

**SELECTION OF SORPTION-RELATED VALUES
FOR UNSATURATED ZONE AND SATURATED ZONE
TRANSPORT IN TOTAL-SYSTEM PERFORMANCE
ASSESSMENT**

Prepared for

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ABSTRACT

The Total-system Performance Assessment (TPA) code is a tool for making informed decisions about the importance of various features, events, and processes that might affect the performance of a potential high-level waste repository at Yucca Mountain, Nevada. In this report, we discuss an approach for treatment of sorption for the actinides americium, neptunium, plutonium, thorium, and uranium. A response surface function approach is proposed to relate the selection of sorption coefficients (K_d values) for these nuclides to sampled variations in geochemical parameters. New field data have been used to update the distribution ranges of pH and P_{CO_2} to make them more specific to conditions at Yucca Mountain. The representation of sorption in the TPA code for other radionuclides has been simplified, while still maintaining geological verisimilitude, by using constant K_d values that were selected as the mean or expected values from U.S. Department of Energy (DOE) sorption datasets for Yucca Mountain. This report describes the parameters relevant to sorption in the TPA code and discusses how the recommended parameter values, ranges, and distribution types were selected.

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: The original CNWRA generated data contained in this report meet quality assurance requirements described in the CNWRA Quality Assurance Manual. Data used to compile this report may be found in CNWRA Scientific Notebooks 252, 523, 556, 628, 653, and 694. Data from the U.S. Department of Energy (DOE) and Nye County sources are presented and were collected according to quality requirements for those organizations. DOE and Nye County sources should be consulted for determining the level of quality for these data.

ANALYSES AND CODES: The geochemical modeling code EQ3/6 Version 7.2b was used to calculate equilibrium chemistry and log fugacity of CO₂ for samples collected by CNWRA. This software package is controlled under CNWRA Quality Assurance Technical Operating Procedure (TOP)-018, Software Configuration Procedure. SYSTAT Version 11 (Systat, Inc., 2004), a statistical analysis software package, was used to perform some calculations, generate some figures, and fit distributions to data. The curve fitting software program TableCurve 2D Version 4.07 (AISN Software Inc., 1996) was used to fit the polynomial response surface function to effective surface area normalized distribution coefficient data. The spreadsheet software program, Microsoft™ Excel 2002, was used in calculations and to generate some figures for this report. These codes (SYSTAT, Excel, TableCurve 2D, GoldSim) are not controlled under CNWRA TOP-018, but their output is recorded and provided as part of the quality assurance record for this report or as part of the scientific notebook record.

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1 INTRODUCTION

The Total-system Performance Assessment (TPA) code (Mohanty, et al., 2002) is a tool used by staff at the U.S. Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA) for making informed decisions about the importance of various features, events, and processes that might affect the performance of a potential high-level waste repository to be sited at Yucca Mountain, Nevada. The TPA code is structured as a set of named computer routines, including an executive module (EXEC) that serves as the program driver, a module that reads the input file (READER), and a number of consequence modules that represent the behavior of various engineered barriers and natural barriers (EBSFAIL, EBSREL, UZFLOW, UZFT, SZFT), particular scenario classes (FAULTO, VOLCANO), direct release from igneous activity (ASHPLUMO, ASHRMOVO), and receptor group doses (DCAGW, DCAGS), among others (Mohanty, et al., 2002).

The TPA code is reviewed and updated as needed to incorporate additional site-specific data, changes in conceptual models, and revised uncertainties in model parameters. This report describes recommendations and potential changes to parameters relevant to sorption in the UZFT and SZFT modules of the TPA code and documents how the parameter values, ranges, and distribution types were selected. In particular, we recommend revisions to implement a more detailed approach to modeling sorption for the actinides Am, Np, Pu, Th, and U. The values and statistical distributions of other sorption-related parameters have also been adjusted.

2 CONCEPTUAL OVERVIEW

2.1 Geological Setting

Yucca Mountain is a series of large north-south trending ridges located in Nye County, Nevada, about 50 km [31 mi] east of Death Valley and about 145 km [90 mi] northwest of Las Vegas. The region surrounding and including Yucca Mountain is characterized by a thick sequence of gently dipping silica-rich volcanic rocks of Miocene age that are underlain by Precambrian and Paleozoic sedimentary rocks (CRWMS M&O, 2002). The entire stratigraphic section has been deformed by extensional basin-and-range faulting to form a series of uplifted ridges, of which Yucca Mountain is an example, separated by basins partially filled with alluvial deposits. The mountain is cut by a subparallel series of near-vertical north-trending faults.

The volcanic rocks are the most important geological units in terms of the design and performance of a potential repository because they would be the host rocks for the repository and would define the groundwater flow pathways beneath and away from the repository. The volcanic sequence at Yucca Mountain consists mainly of welded and nonwelded silica-rich tuffs. The welded tuffs are denser and more subject to fracturing than the nonwelded tuffs. The nonwelded tuffs are generally more porous than the welded tuffs, and water tends to move through the nonwelded tuffs as matrix flow. In contrast, fracture flow is more common in the welded tuffs because of the low permeability of the welded matrix.

The potential repository would be located in the unsaturated zone approximately 350 m [1,150 ft] above the top of the water table. Groundwaters in this region are typically dilute (Bechtel SAIC Company, LLC, 2004a), such that the water generally can be used for human consumption as well as for irrigation and for livestock. The saturated zone in the vicinity of

Yucca Mountain can be divided hydrogeologically into two major aquifer systems: a fractured tuff system below the repository, which extends southwards approximately 5 to 20 km [3 to 12 mi] downgradient; and an alluvial aquifer, which extends into the Amargosa Desert from the terminus of the tuff aquifer. The distance in the saturated zone to the contact between the tuff and the alluvium can be treated as a sampled parameter in performance assessments to account for uncertainties about specific groundwater flow directions and location of the contact in the subsurface. The length of the saturated alluvium flow path is important because the alluvium has a large capacity to retard many radionuclides (Bertetti, et al., 2004; Bechtel SAIC Company, LLC, 2003a).

2.2 Migration of Radionuclides

In the TPA code Version 4.0, the transport of radionuclides in groundwater is focused on a subset of 16 elements from the wasteform inventory (Mohanty, et al., 2002). Radioactive isotopes of these elements (Table 1) would be present in sufficient amounts and would be sufficiently long-lived and mobile in groundwater to be of interest in postclosure performance assessment calculations.

Transport from the repository in groundwater is conceptualized to occur first through the unsaturated zone. Over time, some radionuclides may migrate into the saturated zone. In terms of repository system performance, NRC (2004) concluded that transport distance in the saturated zone has medium risk significance to waste isolation, and retardation in the alluvium has high significance.

Mobile radionuclides will likely be transported through the repository system and geosphere mostly as dissolved ionic species. Some radionuclides also may be transported through the system via association with colloids, either as intrinsic components of the colloids or by sorption onto colloidal surfaces. Colloids are very fine particles, characteristically ranging in size from 1 nanometer to 10 micrometers (0.039 to 39 micrometers), that are suspended in water. Colloids could be derived either within the repository from the wasteform or engineered barriers or within the natural environment (Bechtel SAIC Company, LLC, 2004b). Colloidal transport, including reversible and irreversible sorption in the geosphere, may be included in future TPA code revisions.

2.3 Modeling Sorption Effects in Performance Assessment Studies

Surface interactions between dissolved constituents and solid phases can be complex, particularly in heterogeneous natural systems, and are sensitive to changes in the chemical and physical environment. Although in principle many of the interactions can be expressed thermodynamically by chemical equations, in practice, the complexity of natural systems, the relative scarcity of relevant thermodynamic data for radionuclides, and slow reaction kinetics hinder the use of detailed models in predicting sorption behavior, particularly in combination with the practical need for simplified abstractions to reduce computational burden in performance assessment studies. Instead, sorption is generally expressed in performance

Table 1. Radionuclides (Default Set) for which Transport in Groundwater is Modeled in TPA Version 4.0		
Element	Radionuclide	Half-life (yr)
Americium	Am-241	4.322×10^2
	Am-243	7.380×10^3
Carbon	C-14	5.729×10^3
Chlorine	Cl-36	3.010×10^5
Curium	Cm-245	8.499×10^3
	Cm-245	4.731×10^3
Cesium	Cs-135	2.300×10^6
Iodine	I-129	1.570×10^7
Niobium	Nb-94	2.030×10^4
Nickel	Ni-59	8.000×10^4
Neptunium	Np-237	2.140×10^6
Lead	Pb-210	2.230×10^1
Plutonium	Pu-239	2.406×10^4
	Pu-240	6.537×10^3
Radium	Ra-226	1.600×10^3
Selenium	Se-79	6.496×10^4
Technetium	Tc-99	2.130×10^5
Thorium	Th-230	7.700×10^4
Uranium	U-234	2.445×10^5
	U-238	4.468×10^9

assessment studies by using an empirically determined distribution coefficient, K_d , which can be represented by the simple expression

$$K_d = \frac{S_c}{C} \quad (1)$$

where

S_c = mass of radionuclide sorbed onto the solid phase, relative to the mass of the solid (g/g), and

C = mass of radionuclide remaining in the solution, relative to the solution volume (g/mL)

Application of the linear K_d approach in modeling assumes that the sorption process is reversible, has reached equilibrium, and is independent of variations in water chemistry or mineralogy. It may be difficult to assure that all of these assumptions are met for any given system (Chapman and McKinley, 1987). The empirical approach is limited because it does not convey how sorption may vary in response to changes in groundwater composition, pH,

temperature, properties of the solid substrate on which sorption occurs, or starting concentration of the radionuclide. In particular, the linear sorption approach assumes that there is no set of conditions that produces a maximum value for sorption and site saturation. More sophisticated surface chemistry models that can predict the effects of such changes have been developed, but the complexities of the resulting calculations, the scarcity of appropriate empirical data to calibrate the models, and few examples of model validation for heterogeneous natural settings have limited the application of these more detailed sorption models in performance assessment studies.

In recognition of the uncertainties and variability associated with the simple empirical K_d approach, performance assessment calculations typically sample K_d values from a range of values that are appropriate to sorption for the expected variation in conditions. Over the multiple realizations (typically hundreds or more) of a performance assessment analysis, the predictions cover a broad range of possible sorption outcomes to provide confidence that the uncertainty is bounded by the estimates.

The effect of sorption during movement through rocks or sediment is represented by a retardation factor, which typically is a measure of how the velocity of a contaminant is slowed compared to the velocity of unimpeded groundwater. In its simplest form, the retardation factor can be expressed as

$$R_f = \frac{\text{average groundwater velocity}}{\text{average contaminant velocity}} \quad (2)$$

If a contaminant travels at the same velocity as the groundwater (no retardation; $K_d = 0$), then R_f equals 1.0. If the migration of the contaminant is slowed by sorption, then R_f exceeds 1.0.

In porous media (e.g., in sediments or the porous matrix of a rock), the retardation factor can be calculated from the sorption coefficient and from the porosity and density of the host solid phase by the expression

$$R_f = 1 + \frac{\rho_s(1-\theta)K_d}{\theta} \quad (3)$$

where

R_f	—	retardation factor (dimensionless)
ρ_s	—	particle density of the solid phase (kg/m^3)
θ	—	porosity (dimensionless)
K_d	—	sorption distribution coefficient (m^3/kg)

In Eq. (3), the term $\rho_s(1-\theta)$ is the bulk density of the sorbing substrate (i.e., the matrix), and in unsaturated rocks, moisture content is substituted for porosity. If there is no sorption, then $K_d = 0$, and so $R_f = 1$.

Representing retardation by sorption in fractured rocks tends to be complicated by insufficient information about the properties of the fractures where most groundwater movement occurs.

