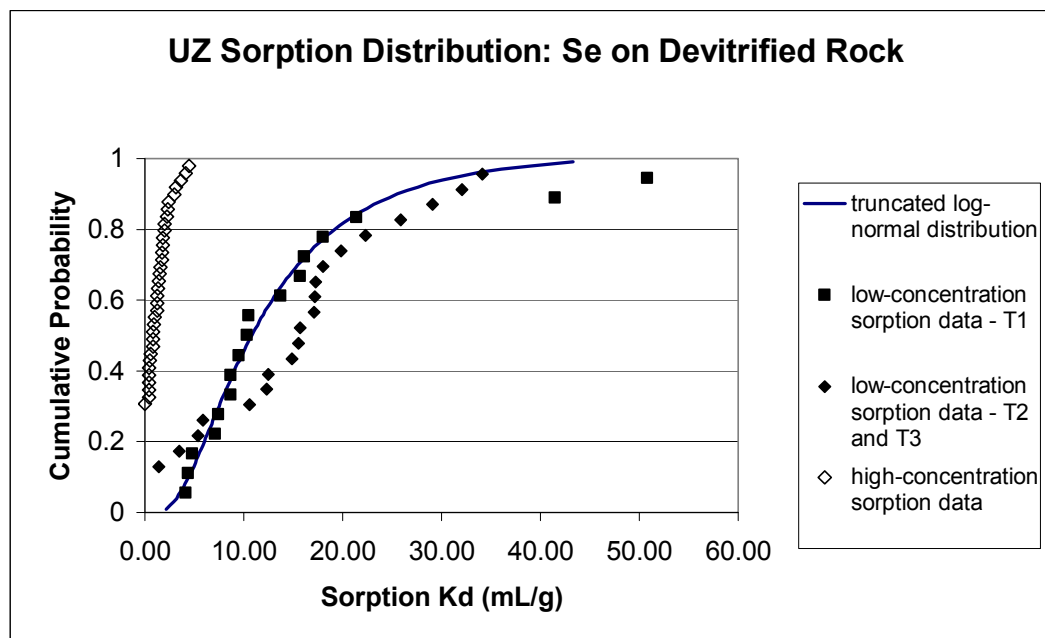
SCI-PRO-002. *Planning for Science Activities.*

SCI-PRO-006. *Models.*

9.3[a] SOURCE DATA, LISTED BY DATA TRACKING NUMBER

- 153323 LA0010JC831341.004. Radionuclide Retardation Measurements of Sorption Distribution Coefficients for Selenium. Submittal date: 10/19/2000.
- 167015 LA0311AM831341.001. Correlation Matrix for Sampling of Sorption Coefficient Probability Distributions. Submittal date: 11/06/2003.
- 171009 LA0407AM831343.001. Modeling Calculations of Radionuclide Sorption via Surface-Complexation Reactions. Submittal date: 07/29/2004.
- 182480 LA0702AM150304.001. Probability Distribution Functions and Cross-Radionuclide Correlations for Sampling of Sorption Coefficient Probability Distributions in the SZ at the YM. Submittal date: 08/16/2007.
- 181561 LA0702MD831232.002. Modeling Calculation of Radionuclide Sorption on Yucca Mountain Volcanic Tuff. Submittal date: 02/27/2007.
- 181562 LA0702MD831232.001. Input Data Sets for Modeling Calculation of Radionuclide Sorption on Yucca Mountain Volcanic Tuff. Submittal date: 02/27/2007.
- 179609 LB0307MR0060R1.002. Ambient Radionuclide Transport - Uniform Instantaneous Release: Data Summaries. Submittal date: 07/19/2003.
- 166225 LB03093RADTRNS.001. Three Way Transport Model Comparison: Input/Output Files. Submittal date: 09/24/2003.
- 166071 LB03093RADTRNS.002. Three Way Transport Model Comparison: Data Summaries. Submittal date: 09/24/2003.
- 180776 LB0702PAUZMTDF.001. Unsaturated Zone Matrix Diffusion Coefficients. Submittal date: 02/20/2007.
- 176868 MO0604SPAPHR25.001. PHREEQC Data 0 Thermodynamic Database for 25 Degrees C - File: PHREEQC DATA025.DAT. Submittal date: 04/10/2006.
- 179925 MO0702PASTREAM.001. Waste Stream Composition and Thermal Decay Histories for LA. Submittal date: 02/15/2007.

Figure A-1[a]. The high-concentration sorption measurements are from DTN: LA0010JC831341.004 [DIRS 153323] and are for aqueous selenium concentrations in excess of 10^{-6} molar. The truncated lognormal distribution was fit to the low-concentration data for use in the unsaturated zone below the TSw, where aqueous selenium concentrations are expected to remain below 10^{-8} molar. The truncated log-normal distribution has a mean of 14 mL/g, a standard deviation of 11.2 mL/g and a range of 1 to 50 mL/g, which provides an adequate fit to the experimental data (DTN: LA0702AM150304.001 [DIRS 182480]). The reduced effective sorption coefficients under higher-concentration conditions are seen in Figure A-1[a].



Output DTN: LB0701PAKDSESN.001.

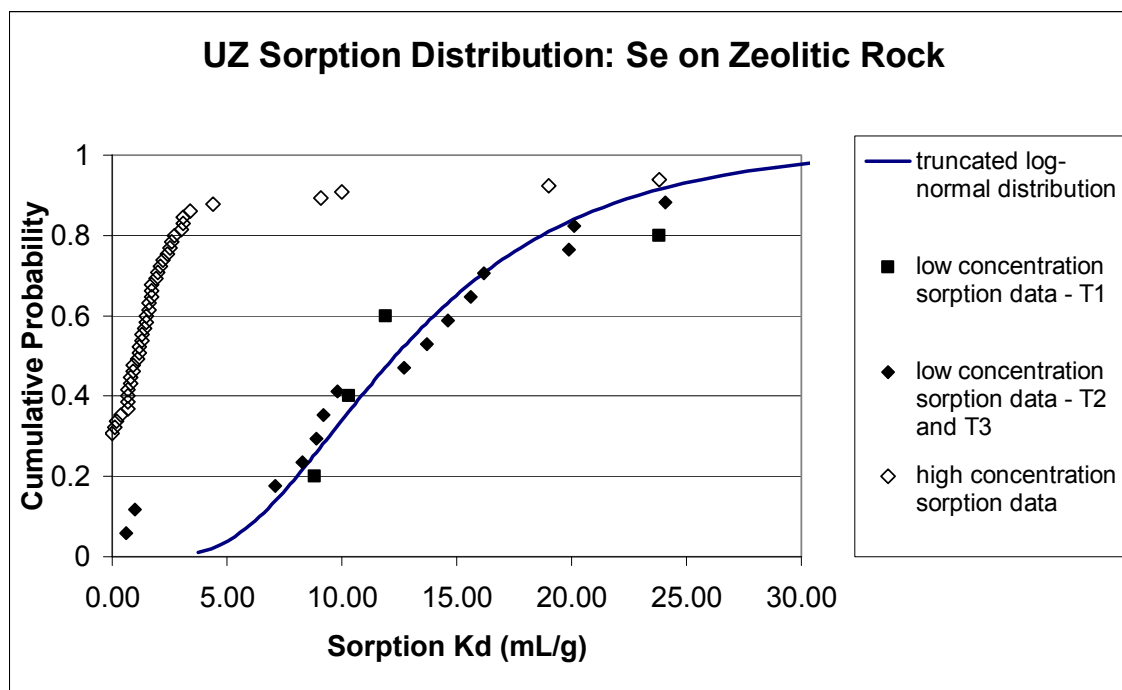
NOTE: T1 refers to data from Table 1 of SNL 2007 [DIRS 179484]; T2 and T3 refer to data from Tables 2 and 3 of SNL 2007 [DIRS 179484].