The available surface area for sorption in fractures depends on the size, shape, and number of individual fractures. These properties are difficult to characterize in natural environments. Also, minerals exposed at fracture faces are likely to differ from those of the rock matrix as a whole, either because they are different minerals altogether (secondary precipitates) or because they have experienced more alteration due to prolonged interaction with water in the fractures.

3 CONCEPTUAL MODELS AND PARAMETER SELECTION

The conceptual models that describe sorption in the unsaturated zone and the saturated zone are structured to consider a number of questions, such as where in the system sorption occurs, how sorption and retardation are represented mathematically, and how uncertainties or differences in the geochemical environment would affect radionuclide transport through the unsaturated zone and through the saturated zone.

3.1 Sorption Substrates

The sorption capacity of rocks and sediments is determined largely by the particular solid phases they contain. Many of the tuffs at Yucca Mountain have abundant volcanic glass shards and pumice fragments and can be described as having vitric sorption properties. Where the volcanic glass inclusions have been altered to finely crystalline minerals such as clays, the tuffs are described as devitrified. In some tuffs, hydrothermal alteration has caused zeolite minerals to form as secondary phases in the matrix. In the TPA conceptual model, tuffs that have more than 10 percent zeolite content by weight are considered to be zeolitized (Winterle, et al., 1999). These distinctions are significant for radionuclide transport because the secondary mineral phases in devitrified and zeolitized tuffs commonly have a greater sorption capacity than the glass particles in vitric tuffs. In addition, migration of radionuclides can be affected because hydrogeological properties such as porosity and permeability typically have been modified in the altered tuffs.

In both the unsaturated zone and the saturated zone, sorption potentially can occur on three types of surfaces: (i) on solid phases in the rock or sediment matrix, (ii) along the walls of fractures in the rock, and (iii) on colloids. In the TPA conceptual model, matrix sorption is considered to be the dominant process. Sorption onto colloids is represented separately in the TPA code and is described in more detail elsewhere (Painter and Cvetkovic, 2004). Although the TPA code has the capability to model sorption in fractures, this option ordinarily is not implemented. The assumption to neglect sorption in fractures is conservative because it may result in faster travel times for certain radionuclides than would be observed in practice. However, compared to sorption in the rock matrix, the overall impact of sorption in fractures is expected to be minor (Mohanty, et al., 2002).

The U.S. Department of Energy (DOE) conceptual model for total system performance assessment makes a similar conservative assumption to neglect sorption in fractures (Bechtel SAIC Company, LLC, 2003b,c). However, in DOE models sorption is associated with fracture flow in the unsaturated and the saturated zones through matrix diffusion, a process in which radionuclides diffuse from the fractures into the rock matrix, where the radionuclides may sorb. The TPA conceptual model includes matrix diffusion in the fractured tuffs of the saturated zone, but it does not include matrix diffusion in the unsaturated zone. It is assumed that radionuclide transport through fractures in the unsaturated zone would be sufficiently rapid, compared to

matrix flow, that there would be minimal opportunity for either matrix diffusion or sorption onto fracture walls. This is a key difference between the DOE and NRC conceptual models for performance assessment.

3.2 Sorption Properties of the Hydrostratigraphic Units

In the TPA code, the unsaturated zone beneath the repository is divided into six conceptual model layers (hydrostratigraphic units) that are present between the base of the potential repository and the top of the water table (Winterle, et al., 1999). A seventh hydrostratigraphic unit representing a hypothetical fault zone is defined as an optional transport pathway for the model. In the lower parts of the stratigraphic section, the same layer of tuff may be part of the unsaturated zone in one subarea of the repository and part of the saturated zone in another due to the gently dipping structural orientation of the volcanic rocks at Yucca Mountain and variations over time in the elevation of the water table.

The six main hydrostratigraphic units in the conceptual model are taken from the actual sequence of volcanic rocks at Yucca Mountain, but characteristics and depositional sequences have been generalized and in some cases rearranged to simplify the model by giving each hydrostratigraphic unit a consistent set of hydrologic properties. The DOE conceptual model similarly represented the Yucca Mountain stratigraphy with conceptual layers but used a more finely divided set of subunits (e.g., Bechtel SAIC Company, LLC, 2004c, Table 2-1). Recommended sorption coefficients for the TPA code for many of the radionuclides in Table 1 have been selected from the DOE dataset of K_d values. In order to use the DOE sorption data, it was necessary to determine which layer sorption property—vitric, devitrified, or zeolitic—best described each generalized hydrostratigraphic unit of the TPA conceptual model. This determination was based on a comparison of the characteristics of the rock formations covered by the hydrostratigraphic unit (Winterle, et al., 1999) and the equivalent subunits in the DOE model (Bechtel SAIC Company, LLC, 2002).

The Topopah Springs-welded hydrostratigraphic unit was assigned vitric layer properties with respect to sorption. Consisting mainly of densely welded, unaltered tuffs, this unit represents the uppermost layer in the UZFT module, and it is the rock type in which the potential repository would be located. Hydrogeologically, this modeled unit would be dominated by fracture flow.

Most of the nonwelded tuffs in the unsaturated zone beneath the potential repository horizon at Yucca Mountain are part of the Calico Hills Formation. Accordingly, two separate hydrostratigraphic units of nonwelded tuffs have been defined based on an observed transition in mineralogy from a predominantly vitric set of Calico Hills tuff layers beneath the southern part of the repository to a zeolitized zone of Calico Hills tuffs beneath the northern part of the repository. This lateral and geographic difference in composition is reflected in the TPA conceptual model by allowing one of the two Calico Hills hydrostratigraphic units to be included in each of the designated subareas below the repository. The Calico Hills-nonwelded vitric hydrostratigraphic unit is porous and dominated hydrogeologically by matrix flow. As indicated by the modifier in its name, the Calico Hills-nonwelded vitric unit has been assigned vitric layer properties with respect to sorption, although it also includes some fine-grained, friable, devitrified tuff layers (Winterle, et al., 1999). The other hydrostratigraphic unit, the Calico Hills-nonwelded zeolitic unit, has lower permeability and is characterized by fracture flow. It has been assigned zeolitic layer properties with respect to sorption. Winterle, et al. (1999), noted that in terms of field relationships, several other nonwelded tuff layers are present in the

unsaturated zone below the Calico Hills Formation, but in the TPA code, all such tuff layers are grouped for simplicity into the Calico Hills-nonwelded vitric and the Calico Hills-nonwelded zeolitic.

The Prow Pass-welded hydrostratigraphic unit is composed entirely of welded tuffs. As described in Bechtel SAIC Company, LLC (2002), the Prow Pass tuffs have both zeolitic and devitrified characteristics. Sorption coefficients for the elements Cm, Ra, Cs, Ni, Pb, Se, and Nb were assigned by comparing the DOE sorption coefficient distribution ranges for zeolitic and devitrified layers. Where a difference between the ranges existed, the more conservative (lower) mean or expected K_d value was selected. The Prow Pass-welded unit is characterized by fracture flow.

For all except one of the conceptual model subareas beneath the potential repository, the remaining tuff layers above the water table are grouped together in the undifferentiated Upper Crater Flat unit (Winterle, et al., 1999). As a hydrostratigraphic unit, the Upper Crater Flat was defined by the TPA flow and transport modelers as an operational unit to allow the user to adjust the total thickness of layers between the repository and the water table for each repository subarea in the model. The rock properties of this unit are poorly defined, except that it does not include any welded tuffs. It is nominally composed of the various Upper Crater Flat nonwelded, partially welded, devitrified, or zeolitic tuffs that are found above the water table within each repository subarea. Other currently assigned geological properties of the Upper Crater Flat hydrostratigraphic unit are similar to those of a nonwelded zeolitized tuff (Winterle, et al., 1999). As a result, the Upper Crater Flat hydrostratigraphic unit has been assigned zeolitic layer properties with respect to sorption.

The Bullfrog Tuff is a welded tuff that is located below the water table in all except one of the repository subareas. In the subarea in which it occurs in the unsaturated zone, the Bullfrog-welded unit is the lowermost hydrostratigraphic unit; in all of the other subareas, it is assigned a thickness of zero. As described in Bechtel SAIC Company, LLC (2002), the stratigraphic subunits that comprise the Bullfrog Tuff have vitric, zeolitic, and devitrified characteristics. The unit as a whole, however, appears to have significant devitrified zones, so it has been assigned devitrified layer properties with respect to sorption. The hydrogeological properties, including fracture-dominated flow, are those associated with welded tuffs.

The Unsaturated Fracture Zone unit is a hypothetical hydrostratigraphic unit in the TPA conceptual model. Ordinarily not used, this seventh unit is available as a user option to simulate a conductive fault zone that extends from the repository to the water table in a specified subarea (Winterle, et al., 1999). This option would be the conservative bound in which all unsaturated zone flow and transport occurs in a fault system. In the parameter input file, the default thickness of the Unsaturated Fracture Zone unit is set to zero. If used in the model, the unit replaces all six of the other hydrostratigraphic units in a given subarea (i.e., the Unsaturated Fracture Zone unit thickness is set equal to the combined thickness of the other six units in the subarea, which in turn are assigned thicknesses of zero). There is no stratigraphic counterpart for the Unsaturated Fracture Zone unit in the DOE conceptual model and no corresponding sorption data. Vitric layer sorption properties have been assumed for this unit. Compared to the devitrified and zeolitic layers, the vitric layers tend to have lower ranges of sorption coefficients. Vitric layer properties, therefore, are typically the most conservative of the three choices.

In the saturated zone, two types of geological media are represented: saturated tuff, much of which is welded and fractured, and saturated alluvium. The saturated fractured tuffs and the saturated alluvium have devitrified layer properties due to their extensive and prolonged exposure to water.

3.3 Methods for Assigning Sorption or Retardation Coefficients (K_d or R_f)

In the unsaturated zone, matrix sorption is represented with simple bulk distribution coefficients (K_d), from which a retardation factor is calculated on the basis of additional parameters that describe physical properties of the rock. Two methods have been used to select the recommended K_d values for potential updates to the UZFT module. Both of these methods are different in some respects from the method used in TPA Version 4.0.

The most important difference is that for 5 of the 16 elements in Table 1—the actinides Am, Np, Pu, Th, and U—the sorption coefficients are determined from sorption response surfaces that correlate K_d values with variations in pH and P_{CO_2} . The sorption response surfaces were developed by applying surface complexation models over a wide range of geochemical conditions to generate a set of effective surface area normalized distribution coefficients (K_a) (Turner, et al., 2002), which are in turn converted to K_d values using the specific surface area properties of the hydrostratigraphic layers. K_a is related to K_d by the equation

$$K_d = K_a \times ESA \quad (4)$$

where

K_d — sorption coefficient
 ESA — effective surface area of a substrate

The effective surface area either is given as a measured property or it can be derived from the geometric relationship (Arthur, 1996)

$$ESA = \frac{3\theta}{\rho_b r} \quad (5)$$

where

θ — porosity (dimensionless)
 ρ_b — bulk density (kg/m³)
 r — average pore radius (m)

In a stochastic performance assessment simulation, each realization samples specific correlated values for pH and P_{CO_2} that, in turn, are used to select the appropriate K_a from the response surface lookup table. Although the approach does not explicitly incorporate geochemistry in the performance assessment transport calculations, it correlates the calculation of K_d values with two key geochemical parameters that affect sorption behavior, providing a stronger technical basis for the treatment of transport for these five significant actinides. In any particular realization of the code, the K_d values for the actinides are calculated separately, but

the calculations for all five are consistent because each value is associated with the same specified pH and P_{CO_2} parameter values.