Figure A-1[a]. Cumulative Probability Distribution for Selenium Sorption on Devitrified Rock

A2.5.2[a] Zeolitic Tuff

Figure A-2[a] shows a comparison between the empirical cumulative distribution for low-concentration sorption measurements, high-concentration sorption measurements and the truncated lognormal distribution for selenium sorption on zeolitic rock. The low-concentration sorption measurements are from *Data Qualification Report for Selenium and Tin Sorption Data Obtained by Los Alamos National Laboratories 1981-1984* (SNL 2007 [DIRS 179484], Tables 1 to 3) and are limited to selenium aqueous concentrations less than 10^{-8} molar. Because of the differences in approach for determining the low-concentration K_d s, the data from Table 1 are shown separately from the data from Tables 2 and 3 in Figure A-2[a]. The high-concentration sorption measurements are from DTN: LA0010JC831341.004 [DIRS 153323] and are for aqueous selenium concentrations in excess of 10^{-6} molar. The truncated lognormal distribution was fit to the low-concentration data for use in the unsaturated zone below the TSw

where aqueous selenium concentrations are expected to remain below 10^{-8} molar. The truncated log-normal distribution has a mean of 14.3 mL/g, a standard deviation of 7.9 mL/g and a range of 1 to 35 mL/g, which provides an adequate fit to the experimental data (DTN: LA0702AM150304.001 [DIRS 182480]). The reduced effective sorption coefficients under higher-concentration conditions are seen in Figure A-2[a].



Output DTN: LB0701PAKDSESN.001.

NOTE: T1 refers to data from Table 1 of SNL 2007 [DIRS 179484]; T2 and T3 refer to data from Tables 2 and 3 of the data qualification report (SNL 2007 [DIRS 179484]).

Figure A-2[a]. Cumulative Probability Distribution for Selenium Sorption on Zeolitic Rock

A2.5.3[a] Vitric Tuff

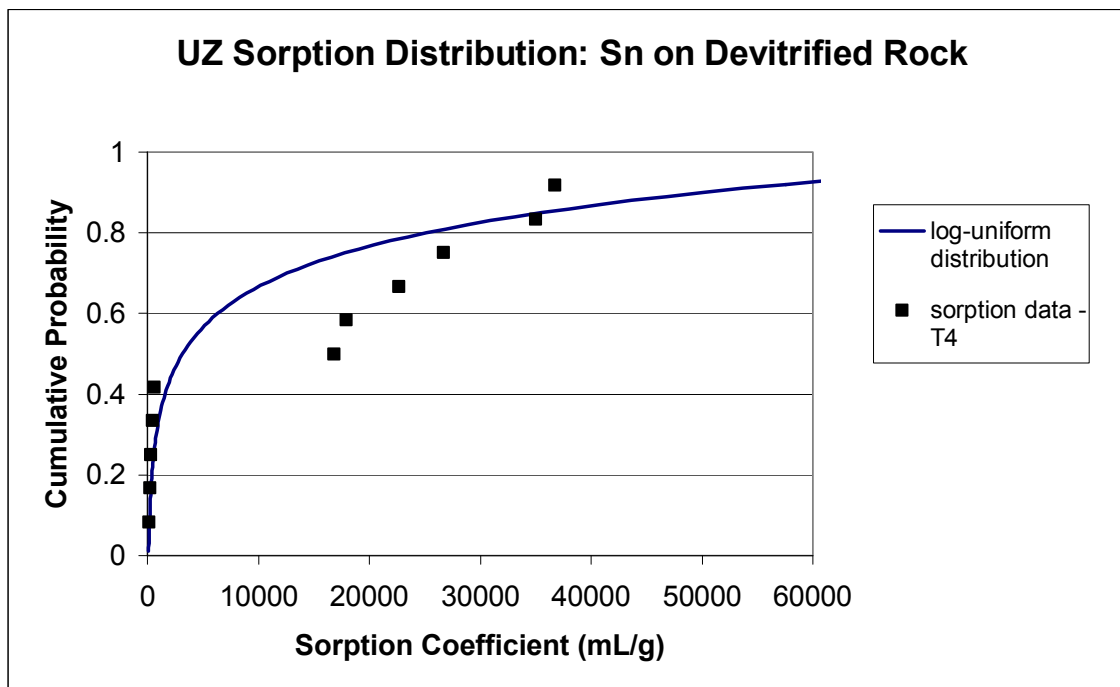
Data for selenium sorption on vitric rock are available only from DTN: LA0010JC831341.004 [DIRS 153323]. The sorption experiments reported in this DTN were carried out at higher aqueous selenium concentrations on the order of 0.1 ppm to 0.5 ppm or 10^{-6} to 5×10^{-6} molar (Triay 1994 [DIRS 179268], pp. C54 to C60; Triay 1996 [DIRS 179266], pp. H44 to H51; Triay 1995 [DIRS 179267], pp. K4 to K5). Unlike the devitrified and zeolitic rock, low-concentration sorption data are available only from Tables 2 and 3 in the data qualification report (SNL 2007 [DIRS 179484]) (see also Sections A2.5.1[a] and A2.5.2[a]). The K_d values obtained at the higher selenium concentrations shown in Figure A-3[a] are similar to values measured at higher selenium concentrations for devitrified and zeolitic rock, shown in Figures A-1[a] and A-2[a]. The higher concentrations result in lower overall values of the sorption coefficient. The parameterization for selenium sorption on vitric rock may be developed using the experimental data for higher selenium concentration sorption on vitric rock shown in Figure A-3[a] and the relationships between sorption coefficients for the higher-concentration data and lower-concentration data, as presented in Figures A-1[a] and A-2[a]. The standard deviation for