For each of the other elements in Table 1, a constant K_d value (i.e., no distribution range) is specified for matrix sorption in each model layer in the unsaturated zone (Table A–1). It is assumed that four of the elements—I, Cl, Tc, and C—are unaffected by sorption. The transport of these elements through the unsaturated zone is represented by assigning a K_d value of zero in each case. This assumption is physically reasonable for I, Cl, and Tc, on the basis of their observed transport behavior in Yucca Mountain rocks. Carbon is subject to more ion exchange and sorption reactions than other anions, so the assumption of no sorption is conservative in this case.

For the remainder of the elements in the list—Cm, Ra, Cs, Ni, Pb, Se, and Nb—non-zero constant K_d values are supplied as input parameters for matrix sorption. Compared to the other elements, few sorption data are available for Cm and Nb. Based on the assumption that Am^{3+} is an adequate trivalent chemical analog for Cm^{3+} and Nb^{3+} , Am sorption coefficients have been substituted for these elements.

Both of the data selection approaches mark a change from TPA Version 4.0, in which the K_d parameter values were either set to zero (no sorption) or sampled from a specified distribution range of K_d values for each model layer. For future TPA code updates, the transport calculations have been simplified by the use of constant K_d values instead of sampled distributions. These simplifications are offset by the introduction of the response surface function that is used to select K_d values for Am, Np, Pu, Th, and U in each realization of a simulation. Using a constant K_d instead of a sampled distribution for the other radionuclides is a risk-informed approach that allows the use of a detailed model for key actinides while providing a simplified but geologically reasonable representation of retardation for the remaining sorbing nuclides, whose overall contribution to dose is less significant.

The selection of input parameters to model matrix sorption in the saturated zone follows the same strategy as in the unsaturated zone. Retardation factors for the actinides Am, Np, Pu, Th, and U are calculated from sorption coefficients ($K_{d,s}$) that are determined by the response surface functions on the basis of sampled pH and P_{CO_2} values (see Section 3.5.1). For the other nuclides, sorption coefficients have been selected as constant-value $K_{d,s}$ from the mean or expected values of the distribution ranges of DOE sorption coefficients for the same elements, with Am sorption coefficients used as a trivalent analog for Cm and Nb. Bechtel SAIC Company, LLC (2003b), summarizes the DOE ranges of sorption coefficients for saturated fractured tuff. Depending on the nuclide, the sorption properties for saturated alluvium in the TPA code were selected from distributions for saturated alluvium or saturated fractured tuff in various DOE reports (e.g., Bechtel SAIC Company, LLC, 2003c,d, 2001). For example, data for Ni, Se, and Pb for saturated alluvium are not presented in recent DOE reports and, therefore, have been taken from older compilations of sorption data on saturated fractured tuff with devitrified characteristics (Bechtel SAIC Company, LLC, 2001).

The SZFT module differs from the UZFT module in that K_d is not supplied directly as a parameter value. Instead, K_d values have been used outside the code to calculate specific retardation factors (R_f s) for the saturated tuff unit and the saturated alluvium unit using Eq. (3). It is the R_f value, not the K_d value, that is then supplied as a TPA code input file parameter for sorption in the SZFT module (Table A–2).

Although the TPA conceptual model conservatively assumes no radionuclide sorption in fractures, parameters are included to allow a user to include this process if desired. Sorption in fractures for the actinides Am, Np, Pu, Th, and U is represented by the response surface function method and is activated by input file switches UZFractureForceFactorForKdtoRd and SZFractureForceFactorForKdtoRd for the unsaturated zone and the saturated zone, respectively. These switches are ordinarily set to zero (no sorption). Separate retardation factors for the remainder of the nuclides are specified for sorption in fractures of the unsaturated zone and saturated zone. All of these retardation factors are ordinarily set to values of 1.0 (no sorption) in the input file.

3.4 Other Physical Properties Relevant to Sorption

As indicated by Eq. (3), particle density and porosity values are needed, in addition to K_d values, to calculate the retardation factor R_f for each hydrostratigraphic unit in the unsaturated zone. (For the saturated zone, retardation factors are given as input parameters in the TPA code, but density and porosity values still are needed external to the code to calculate the supplied R_f values.) Recommended particle density and porosity values are shown in Table A–1 of Appendix A as the TPA input parameters MatrixGrainDensity_layer and MatrixPorosity_layer, where the suffix “_layer” in each parameter name stands for the three- or four-letter abbreviation of each hydrostratigraphic unit as listed in Table 2. In the saturated zone, the equivalent density and porosity parameters are termed ImmobileGrainDensity_STFF and ImmobilePorosity_STFF for the saturated tuff and AlluviumMatrixGrainDensity_SAV and AlluviumTotalPorosity_SAV for the saturated alluvium (Table A–2, Appendix A).

For the actinides Am, Np, Pu, Th, and U, Eq. (4) is used to calculate K_d values from the K_a values generated by the response surface function approach for each actinide (Bertetti, et al., 2004). The other rock property that must be known to use Eq. (4) is the effective surface area. For consolidated rock layers, such as the Yucca Mountain tuffs, the effective surface area can be derived from Eq. (5), by using the particle density and porosity parameters to calculate bulk density as indicated in Eq. (3). The third parameter needed in Eq. (5), the average pore radius, is defined as the term MatrixPoreRadius_layer for the unsaturated zone hydrostratigraphic units and as ImmobilePoreRadius_STFF for the saturated tuff.

Although Eq. (5) produces reasonable estimates of effective specific surface areas for consolidated rocks, based on comparisons to DOE-measured surface areas (Triay, et al., 1996), the approach is not generally applicable to unconsolidated material such as the saturated alluvium. The specific surface area value for alluvium would be supplied directly to the TPA code as an input parameter, AlluviumMatrixSpecificSurfaceArea, that has a sampled distribution range based on field measurements of alluvium samples (Bertetti, et al., 2004).

Each of these physical parameters has been assigned an individual constant value for the recommended TPA code input file (Tables A–1 and A–2). For the MatrixPoreRadius_layer parameters, a constant value of 5.0×10^{-8} m [2.0×10^{-6} in] has been assigned for each of the tuff units. This pore radius value is consistent with the median value used by DOE, based on moisture retention curves from work by Travis and Nuttall (1987). Bechtel SAIC Company, LLC (2003e), indicates a more complex distribution of pore sizes depending on the rock unit, but the assigned value of 5.0×10^{-8} m [2.0×10^{-6} in] is conservative with respect to surface area uncertainties. Similarly, the individual values for MatrixGrainDensity_layer and MatrixPorosity_layer for the tuffs are estimated from averaged data for stratigraphically

Table 2. Sorption Layer Properties for TPA Hydrostratigraphic Units		
Abbreviation	Name	Sorption Layer Property
TSw	Topopah Spring welded tuff	Based on a review of stratigraphy* the units that make up the Topopah Spring welded tuff in the unsaturated zone are mostly vitric.
CHnv	Calico Hills nonwelded vitric tuff	Based on a review of stratigraphy* the Calico Hills-nonwelded vitric tuff has vitric layer properties with respect to sorption.
CHnz	Calico Hills nonwelded zeolitic tuff	Based on a review of stratigraphy* the Calico Hills-nonwelded zeolitic has zeolitic characteristics for sorption.
PPw	Prow Pass welded tuff	Based on review of stratigraphy* the Prow Pass tuffs have both zeolitic and devitrified characteristics. Zeolitic layer properties are assumed for this unit because they tend to be more conservative than devitrified layer properties.
UCF	Upper Crater Flat tuff	In the TPA model, Upper Crater Flat tuff represents all the non-to-partially welded, devitrified, and zeolitized Crater Flat tuff layers above the water table in each repository subarea†. Zeolitic layer properties are assumed for this unit because they generally are more conservative than devitrified layer properties.
BFw	Bullfrog welded tuff	Based on a review of stratigraphy* the subunits that comprise the Bullfrog welded tuff have vitric, zeolitic and devitrified characteristics. The unit as a whole, however, appears to have significant devitrified zones, so it is assumed to have devitrified sorption layer properties.
UFZ	Unsaturated Fracture Zone	Unsaturated Fracture Zone is a hypothetical unit used in TPA to represent a fault zone. Vitric sorption properties are assumed for this layer/region because DOE vitric K_d values are typically the most conservative.
<p>*Bechtel SAIC Company, LLC, 2002. "Mineralogic Model (MM3.0) Analysis Model Report." MDL-NBS-GS-000003. Rev. 00 ICN 02. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2002. †Winterle, J.R., R.W. Fedors, D.L. Hughson, and S. Stothoff. "Update of Hydrologic Parameters for the Total-system Performance Assessment Code." San Antonio, Texas: CNWRA. 1999.</p>		

equivalent subunits as reported by Flint (1998). The corresponding parameter values for saturated alluvium, AlluviumMatrixSpecificSurfaceArea, AlluviumMatrixGrainDensity_SAV and AlluviumTotalPorosity_SAV, are estimated from field measurements at Fortymile Wash and from published DOE averages (Bechtel SAIC Company, LLC, 2003c). See Table A–2 for additional information about the sources of data and rationale for selection of specific values.

Sorption in fractures ordinarily is neglected in the TPA code, but it can be implemented optionally for Am, Np, Pu, Th, and U. In that case, the retardation factor is calculated from the relationship

$$R_f = 1 + \frac{2 K_a}{b} \quad (6)$$

where

- R_f — retardation factor (unitless)
- K_a — modified sorption coefficient, normalized to surface area (mL/m²)
- b — fracture aperture width (m)

The value of K_a is obtained from the relevant response surface function for each actinide. The fracture aperture width parameter, which is termed FractureAperture_layer in the TPA code, specifies the size of the opening, or gap, between the fracture faces of an open fracture. During transport of a sorbing radionuclide in a fracture, the extent of retardation is influenced by the ratio of the exposed fracture surface area relative to the void-space (volume) of the opening (aperture) through which the solute is being transported. The retardation of the solute would be greater in a small-aperture fracture than in a large-aperture fracture. The FractureAperture_layer parameter has been assigned the same constant value $\{(1.0 \times 10^{-4} \text{ m}) [4.0 \times 10^{-3} \text{ in}]\}$ for each of the hydrostratigraphic units and for the saturated tuff. This estimate originally was based on early DOE site characterization data for Yucca Mountain. Subsequent field data obtained by DOE are similar to the original estimated value (Table 3).

3.5 Geochemical Properties Relevant to Sorption

The sorption of many contaminants, including radionuclides, is particularly sensitive to variations in pH. For actinides, sensitivity to pH values in terms of sorption is related to their typically complicated hydrolysis behavior. The concentration of carbonate species in groundwater also has a pronounced effect on complexation and sorption of actinides, particularly at pH values above about 7 (Bertetti, et al., 1998; Pabalan and Turner, 1997; Davis, 2001).

For TPA Version 4.0 (Mohanty, et al., 2002), the selection of sorption modeling parameters was informed by a regional compilation of groundwater chemistry analyses for southwestern Nevada (Perfect, et al., 1995) and by a screened subset of the Perfect, et al. (1995), data set that focused on a smaller region in the vicinity of Yucca Mountain (Turner and Pabalan, 1999).