water is described in Appendix A, Section A4, of the parent report. In general, the concentration of dissolved constituents in J-13 well water tends to be lower than in unsaturated zone pore waters, as shown in Appendix A, Table A-2. However, the sorption measurements indicate that sorption of tin lies within the same range using both waters.

A2.6.1[a] Devitrified Tuff

Figure A-4[a] shows a comparison between the empirical cumulative distribution for sorption measurements and the log-uniform distribution for tin sorption on devitrified rock. The sorption measurements are from *Data Qualification Report for Selenium and Tin Sorption Data Obtained by Los Alamos National Laboratories 1981-1984* (SNL 2007 [DIRS 179484]). The log-uniform distribution was fit to the sorption data for use in the unsaturated zone. This distribution has a range of 100 to 100,000 mL/g based on the experimental data. This distribution goes to a higher upper bound than reported in DTN: LA0702AM150304.001 [DIRS 182480], Table 4 for SZ transport. This is because the SZ distribution treats the combination of devitrified and zeolitic rock as a composite volcanic rock type. The SZ transport simulations use the sorption distribution on devitrified rock as representative of the composite volcanic rock (SNL 2007 [DIRS 177392] Section A7.10.1). As shown in Section A2.6.2[a], the sorption distribution for tin on zeolitic rock is characterized by a log-uniform distribution from 100 to 5,000 mL/g.

The data fall into two distinct ranges, less than 1,000 mL/g and over 10,000 mL/g. The experiments that fall into the lower range are likely to have been affected by colloids. The final solution concentrations in the sorption experiments are quite low (3.5×10^{-14} to 4.4×10^{-12} M; SNL 2007 [DIRS 179484]); it would not take much colloidal material with adsorbed tin, accounted for as dissolved tin, to significantly reduce the resulting estimated sorption coefficients from the experiments. Four of the six experiments that fell into the higher range were conducted with p#1 water. All of the tests with sorption in the lower range were conducted using J-13 water. Colloidal materials are destabilized by calcium and magnesium ions in solution. The p#1 water is from a carbonate aquifer with higher calcium and magnesium concentrations than in J-13 water (see Table A-2), which is from a volcanic aquifer.



Output DTN: LB0701PAKDSESN.001.