For TPA updates, the sorption coefficients for five significant actinides—Am, Np, Pu, Th, U—would be determined in each simulation from a response surface function that correlates effective surface area normalized distribution coefficients with sampled ranges of groundwater

Table 3. Mean Fracture Aperture Widths for the U.S. Department of Energy Unsaturated Zone Flow Model Layers at and below the Potential Repository Horizon*							
Stratigraphic Unit	Unsaturated Zone Flow Model Layer	Mean Permeability k_f (m ²)	Mean Permeability k_f (ft ²)	Mean Fracture Frequency f (1/m)	Mean Fracture Frequency f (1/m)	Mean Fracture Aperture* b (m)	Mean Fracture Aperture* b (in)
Topopah Spring	tsw31	8.1×10^{-13}	8.7×10^{-12}	2.17	0.66	0.0002	0.006
	tsw32	7.1×10^{-13}	7.6×10^{-12}	1.12	0.34	0.0002	0.008
	tsw33†	7.8×10^{-13}	8.4×10^{-12}	0.81	0.25	0.0002	0.009
	tsw34†	3.3×10^{-13}	3.6×10^{-12}	4.32	1.32	0.0001	0.004
	tsw35†	9.1×10^{-13}	9.8×10^{-12}	3.16	0.96	0.0002	0.006
	tsw36†	1.3×10^{-12}	9.8×10^{-12}	4.02	1.23	0.0002	0.006
	tsw37	1.3×10^{-12}	1.4×10^{-11}	4.02	1.23	0.0002	0.006
	tsw38	8.1×10^{-13}	8.7×10^{-12}	4.36	1.33	0.0001	0.005
	tsw39	8.1×10^{-13}	8.7×10^{-12}	0.96	0.29	0.0002	0.009
Calico Hills	ch1Ze	2.5×10^{-14}	2.7×10^{-13}	0.04	0.01	0.0002	0.008
	ch1VI	2.2×10^{-13}	2.4×10^{-12}	0.10	0.03	0.0003	0.012
	ch[23456]VI	2.2×10^{-13}	2.4×10^{-12}	0.14	0.04	0.0003	0.010
	ch[2345]Ze	2.5×10^{-13}	2.7×10^{-12}	0.14	0.04	0.0003	0.011
	ch6	2.5×10^{-14}	2.7×10^{-13}	0.04	0.01	0.0002	0.008
Prow Pass	pp4	2.5×10^{-14}	2.7×10^{-13}	0.14	0.04	0.0001	0.005
	pp3	2.2×10^{-13}	2.4×10^{-12}	0.20	0.06	0.0002	0.009
	pp2	2.2×10^{-13}	2.4×10^{-12}	0.20	0.06	0.0002	0.009
	pp1	2.5×10^{-14}	2.7×10^{-13}	0.14	0.04	0.0001	0.005
Bullfrog	bf3	2.2×10^{-13}	2.4×10^{-12}	0.20	0.06	0.0002	0.009
	bf2	2.5×10^{-14}	2.7×10^{-13}	0.14	0.04	0.0001	0.005
	tr3	2.2×10^{-13}	2.4×10^{-12}	0.20	0.06	0.0002	0.009
	tr2	2.5×10^{-14}	2.7×10^{-13}	0.14	0.04	0.0001	0.005

*Calculated from Eq. (7), Section 6.1.2 and the geometric means of field data presented in Table 7 (Bechtel SAIC Company, LLC). "Analysis of Hydrologic Properties Data." MDL-NBS-HS-000014. Rev. 00. Las Vegas, Nevada: Bechtel SAIC Company, LLC. p. 40. April 2003.
†Unit intersected by the repository horizon (TBD No. 2, Fig. 2-3).

pH and carbonate concentrations. The usefulness of this approach has been strengthened by updating the distribution ranges of these important geochemical parameters to make them more site-specific by including new groundwater analyses from wells in the saturated alluvium of Fortymile Wash south of Yucca Mountain (Bertetti, et al., 2004) and by screening the data set of Turner and Pabalan (1999) to eliminate wells outside the boundaries of the DOE site-scale flow and transport model (Bechtel SAIC Company, LLC, 2003f).

3.5.1 Distributions for pH and P_{CO_2}

Recently published results and analyses of groundwater chemistries sampled as part of the DOE site characterization activities (Bechtel SAIC Company, LLC, 2004a), supplemented with groundwater chemistry data collected from the Nye County Early Warning Drilling Program wells (Bertetti, et al., 2004), provide a representative data set for updated groundwater chemistry parameters (Bertetti, et al., 2004). However, even with this data set, selection of appropriate ranges and distribution types from which to sample pH and P_{CO_2} for use in calculating retardation factors for the five actinides mentioned previously is not a simple task. The ranges must be consistent with observations of pH and P_{CO_2} in groundwater from the Yucca Mountain vicinity and must be broad enough to account for uncertainties in field measurements while narrow enough to prevent undue risk dilution effects. The distribution types should be representative of collected data and also be reflective of populations observed in nature. The recommended approach samples only one set of chemistry values per realization for the unsaturated zone and the saturated zone, so the ranges and distributions must be representative of both.

To develop the pH and P_{CO_2} distributions, a multi-step process was used. First, available data were plotted, culled, and statistically analyzed to provide a basic understanding of the ranges and trends in the data. Second, several potential distribution types were fitted to an appropriate data subset, representative of groundwaters in the Yucca Mountain vicinity, in an effort to determine the most applicable distribution type for pH and P_{CO_2} . Finally, the selected distribution types were customized by creating user-specified piecewise distributions that represented the slightly skewed and truncated characteristics of the observed data sets.

Geochemical data (pH and P_{CO_2}) from the Yucca Mountain region provided in Bechtel SAIC Company, LLC (2004a), and Bertetti, et al. (2004), are plotted in Figure 1. Of the more than 200 data values represented in this figure, only 107 are from groundwater sampling points located within the site-scale model boundary used by DOE (Bechtel SAIC Company, LLC, 2003f). Data from wells within the site-scale model boundary are plotted separately in Figure 2. The site-scale model boundary is large enough to encompass all plausible groundwater flow paths from the repository to the accessible environment, and the number and location of sampling points within the site-scale boundary appear to provide sufficient data to adequately represent groundwater chemistry relevant to the performance of the potential repository. Moreover, as noted in Bertetti, et al. (2004), the range and median values of pH and P_{CO_2} for groundwater samples from the regional data set (Bechtel SAIC Company, LLC, 2004a), as well as from older regional data compilations (Turner and Pabalan, 1999), are quite similar to those of the site-scale data set. Summary statistics for the site-scale pH and P_{CO_2} data are shown in Table 4.

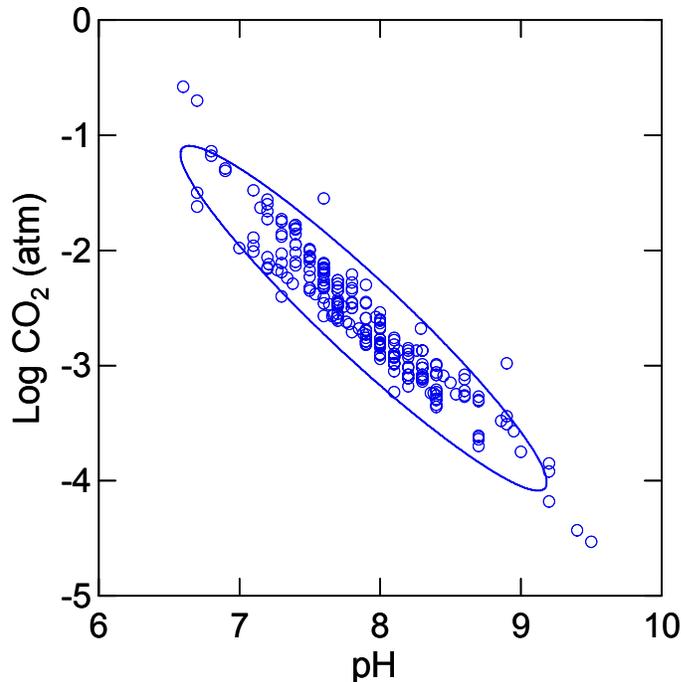


Figure 1. Plot of Water Chemistry Data for Groundwater Samples from the Yucca Mountain Region. The Blue Line Represents the 95-Percent Confidence Ellipse for the Samples. The pH and CO₂ Data Have a Correlation Factor of About -0.95 (Bechtel SAIC Company, LLC, 2004a; Bertetti, et al., 2004).

Analysis of Figure 2 indicates that the pH and P_{CO_2} data are highly correlated (correlation factor of -0.95). The correlated nature of pH and P_{CO_2} data is maintained in the recommended modeling approach for the TPA code. A 95-percent confidence ellipse, calculated assuming the pH and P_{CO_2} data are normally distributed, is also shown in Figure 2. The confidence ellipse provides a convenient graphical means to identify the more extreme data values for further discussion. Note that in Figure 2 only three data points fall outside the 95-percent confidence ellipse. The two points outside the 95-percent confidence ellipse with low pH and high P_{CO_2} concentrations represent samples collected from Wells UE25-p#1 and NC-EWDP-1DX (Bechtel SAIC Company, LLC, 2004a). The UE25-p#1 sample was taken from a zone completed in carbonate-rich rocks of the deep Paleozoic aquifer underlying the Yucca Mountain region, and the sample from NC-EWDP-1DX was taken from a deep zone that also is believed to represent water from the Paleozoic aquifer. Although hydrologic studies of the Yucca Mountain saturated zone (Bechtel SAIC Company, LLC, 2003c) indicate that potential flow paths emanating from Yucca Mountain would not enter the deep Paleozoic aquifer, these two sample points were retained in subsequent statistical analyses to represent the possible geochemical mixing influence of carbonate-rich rocks in the Yucca Mountain saturated zone. This is consistent with bounding assumptions used by Triay, et al. (1996) to establish some of the DOE K_d distributions. The third point outside the 95-percent confidence ellipse in Figure 2 has high pH and low P_{CO_2} relative to all other data from the site-scale subset. This sample point represents Well NC-EWDP-4PB (Bechtel SAIC Company, LLC, 2004a), and as discussed in Bertetti, et al. (2004), very likely represents water contaminated by cementitious grout materials during well construction and completion.

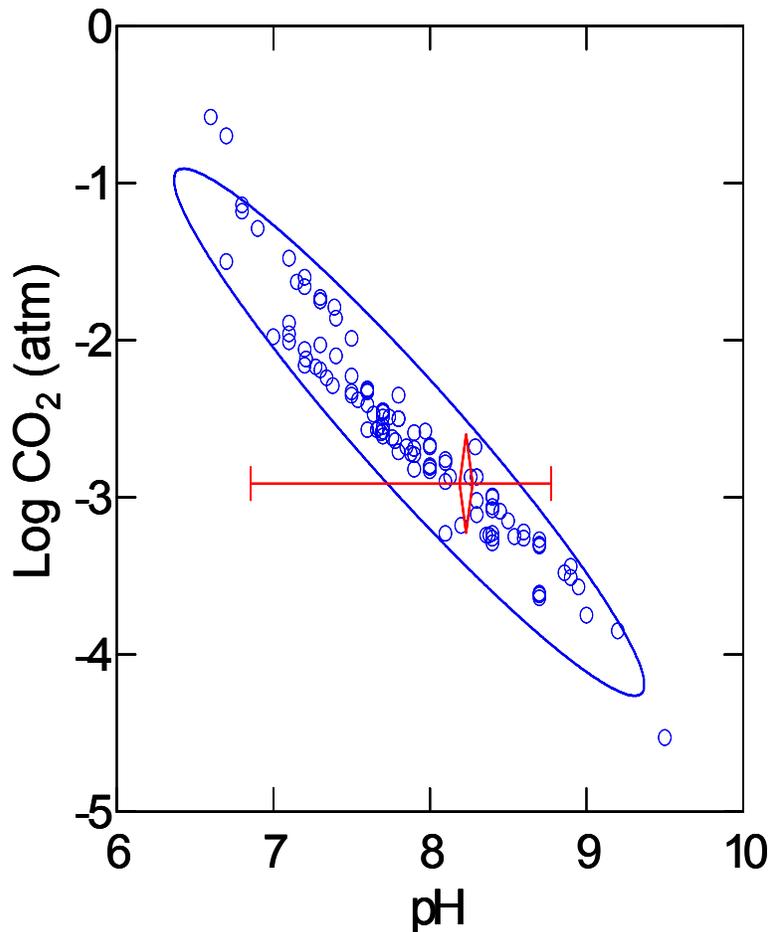


Figure 2. Plot of Water Chemistry Data from Wells Located Within the Site-Scale Model Area (Bechtel SAIC Company, LLC, 2003a) in the Yucca Mountain Vicinity. The 95% Confidence Ellipse (Blue Line) is Shown for the pH and CO₂ Data. The Red Bar Approximately Indicates the Range of pH Values from an Analysis of Unsaturated Zone Waters (103 Samples) from Yucca Mountain (Browning and Murphy, 2002) While the Red Diamond Approximately Indicates the Median pH Value from the Same Study.