NOTE: T4 refers to data from Table 4 of the data qualification report (SNL 2007 [DIRS 179484]).

Figure A-4[a]. Cumulative Probability Distribution for Tin Sorption on Devitrified Rock

A2.6.2[a] Zeolitic Tuff

Figure A-5[a] shows a comparison between the empirical cumulative distribution for sorption measurements and an estimated log-uniform distribution for tin sorption on zeolitic rock. The sorption measurements are from *Data Qualification Report for Selenium and Tin Sorption Data Obtained by Los Alamos National Laboratories 1981-1984* (SNL 2007 [DIRS 179484]). The experimental results for tin sorption on zeolitic rock are thought to be reduced because of the experimental methods used. The sorption experiments are conducted on crushed rock, and zeolitic rock tends to create more colloid-sized material. If not completely removed, the colloidal material could carry sorbed tin as a suspended material, leading to reduced values of the apparent sorption coefficient (SNL 2007 [DIRS 179484]). The sorption experiments carried out with UE-25 p#1 water show the tin sorption coefficient values at the high end of the range (SNL 2007 [DIRS 179484]), which is consistent with the interpretation that colloidal interference has occurred. See also the discussion in Section A2.6.1[a]. Therefore, the estimated log-uniform distribution was used to represent uncertainty in unsaturated zone sorption. This distribution has a range of 100 to 5,000 mL/g (DTN: LA0702AM150304.001 [DIRS 182480], Table 4). The upper range was chosen because tin is expected to sorb as readily to zeolitic tuff as to vitric and devitrified tuffs. The value of 5,000 mL/g is the same as the upper bound for sorption of tin on vitric rock and is less than the upper bound for tin sorption on devitrified rock.

APPENDIX B[a]
CORRELATIONS FOR SAMPLING OF SORPTION COEFFICIENT
PROBABILITY DISTRIBUTIONS

shown in Figure A-45 (Appendix A of the parent report) for barium sorption on zeolite indicates that solution concentration is not an important factor.

Radium sorption on devitrified and vitric rock is analogous to cesium sorption; hence the controlling factors follow the same order.

Strontium, like cesium and radium, shows significantly stronger sorption behavior on zeolitic rock than on devitrified or vitric rock. As for radium, however, this dependence on zeolite is not as strong as for cesium. Water-composition effects similar to those for radium were found for strontium when testing sorption behavior using J-13 and p#1 water. The analogy between strontium and radium for sorption on zeolite carries through all the factors.

Strontium sorption on devitrified and vitric rock is also similar to radium sorption on these rock types. Strontium sorption shows somewhat stronger dependence on water chemistry than radium. The primary difference is that strontium solution concentration effects appear only when the solution concentrations are close to the solubility limit (Triay et al. 1996 [DIRS 101014], p. III.3-4). Thus the effect of this factor is reduced, resulting in greater dependence for strontium sorption on devitrified and vitric rock on surface area and water chemistry.

Thorium sorption coefficients, as with those for protactinium, are based on a relatively small number of measurements compared with the other radioelements. Thorium is a strong sorbing radioelement on all rock types (Table 6-1[a]). Given this behavior, the dominant control on sorption behavior is expected to be surface area. Some evidence also exists for the dependence of thorium sorption behavior on water chemistry, although this dependence is not strong (Section A8.5.1, Appendix A). No correlations were found between thorium sorption behavior and pH (Triay et al. 1996 [DIRS 101014], p. III.3-4).

Uranium sorption has been found to be sensitive to a number of water chemistry factors. The dominant compositional controls are pH, carbonate, calcium, and magnesium (Triay et al. 1996 [DIRS 101014], p. III.3-68). Uranium also displays nonlinear sorption behavior, indicating sensitivity of the sorption coefficients to aqueous concentrations (Triay et al. 1996 [DIRS 101014], p. III.3-66). The effects of surface area are shown in Figures A-62 and A-66 (Appendix A of the parent report), although these tend to be smaller in the pH range of 7 to 9 that is characteristic of unsaturated-zone pore waters.

The rankings in Table 6-2 of the parent report for selenium are based on the analogy of sorption of SeO_3^{2-} with $(\text{UO}_2)(\text{CO}_3)_3^{4-}$, the expected aqueous forms (DTN: LB0702PAUZMTDF.001 [DIRS 180776]; Thomas 1987 [DIRS 101361], p. 20). The sorption behavior of these two elements has been found to be similar. Rock composition was found to have more influence on sorption of selenium as compared with uranium.

The rankings in Table 6-2 for tin are based on observations presented in *Data Qualification Report for Selenium and Tin Sorption Data Obtained by Los Alamos National Laboratories 1981-1984* (SNL 2007 [DIRS 179484]) for tin sorption on granite and volcanic tuffs, as well as pH effects on sorption. Although water chemistry was found to have some effect, the influence is deemed to be an artifact of colloid interactions (SNL 2007 [DIRS 179484]).

The rating system presented in Table B-1[a] was used to develop correlations between the sorption coefficient probability distributions for the elements of interest. Identical parameter ratings resulted in a correlation of 100%. If the two highest ratings were for the same parameters in the same order, a correlation of 75% was assigned. If the two highest ratings were for the same parameters but not in the same order, a correlation of 50% was assigned. If the three highest ratings were for the same parameters but not in the same order, a correlation of 25% was assigned. If the four highest ratings were for the same parameters but not in the same order, a correlation of 10% was assigned. If the three highest ratings were not for the same parameters, a correlation of zero percent was assigned.

Based on these rankings, correlations between selenium and tin sorption, as well as with other sorbing radioelements, were developed. The full correlation matrix contains many redundant columns and rows where the same correlations are repeated. To produce a nonsingular correlation matrix, the redundant columns and rows need to be removed by sequentially comparing the columns (e.g., comparing the first column with the second column, then the first column with the third column and so on) and eliminating any column that was a multiple of the comparison column. The corresponding row was also deleted. The correspondence between redundant columns and rows and the reduced (nonsingular) correlation matrix is provided in Output DTN: LB0701PAKDSESN.001, *UZ sorption correlation table.xls*. The final nonsingular correlation matrix is presented in Table B-2[a]. Some of the correlations differ from those presented in DTN: LA0702AM150304.001 [DIRS 182480] for the saturated zone. These differences are a result of different water compositions and radionuclide concentrations in the unsaturated and saturated zones.

Methodology for Implementing the Correlation Matrix

To implement the correlation in the total system performance assessment for the license application (TSPA-LA) model, the approach described below is used to generate the desired rank correlation among the simulated variables while maintaining their marginal distributions. For the case of normal random variables, a multivariate normal vector with the correct correlation structure can be produced using a linear combination of independent normal variables (Iman and Conover 1982 [DIRS 124158], pp. 313 to 320; Anderson 1984 [DIRS 169668], Section 2.4). In the description that follows, this linear combination is expressed as a matrix-vector multiplication.

The random vector is created using a linear combination of independent standard normal random variables. This method uses the Cholesky factorization of \mathbf{C} (Press et al. 1992 [DIRS 103316], Section 2.9), which is a lower triangular matrix, \mathbf{P} , such that $\mathbf{P}\mathbf{P}^T = \mathbf{C}$ (actually any factorization or “square root” of \mathbf{C} will do) where \mathbf{P}^T is the transpose of matrix, \mathbf{P} . The Cholesky factorization always exists whenever \mathbf{C} is positive definite (Press et al. 1992 [DIRS 103316], Section 2.9), as are all valid correlation matrices. Forming a vector of independent standard normal random variables and multiplying by the matrix, \mathbf{P} , results in a vector from a multivariate-normal distribution with mean vector zero and covariance matrix, \mathbf{C} .

Extending this method to nonnormal distributions, the marginal distributions are used in a way such that the rank correlation structure is preserved in the transform. The marginal distribution of any variable of a multivariate normal is normal (Anderson 1984 [DIRS 169668], Section 2.4).