Because the contaminated sample is not representative of naturally occurring Yucca Mountain groundwater, data from NC-EWDP-4PB were excluded from subsequent statistical analyses to determine the range and distribution type for geochemical parameters.

The statistical software package SYSTAT Version 11 was used to fit the site-scale pH and P_{CO_2} data to a number of candidate distribution types. Goodness-of-fit parameters, such as the Chi-square test and the Kolmogorov-Smirnov test, were used along with visual inspection of the fitted distributions, and data histograms were used to evaluate the quality of the fits. Beta and lognormal distributions did not adequately represent the data. Triangular distributions best fit the data, although normal distributions also had excellent fit statistics and provided a

Table 4. Summary Statistics for Yucca Mountain Groundwater Data Collected from within the Site-Scale Model Boundary of DOE*†. Statistics for the Site-Scale Subset with and without Data from Well NC–EWDP–4PB Are Shown for Comparison. Recommended Updated pH and CO₂ Distributions are Based on the Data Set without Well NC–EWDP–4PB.

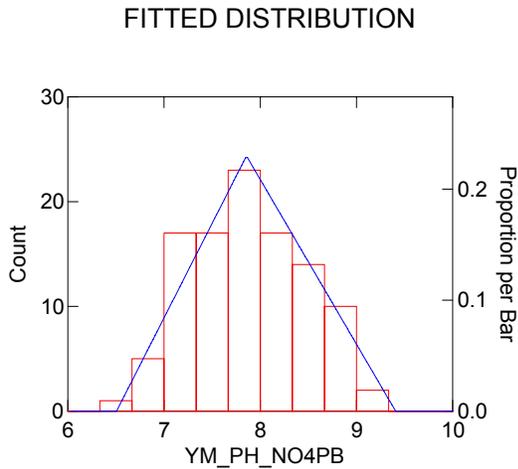
	Site-Scale pH	Site-Scale CO ₂ (log atm)	Site-Scale pH no 4PB	Site-Scale CO ₂ (log atm) no 4PB
Number of cases	107	107	106	106
Minimum	6.60	-4.53	6.60	-3.85
Maximum	9.50	-0.58	9.20	-0.58
Range	2.90	3.95	2.60	3.27
Mean	7.868	-2.585	7.852	-2.567
Standard deviation	0.602	0.672	0.584	0.648
Skewness	0.199	0.331	0.089	0.549
Pearson correlation	-0.958		-0.955	

*Bechtel SAIC Company, LLC. "Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing, and Recharge at Yucca Mountain, Nevada." NAL†NBS†HS†000021. Rev. 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2004.
†———. "Bechtel SAIC Company, LLC. "SZ Flow and Transport Model Abstraction." MDL–NBS–HS–000021. Rev. 00. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003.

reasonable match of predicted versus observed data over the entire range of pH and P_{CO2}. This is illustrated by Figure 3, which is a comparison of normal and triangular fitted distributions for the site-scale pH data.

Triangular distributions typically are not observed in natural systems, but normally distributed data are common. Part of the purpose of the TPA code is to provide an accurate representation of system characteristics (e.g., pH and P_{CO2} values) while maintaining a reasonable theoretical and mechanistic basis for those characteristics. This purpose appeared to be best achieved by the use of the normal distributions, so they were selected to specify pH and P_{CO2} parameter values.

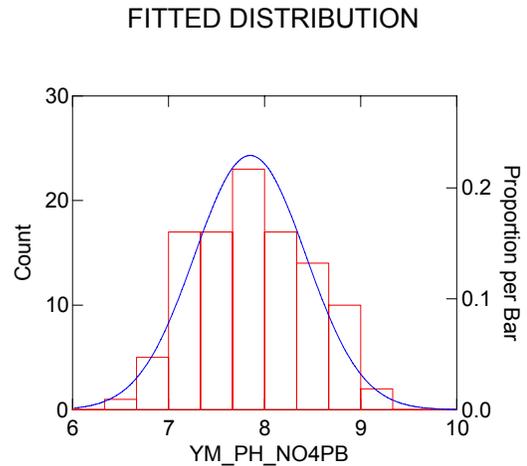
Because the pH and P_{CO2} data are slightly skewed, applying non-truncated normal distributions would produce a small set of sampled values from the tails of both the pH and P_{CO2} distributions that fall outside the observed range of data (e.g., Figure 3). The use of truncated normal distributions would provide an adequate solution to this problem, but the TPA code sampling routine does not support truncated normal distributions. However, the TPA code does allow for sampling from a user-specified piecewise distribution. Using an Excel spreadsheet,



Variable Name: YM_PH_NO4PB
 Distribution: Triangular
 Specified: Low (a)=6.500000 High
 (b) = 9.400000 Mode (c) = 7.850000
 Test Results:

LimitL	LimitU	Observed	Expected
.	7.120	11.0	10.408
7.120	7.380	13.0	10.559
7.380	7.640	14.0	14.220
7.640	7.900	20.0	17.754
7.900	8.160	15.0	16.800
8.160	8.420	16.0	13.611
8.420	8.680	5.0	10.423
8.680	.	12.0	12.225
		106.0	106.0

Chi-square test statistic = 4.323096 df = 7
 p-value = 0.74190
 Kolmogorov-Smirnov test statistic = 0.096629
 p-value(2-tail) = 0.27555



Variable Name: YM_PH_NO4PB
 Distribution: Normal
 Specified: Location or mean (mu) = 7.850000
 Scale or SD (sigma) = 0.580000
 Test Results:

LimitL	LimitU	Observed	Expected
.	7.120	11.0	11.033
7.120	7.380	13.0	11.107
7.380	7.640	14.0	15.877
7.640	7.900	20.0	18.624
7.900	8.160	15.0	17.930
8.160	8.420	16.0	14.166
8.420	8.680	5.0	9.185
8.680	.	12.0	8.078
		106.0	106.0

Chi-square test statistic = 5.173008 df = 7
 p-value = 0.638859
 Kolmogorov-Smirnov test statistic = 0.068413
 p-value(2-tail) = 0.703972
 Shapiro-Wilk test statistic for normality = 0.985801
 p-value = 0.321952

Figure 3. Comparison of Triangular (Left) and Normal (Right) Fitted Distributions to pH Values for the Site-Scale Data Set (Without Data for Well NC-EWDP-4PB). SYSTAT Version 11 Was Used to Fit the Data and Fit Statistics Are Provided Below Each Graph. In the Tables, Observed Indicates Number Of Data Points from the Site-Scale Data Set Contained Within the Specified Interval, While Expected Indicates the Number of Data Points Occurring in the Same Interval as Predicted by the Fit. Although Both Distribution Types Adequately Represent the Data, the Normal Distribution (as Modified, See Text) Was Selected for Use in Potential TPA Code Updates.

user-specified piecewise distributions were generated for pH and P_{CO_2} using the mean and standard deviation parameters from the fitted normal distributions (see Appendix B). The distributions were truncated at maximum and minimum values that provided coverage of the full range of pH or P_{CO_2} data and prevented sampling of values outside the observed data ranges. The user-specified distributions are listed in Appendix B as the parameters pH_AllUZ_SZLayers and LogCO2PartialPressure_AllUZ_SZLayers.

3.5.2 Response Surface Functions

The response surface functions used to correlate distribution coefficients with sampled groundwater chemistries are based on an application of surface complexation model predictions of sorption for each of the five actinides over a range of pH values and P_{CO_2} concentrations (Turner, et al., 2002). The surface complexation model predictions are based on analyses of data derived from sorption experiments conducted using minerals and solutions relevant to conditions at Yucca Mountain (e.g., Pabalan, et al., 1998; Bertetti, et al., 1998, Turner, et al., 1998). Detailed descriptions of the methods and philosophy used to develop the surface complexation model predictions can be found in Turner, et al. (2002); Turner (1995); and Turner and Pabalan (1999).

The surface complexation model predictions are represented by a fifth-order polynomial fit (response surface function) to the logarithm (base 10) of the K_a values (the surface complexation model output) calculated for each nuclide at a discrete concentration of P_{CO_2} and over a range of pH values. Fitting the response surface function to multiple P_{CO_2} concentrations over a range of pH values produces a series of curves that, together, represent the sorption response surface for a particular radionuclide. An example of a sorption response surface for Np is shown in Figure 4. During each realization in the recommended approach, the coefficients of the polynomial response surface functions and sampled values of pH and P_{CO_2} to calculate a K_a value for each of the five actinides. The coefficients for the response surface functions, along with the range of pH values appropriate for each fitted curve (at a particular P_{CO_2} concentration), are stored in an auxiliary data file.

In practice, at a given P_{CO_2} , the response surface polynomial is

$$y = a + bx + cx^2 + dx^3 + ex^4 + fx^5 \quad (7)$$

where x represents the pH value, $a-f$ are the coefficients, and y is the calculated K_a value, fit to surface complexation model predictions using the curve-fitting software package TableCurve 2D Version 4.07. Fits were optimized by limiting the range of pH over which the response surface function was applied. The limited pH ranges were selected to be consistent with observed values of pH for given P_{CO_2} concentrations in groundwaters from the saturated zone in the Yucca Mountain vicinity (Figure 2) and to minimize the residuals between the curve fit and the surface complexation model output. An example fit of surface complexation model K_a values for Np at a P_{CO_2} concentration of $10^{-1.5}$ atm is shown in Figure 5. In this case, although the surface complexation model includes predictions over a range of pH from 5 to 10, pH values for the fit are limited to the range 5.5 to 8.25, consistent with the minimum pH value observed in the field and the range of pH observed for a P_{CO_2} concentration of $10^{-1.5}$ atm (Figure 2). A complete listing of the response surface function coefficients is provided in Appendix C.

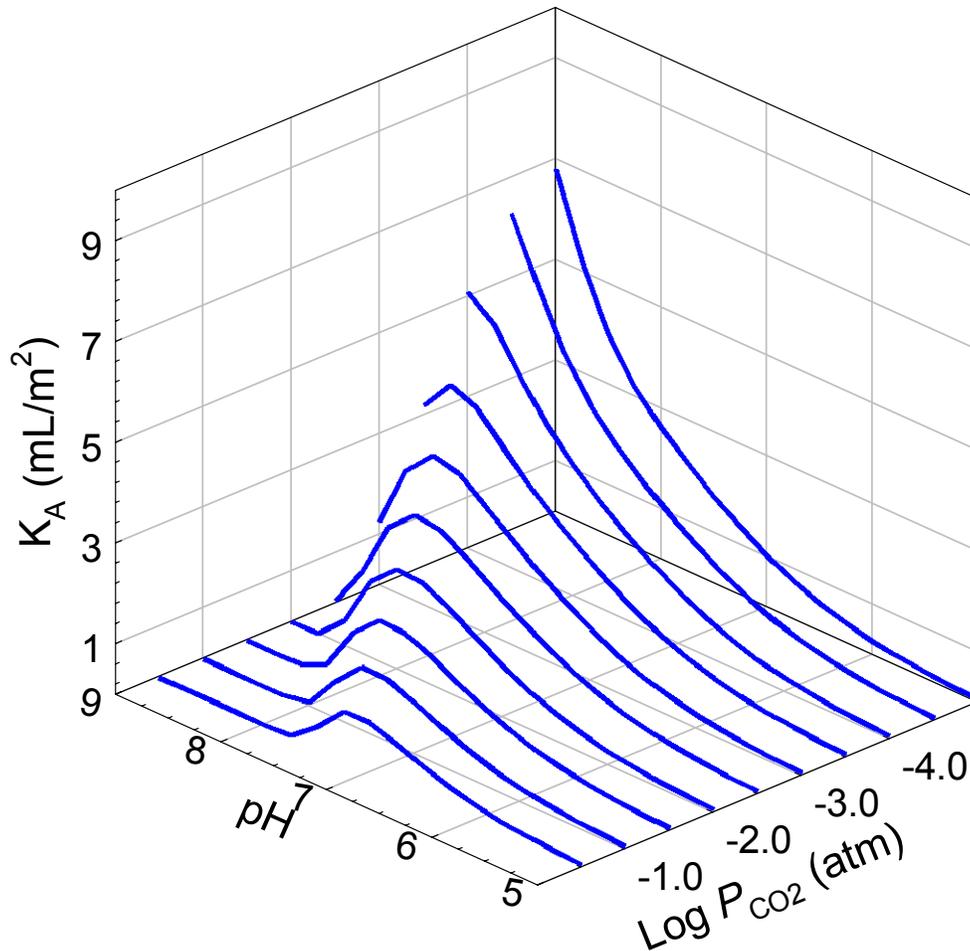


Figure 4. Sorption Response Surface for Neptunium Plotted in Terms of Effective Surface Area Normalized Distribution Coefficient (K_a) At Discrete Values of CO_2 Concentrations and Over a Range of pH Values.

To implement the response surface model in the TPA code, one would sample pH and P_{CO_2} values from continuous distribution functions (the user-specified truncated normal distributions discussed previously). When a sampled P_{CO_2} concentration for a given realization falls between the discrete values listed in the auxiliary data file, the code would calculate an appropriate K_a value through a linear interpolation of the coefficients from the next highest and next lowest P_{CO_2} values found in the auxiliary data file. Should the sampled pH fall outside the applicable range of pH for a response surface function for the sampled P_{CO_2} concentration, or if the sampled P_{CO_2}

Fit of Np Sorption at $\text{Log } P_{\text{CO}_2} = -1.5$ (atm)

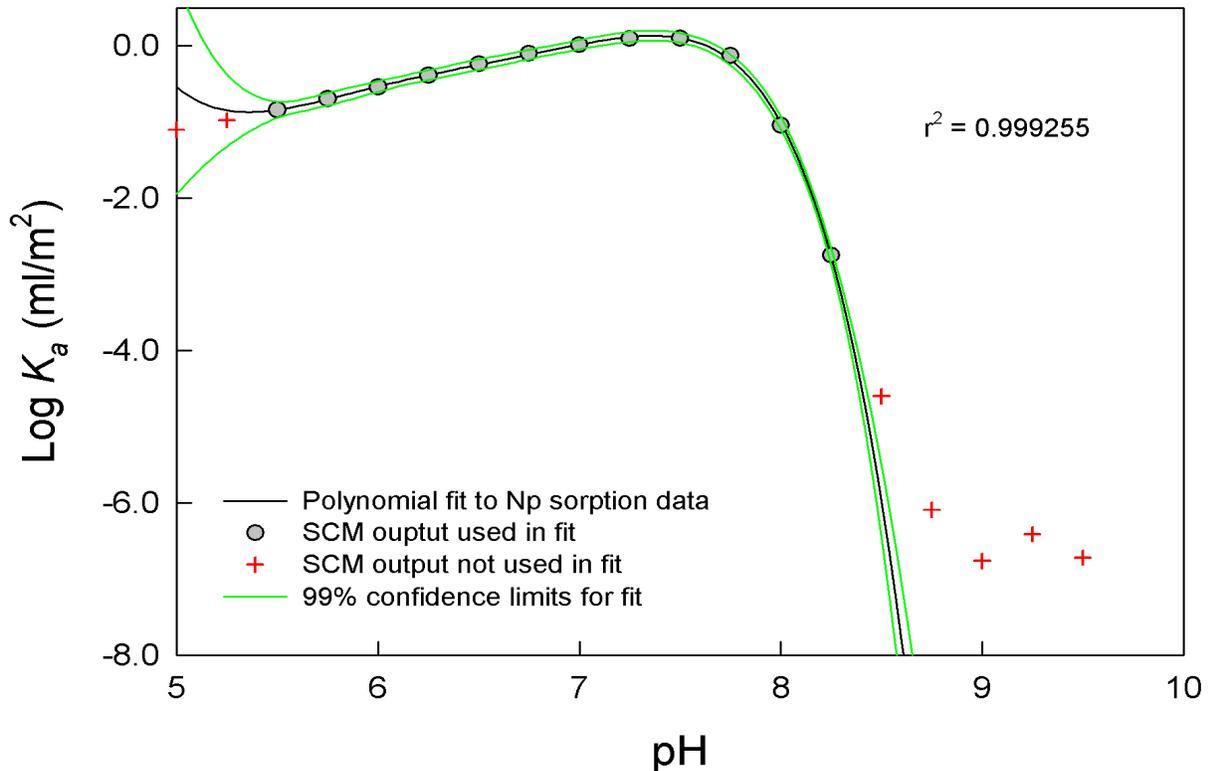


Figure 5. Example Curve-Fit (Black Line) of Neptunium (Np) Sorption Data (Gray Circles) Using the Polynomial Response Surface Function (See Text). Ninety-Nine Percent Confidence Limits for the Fit Are Shown by the Green Lines. Coefficients Derived from This Fit Are Incorporated Into the *coefkdeq.dat* File and Used to Calculate K_a Values from TPA-Sampled pH and CO_2 Concentrations. As Exemplified in This Plot, the Fits Were Optimized to Focus On a pH Region Appropriate for the CO_2 Concentration (See Figure 2), So Some Surface Complexation Model Data (Red Crosshairs) Were Eliminated from the Fit. In This Case, the Resulting Applicable pH Range is Limited from 6.0 to 8.25 Within *coefkdeq.dat*. Note That $\text{Log } K_a$ Values Below About -2.0 Would Produce Retardation Factors Near 1.0 (No Retardation).

is outside the represented range of P_{CO_2} values, then a K_a value of zero (corresponding to a K_d value of 0 and an R_f of 1, no retardation) would be produced.

There is less of a direct connection between the groundwater chemistry and the selection of sorption coefficients and retardation factors for the other nuclides, given that constants are used for the parameter values in each case and, therefore, are not affected by the sampled differences in pH and P_{CO_2} . However, the mean or expected value was selected from the DOE range of distribution coefficients, which included the effect of groundwater chemistry on sorption behavior. This approach provides a simplified but geologically reasonable representation of

sorption for the other radionuclides. Risk-significant nuclides Tc-99 and I-129, which are the primary contributors to dose at long times (CRWMS M&O, 2000), are still treated conservatively by assuming that their transport is unretarded by sorption or by solubility constraints.

4 CONCLUSIONS

Recommended sorption-related changes for future updates after TPA Version 4.0 include a more detailed treatment of matrix sorption for the five important actinides Am, Np, Pu, Th, and U. A response surface function approach is proposed for these nuclides to relate the selection of sorption coefficients to sampled variations in the geochemical parameters pH and P_{CO_2} . New field data was used to update the distribution ranges of these two parameters to make them more specifically related to conditions at Yucca Mountain. To balance the increased computational demand introduced by the more detailed treatment of sorption for the five actinides, the representation of sorption for minor nuclides has been simplified, while still maintaining geological realism, by using constant sorption coefficients that were selected as the means or expected values from DOE sorption datasets for Yucca Mountain. Other parameters related to the calculation of retardation factors would remain unchanged from TPA Version 4.0 or be revised slightly to incorporate additional field data.

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APPENDIX A

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
Matrix Kds						
MatrixKD_TSw_I	m ³ /kg	Sorption coefficient (K_d) for iodine in matrix of TSw	constant	0.0	No significant retardation for iodine (anionic species).	1007
MatrixKD_CHnvI	m ³ /kg	Sorption coefficient (K_d) for iodine in matrix of CHnv	constant	0.0	Same as for MatrixKD_TSw_I.	1008
MatrixKD_CHnzI	m ³ /kg	Sorption coefficient (K_d) for iodine in matrix of CHnz	constant	0.0	Same as for MatrixKD_TSw_I.	1009
MatrixKD_PPw_I	m ³ /kg	Sorption coefficient (K_d) for iodine in matrix of PPw	constant	0.0	Same as for MatrixKD_TSw_I.	1010
MatrixKD_UCF_I	m ³ /kg	Sorption coefficient (K_d) for iodine in matrix of UCF	constant	0.0	Same as for MatrixKD_TSw_I.	1011
MatrixKD_BFw_I	m ³ /kg	Sorption coefficient (K_d) for iodine in matrix of BFw	constant	0.0	Same as for MatrixKD_TSw_I.	1012
MatrixKD_UFZ_I	m ³ /kg	Sorption coefficient (K_d) for iodine in matrix of UFZ	constant	0.0	Same as for MatrixKD_TSw_I.	1013
MatrixKD_TSw_Tc	m ³ /kg	Sorption coefficient (K_d) for technetium in matrix of TSw	constant	0.0	No Tc retardation assumed; consistent with experimental evidence.	1014
MatrixKD_CHnvTc	m ³ /kg	Sorption coefficient (K_d) for technetium in matrix of CHnv	constant	0.0	Same as for MatrixKD_TSw_Tc.	1015
MatrixKD_CHnzTc	m ³ /kg	Sorption coefficient (K_d) for technetium in matrix of CHnz	constant	0.0	Same as for MatrixKD_TSw_Tc.	1016
MatrixKD_PPw_Tc	m ³ /kg	Sorption coefficient (K_d) for technetium in matrix of PPw	constant	0.0	Same as for MatrixKD_TSw_Tc.	1017
MatrixKD_UCF_Tc	m ³ /kg	Sorption coefficient (K_d) for technetium in matrix of UCF	constant	0.0	Same as for MatrixKD_TSw_Tc.	1018
MatrixKD_BFw_Tc	m ³ /kg	Sorption coefficient (K_d) for technetium in matrix of BFw	constant	0.0	Same as for MatrixKD_TSw_Tc.	1019
MatrixKD_UFZ_Tc	m ³ /kg	Sorption coefficient (K_d) for technetium in matrix of UFZ	constant	0.0	Same as for MatrixKD_TSw_Tc.	1020
MatrixKD_TSw_Cl	m ³ /kg	Sorption coefficient (K_d) for chlorine in matrix of TSw	constant	0.0	No significant retardation for chlorine (anionic species).	1021
MatrixKD_CHnvCl	m ³ /kg	Sorption coefficient (K_d) for chlorine in matrix of CHnv	constant	0.0	Same as for MatrixKD_TSw_Cl.	1022
MatrixKD_CHnzCl	m ³ /kg	Sorption coefficient (K_d) for chlorine in matrix of CHnz	constant	0.0	Same as for MatrixKD_TSw_Cl.	1023

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixKD_PPw_Cl	m ³ /kg	Sorption coefficient (K_d) for chlorine in matrix of PPw	constant	0.0	Same as for MatrixKD_TSw_Cl.	1024
MatrixKD_UCF_Cl	m ³ /kg	Sorption coefficient (K_d) for chlorine in matrix of UCF	constant	0.0	Same as for MatrixKD_TSw_Cl.	1025
MatrixKD_BFw_Cl	m ³ /kg	Sorption coefficient (K_d) for chlorine in matrix of BFw	constant	0.0	Same as for MatrixKD_TSw_Cl.	1026
MatrixKD_UFZ_Cl	m ³ /kg	Sorption coefficient (K_d) for chlorine in matrix of UFZ	constant	0.0	Same as for MatrixKD_TSw_Cl.	1027
MatrixKD_TSw_Cm	m ³ /kg	Sorption coefficient (K_d) for curium in matrix of TSw (vitric sorption properties)	constant	0.4	By trivalent analogy, americium K_d s are substituted for curium. Bechtel SAIC Company, LLC (2003a), lists the K_d values for Am for vitric layer properties as 0.1 to 1.0 m ³ /kg, in a piecewise distribution range such that 0.1 = 0%, 0.4 = 50%, and 1.0 = 100%. The median (expected) value is used for TPA.	1028
MatrixKD_CHnvCm	m ³ /kg	Sorption coefficient (K_d) for curium in matrix of CHnv (vitric sorption properties)	constant	0.4	Same as for MatrixKD_TSw_Cm	1029
MatrixKD_CHnzCm	m ³ /kg	Sorption coefficient (K_d) for curium in matrix of CHnz (zeolitic sorption properties)	constant	0.55	By trivalent analogy, americium K_d s are substituted for curium. Bechtel SAIC Company, LLC (2003a), lists the K_d values for Am for zeolitic layer properties as 0.1 to 1.0 m ³ /kg, in a uniform distribution. The mean (expected) value of 0.55 is used for TPA.	1030
MatrixKD_PPw_Cm	m ³ /kg	Sorption coefficient (K_d) for curium in matrix of PPw (assumed zeolitic sorption properties)	constant	0.55	Same as for MatrixKD_CHnzCm.	1031
MatrixKD_UCF_Cm	m ³ /kg	Sorption coefficient (K_d) for curium in matrix of UCF (assumed zeolitic sorption properties)	constant	0.55	Same as for MatrixKD_CHnzCm.	1032
MatrixKD_BFw_Cm	m ³ /kg	Sorption coefficient (K_d) for curium in matrix of BFw (assumed devitrified sorption properties)	constant	1.05	By trivalent analogy, americium K_d s are substituted for curium. Bechtel SAIC Company, LLC (2003a), lists the K_d values for Am for devitrified layer properties as 0.1 to 2.0 m ³ /kg, in a uniform distribution. The mean (expected) value is used for TPA.	1033
MatrixKD_UFZ_Cm	m ³ /kg	Sorption coefficient (K_d) for curium in matrix of UFZ (assumed vitric sorption properties)	constant	0.4	Same as for MatrixKD_TSw_Cm.	1034

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixKD_TSw_Ra	m ³ /kg	Sorption coefficient (K_d) for radium in matrix of TSw (vitric sorption properties)	constant	0.325	Bechtel SAIC Company, LLC (2003a) gives K_d values for Ra sorption onto vitric tuff that range from 0.05 to 0.6 m ³ /kg, in a uniform distribution. The mean (expected) value is used in TPA.	1035
MatrixKD_CHnvRa	m ³ /kg	Sorption coefficient (K_d) for radium in matrix of CHnv (vitric sorption properties)	constant	0.325	Same as for MatrixKD_TSw_Ra.	1036
MatrixKD_CHnzRa	m ³ /kg	Sorption coefficient (K_d) for radium in matrix of CHnz (zeolitic sorption properties)	constant	3.0	Bechtel SAIC Company, LLC (2003a) gives K_d values for Ra sorption onto zeolitic tuff that range from 1.0 to 5.0 m ³ /kg, uniform distribution. The mean (expected) value is used in TPA.	1037
MatrixKD_PPw_Ra	m ³ /kg	Sorption coefficient (K_d) for radium in matrix of PPw (assumed devitrified sorption properties)	constant	0.55	K_d s for devitrified tuffs more conservative than for zeolitic.	1038
MatrixKD_UCF_Ra	m ³ /kg	Sorption coefficient (K_d) for radium in matrix of UCF (assumed zeolitic sorption properties)	constant	0.55	Same as for MatrixKD_PPw_Ra.	1039
MatrixKD_BFw_Ra	m ³ /kg	Sorption coefficient (K_d) for radium in matrix of BFw (assumed devitrified sorption properties)	constant	0.55	Bechtel SAIC Company, LLC (2003a) gives K_d values for Ra sorption onto devitrified tuff that range from 0.1 to 1.0 m ³ /kg (uniform distribution). The mean (expected) K_d for devitrified layers is used in TPA.	1040
MatrixKD_UFZ_Ra	m ³ /kg	Sorption coefficient (K_d) for radium in matrix of UFZ (assumed vitric sorption properties)	constant	0.325	Same as for MatrixKD_TSw_Ra.	1041
MatrixKD_TSw_Pb	m ³ /kg	Sorption coefficient (K_d) for lead in matrix of TSw (vitric sorption properties)	constant	0.3	For Pb, Bechtel SAIC Company, LLC (2001) has the same K_d distribution range of 0.1 to 0.5 m ³ /kg, uniform distribution, for all rock types. The mean (expected) value is used in TPA.	1042
MatrixKD_CHnvPb	m ³ /kg	Sorption coefficient (K_d) for lead in matrix of CHnv (vitric sorption properties)	constant	0.3	Same as for MatrixKD_TSw_Pb.	1043
MatrixKD_CHnzPb	m ³ /kg	Sorption coefficient (K_d) for lead in matrix of CHnz (zeolitic sorption properties)	constant	0.3	Same as for MatrixKD_TSw_Pb.	1044
MatrixKD_PPw_Pb	m ³ /kg	Sorption coefficient (K_d) for lead in matrix of PPw (assumed zeolitic sorption properties)	constant	0.3	Same as for MatrixKD_TSw_Pb.	1045

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixKD_UCF_Pb	m ³ /kg	Sorption coefficient (K_d) for lead in matrix of UCF (assumed zeolitic sorption properties)	constant	0.3	Same as for MatrixKD_TSw_Pb.	1046
MatrixKD_BFw_Pb	m ³ /kg	Sorption coefficient (K_d) for lead in matrix of BFw (assumed devitrified sorption properties)	constant	0.3	Same as for MatrixKD_TSw_Pb.	1047
MatrixKD_UFZ_Pb	m ³ /kg	Sorption coefficient (K_d) for lead in matrix of UFZ (assumed vitric sorption properties)	constant	0.3	Same as for MatrixKD_TSw_Pb.	1048
MatrixKD_TSw_Cs	m ³ /kg	Sorption coefficient (K_d) for cesium in matrix of TSw (vitric sorption properties)	constant	0.002	Bechtel SAIC Company, LLC (2003a) lists K_d values for Cs sorption onto vitric rocks as a user-defined distribution, 0 = 0%, 0.002 = 50%, 0.1 = 100%. The median (expected) value is used for TPA.	1049
MatrixKD_CHnvCs	m ³ /kg	Sorption coefficient (K_d) for cesium in matrix of CHnv (vitric sorption properties)	constant	0.002	Same as for MatrixKD_TSw_Cs.	1050
MatrixKD_CHnzCs	m ³ /kg	Sorption coefficient (K_d) for cesium in matrix of CHnz (zeolitic sorption properties)	constant	5.0	Bechtel SAIC Company, LLC (2003a) lists K_d values for Cs sorption onto zeolitic rocks as a user-defined distribution, 0.425 = 0%, 5.0 = 50%, 20.0 = 100%. The median (expected) value is used for TPA.	1051
MatrixKD_PPw_Cs	m ³ /kg	Sorption coefficient (K_d) for cesium in matrix of PPw (assumed devitrified sorption properties)	constant	.008	Used K_d s for devitrified tuffs; more conservative than for zeolitic.	1052
MatrixKD_UCF_Cs	m ³ /kg	Sorption coefficient (K_d) for cesium in matrix of UCF (assumed devitrified sorption properties)	constant	.008	Same as for MatrixKD_PPw_Cs.	1053
MatrixKD_BFw_Cs	m ³ /kg	Sorption coefficient (K_d) for cesium in matrix of BFw (assumed devitrified sorption properties)	constant	.008	For Cs sorption onto devitrified rocks, K_d values listed in Bechtel SAIC Company, LLC (2003a) range from 0.001 to 0.015 m ³ /kg, uniform distribution. The mean (expected) value is used for TPA.	1054
MatrixKD_UFZ_Cs	m ³ /kg	Sorption coefficient (K_d) for cesium in matrix of UFZ (assumed vitric sorption properties)	constant	0.002	Same as for MatrixKD_TSw_Cs.	1055
MatrixKD_TSw_Ni	m ³ /kg	Sorption coefficient (K_d) for nickel in matrix of TSw (vitric sorption properties)	constant	0.03	For Ni sorption onto vitric rocks, K_d values in Bechtel SAIC Company, LLC (2001) range from 0 to 0.05 m ³ /kg, beta distribution, with expected value 0.03, stdev = 0.01, and COV = 0.33. The expected value is used for TPA.	1056

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixKD_CHnvNi	m ³ /kg	Sorption coefficient (K_d) for nickel in matrix of CHnv (vitric sorption properties)	constant	0.03	Same as for MatrixKD_TSw_Ni.	1057
MatrixKD_CHnzNi	m ³ /kg	Sorption coefficient (K_d) for nickel in matrix of CHnz (zeolitic sorption properties)	constant	0.05	Bechtel SAIC Company, LLC (2001) AMR lists K_d values for Ni sorption onto zeolitic rocks and devitrified rocks as 0.0 to 0.2, beta distribution, expected value 0.05, COV = 0.33, and stdev = 0.01. The expected value is used for TPA	1058
MatrixKD_PPw_Ni	m ³ /kg	Sorption coefficient (K_d) for nickel in matrix of PPw (assumed zeolitic sorption properties)	constant	0.05	Same as for MatrixKD_CHnz.	1059
MatrixKD_UCF_Ni	m ³ /kg	Sorption coefficient (K_d) for nickel in matrix of UCF (assumed zeolitic sorption properties)	constant	0.05	Same as for MatrixKD_CHnz.	1060
MatrixKD_BFw_Ni	m ³ /kg	Sorption coefficient (K_d) for nickel in matrix of BFw (assumed devitrified sorption properties)	constant	0.05	Same as for MatrixKD_CHnz.	1061
MatrixKD_UFZ_Ni	m ³ /kg	Sorption coefficient (K_d) for nickel in matrix of UFZ (assumed vitric sorption properties)	constant	0.03	Same as for MatrixKD_TSw_Ni.	1062
MatrixKD_TSw_C	m ³ /kg	Sorption coefficient (K_d) for carbon in matrix of TSw	constant	0.0	No retardation assumed. Carbon is subject to more exchange and sorption reactions than other anions, but the assumption is conservative (Bechtel SAIC Company, LLC, 2001).	1063
MatrixKD_CHnvC	m ³ /kg	Sorption coefficient (K_d) for carbon in matrix of CHnv	constant	0.0	Same as for MatrixKD_TSw_C.	1064
MatrixKD_CHnzC	m ³ /kg	Sorption coefficient (K_d) for carbon in matrix of CHnz	constant	0.0	Same as for MatrixKD_TSw_C.	1065
MatrixKD_PPw_C	m ³ /kg	Sorption coefficient (K_d) for carbon in matrix of PPw	constant	0.0	Same as for MatrixKD_TSw_C.	1066
MatrixKD_UCF_C	m ³ /kg	Sorption coefficient (K_d) for carbon in matrix of UCF	constant	0.0	Same as for MatrixKD_TSw_C.	1067
MatrixKD_BFw_C	m ³ /kg	Sorption coefficient (K_d) for carbon in matrix of BFw	constant	0.0	Same as for MatrixKD_TSw_C.	1068
MatrixKD_UFZ_C	m ³ /kg	Sorption coefficient (K_d) for carbon in matrix of UFZ	constant	0.0	Same as for MatrixKD_TSw_C.	1069

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixKD_TSw_Se	m ³ /kg	Sorption coefficient (K_d) for selenium in matrix of TSw (vitric sorption properties)	constant	0.0001	For Se, Bechtel SAIC Company, LLC (2001) gives same range of K_d values for all rock types, from 0 to 0.001 m ³ /kg, beta distribution, expected value = 0.0001, stdev = 0.0001, COV = 1.0. Expected value is used for TPA.	1070
MatrixKD_CHnvSe	m ³ /kg	Sorption coefficient (K_d) for selenium in matrix of CHnv (vitric sorption properties)	constant	0.0001	Same as for MatrixKD_TSw_Se.	1071
MatrixKD_CHnzSe	m ³ /kg	Sorption coefficient (K_d) for selenium in matrix of CHnz (zeolitic sorption properties)	constant	0.0001	Same as for MatrixKD_TSw_Se.	1072
MatrixKD_PPw_Se	m ³ /kg	Sorption coefficient (K_d) for selenium in matrix of PPw (assumed zeolitic sorption properties)	constant	0.0001	Same as for MatrixKD_TSw_Se.	1073
MatrixKD_UCF_Se	m ³ /kg	Sorption coefficient (K_d) for selenium in matrix of UCF (assumed zeolitic sorption properties)	constant	0.0001	Same as for MatrixKD_TSw_Se.	1074
MatrixKD_BFw_Se	m ³ /kg	Sorption coefficient (K_d) for selenium in matrix of BFw (assumed devitrified sorption properties)	constant	0.0001	Same as for MatrixKD_TSw_Se.	1075
MatrixKD_UFZ_Se	m ³ /kg	Sorption coefficient (K_d) for selenium in matrix of UFZ (assumed vitric sorption properties)	constant	0.0001	Same as for MatrixKD_TSw_Se.	1076
MatrixKD_TSw_Nb	m ³ /kg	Sorption coefficient (K_d) for niobium in matrix of TSw (vitric sorption properties)	constant	0.4	By trivalent analogy, americium K_d s are substituted for niobium. Bechtel SAIC Company, LLC (2003a) lists the K_d values for Am for vitric layer properties as 0.1 to 1.0 m ³ /kg, in a piecewise distribution range such that 0.1 = 0%, 0.4 = 50%, and 1.0 = 100%. The median (expected) value is used for TPA.	1077
MatrixKD_CHnvNb	m ³ /kg	Sorption coefficient (K_d) for niobium in matrix of CHnv (vitric sorption properties)	constant	0.4	Same as for MatrixKD_TSw_Nb.	1078
MatrixKD_CHnzNb	m ³ /kg	Sorption coefficient (K_d) for niobium in matrix of CHnz (zeolitic sorption properties)	constant	0.55	By trivalent analogy, americium K_d s are substituted for curium. Bechtel SAIC Company, LLC (2003a) lists the K_d values for Am for zeolitic layer properties as 0.1 to 1.0 m ³ /kg, in a uniform distribution. The mean (expected) value of 0.55 is used for TPA.	1079

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixKD_PPw_Nb	m ³ /kg	Sorption coefficient (K_d) for niobium in matrix of PPw (zeolitic sorption properties)	constant	0.55	Same as for MatrixKD_CHnzNb.	1080
MatrixKD_UCF_Nb	m ³ /kg	Sorption coefficient (K_d) for niobium in matrix of UCF (assumed zeolitic sorption properties)	constant	0.55	Same as for MatrixKD_CHnzNb.	1081
MatrixKD_BFw_Nb	m ³ /kg	Sorption coefficient (K_d) for niobium in matrix of BFw (assumed devitrified sorption properties)	constant	1.05	By trivalent analogy, americium K_d s are substituted for niobium. Bechtel SAIC Company, LLC (2003a) lists the K_d values for Am for devitrified layer properties as 0.1 to 2.0 m ³ /kg, in a uniform distribution. The mean (expected) value is used for TPA.	1082
MatrixKD_UFZ_Nb	m ³ /kg	Sorption coefficient (K_d) for niobium in matrix of UFZ (assumed vitric sorption properties)	constant	0.4	Same as for MatrixKD_TSw_Nb.	1083
Other Matrix Properties						
MatrixPoreRadius_TSw_	m	Size of average pore, used to estimate surface area for sorption in rock matrix	constant	5.0E-8	Consistent with TSw median value as reported in U0065 AMR.	1196
MatrixPoreRadius_CHnv	m	Size of average pore, used to estimate surface area for sorption in rock matrix	constant	5.0E-8	Actual median value for CHnv is probably closer to 4.5E-7 m [Bechtel SAIC Company, LLC. (2003b)].	1197
MatrixPoreRadius_CHnz	m	Size of average pore, used to estimate surface area for sorption in rock matrix	constant	5.0E-8	CHnz has a median value about 5 E-8 m, comparable to that of TSw, but with a broader distribution (Bechtel SAIC Company, LLC, 2003b).	1198
MatrixPoreRadius_PPw_	m	Size of average pore, used to estimate surface area for sorption in rock matrix	constant	5.0E-8	Almost all of the pore sizes (96%) in some Prow Pass tuffs have a radius less than 5 E-8 m (Bechtel SAIC Company, LLC, 2003b). In other Prow Pass tuffs, few of the sizes (~16%) are less than 5 E-8 m. On average for PPw, about half of the pore sizes are less than 5 E-8 m.	1199
MatrixPoreRadius_UCF_	m	Size of average pore, used to estimate surface area for sorption in rock matrix	constant	5.0E-8	In TPA model, this unit arbitrarily represents the non-to-partially welded, devitrified, and zeolitized tuffs in the Crater Flat Group that are above the water table.	1200

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixPoreRadius_BFw_	m	Size of average pore, used to estimate surface area for sorption in rock matrix	constant	5.0E-8	Consistent with Bullfrog median value as reported in Bechtel SAIC Company, LLC (2003b).	1201
MatrixPoreRadius_UFZ_	m	Size of average pore, used to estimate surface area for sorption in rock matrix	constant	5.0E-8	This is a hypothetical UZFT unit to represent transport through a fault zone. Constant value of 5E-8 is consistent with median value used for the other UZ hydrostratigraphic units.	1202
MatrixGrainDensity_TSw_	kg/m ³	Density of TSw unit; used in retardation calculations	constant	2460.0	Best estimate, based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, cancel out so that only matrix porosity is important in determining the retardation factor as it is calculated by TPA code.	1189
MatrixGrainDensity_CHnv	kg/m ³	Density of CHnv unit; used in retardation calculations	constant	2260.0	Best estimate, based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data.	1190
MatrixGrainDensity_CHnz	kg/m ³	Density of CHnz unit; used in retardation calculations	constant	2400.0	Best estimate, based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data.	1191
MatrixGrainDensity_PPw_	kg/m ³	Density of PPw unit; used in retardation calculations	constant	2540.0	Best estimate, based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data.	1192
MatrixGrainDensity_UCF_	kg/m ³	Density of UCF unit; used in retardation calculations	constant	2420.0	Best estimate, based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data.	1193
MatrixGrainDensity_BFw_	kg/m ³	Density of BFw unit; used in retardation calculations	constant	2570.0	Best estimate, based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data.	1194
MatrixGrainDensity_UFZ_	kg/m ³	Density of UFZ unit; used in retardation calculations	constant	2630.0	Constant values assumed because little variation exists in reported data.	1195
MatrixPorosity_TSw_	-	Porosity of TSw unit; used in retardation calculations	constant	0.08	Constant values assumed because measured variations are small; estimates based on data in Flint (1998).	1175
MatrixPorosity_CHnv	-	Porosity of CHnv unit; used in retardation calculations	constant	0.32	Same comment as for MatrixPorosity_TSw_.	1176
MatrixPorosity_CHnz	-	Porosity of CHnz unit; used in retardation calculations	constant	0.24	Same comment as for MatrixPorosity_TSw_.	1177

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
MatrixPorosity_PPw_	–	Porosity of PPw unit; used in retardation calculations	constant	0.25	Same comment as for MatrixPorosity_TSw_.	1178
MatrixPorosity_UCF_	–	Porosity of UCF unit; used in retardation calculations	constant	0.22	Same comment as for MatrixPorosity_TSw_.	1179
MatrixPorosity_BFw_	–	Porosity of BFw unit; used in retardation calculations	constant	0.10	Same comment as for MatrixPorosity_TSw_.	1180
MatrixPorosity_UFZ_	–	Porosity of UFZ unit; used in retardation calculations	constant	0.12	Hypothetical unit to model transport through a fault zone. Parameter value retained from TPA Version 4.0 for consistency.	1181
Fracture Rds						
FractureRD_TSw_I	–	Fracture retardation coefficient for iodine in TSw	constant	1.0	Value assumes no fracture retardation ($K_d = 0, R_d = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport.	1091
FractureRD_CHnvI	–	Fracture retardation coefficient for iodine in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1092
FractureRD_CHnzI	–	Fracture retardation coefficient for iodine in CHnz	constant	1	Same as for FractureRD_TSw_I.	1093
FractureRD_PPw_I	–	Fracture retardation coefficient for iodine in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1094
FractureRD_UCF_I	–	Fracture retardation coefficient for iodine in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1095
FractureRD_BFw_I	–	Fracture retardation coefficient for iodine in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1096
FractureRD_UFZ_I	–	Fracture retardation coefficient for iodine in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1097
FractureRD_TSw_Tc	–	Fracture retardation coefficient for technetium in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1098
FractureRD_CHnvTc	–	Fracture retardation coefficient for technetium in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1099
FractureRD_CHnzTc	–	Fracture retardation coefficient for technetium in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1100
FractureRD_PPw_Tc	–	Fracture retardation coefficient for technetium in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1101
FractureRD_UCF_Tc	–	Fracture retardation coefficient for technetium in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1102

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
FractureRD_BFw_Tc	–	Fracture retardation coefficient for technetium in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1103
FractureRD_UFZ_Tc	–	Fracture retardation coefficient for technetium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1104
FractureRD_TSw_Cl	–	Fracture retardation coefficient for chlorine in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1105
FractureRD_CHnvCl	–	Fracture retardation coefficient for chlorine in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1106
FractureRD_CHnzCl	–	Fracture retardation coefficient for chlorine in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1107
FractureRD_PPw_Cl	–	Fracture retardation coefficient for chlorine in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1108
FractureRD_UCF_Cl	–	Fracture retardation coefficient for chlorine in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1109
FractureRD_BFw_Cl	–	Fracture retardation coefficient for chlorine in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1110
FractureRD_UFZ_Cl	–	Fracture retardation coefficient for chlorine in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1111
FractureRD_TSw_Cm	–	Fracture retardation coefficient for curium in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1112
FractureRD_CHnvCm	–	Fracture retardation coefficient for curium in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1113
FractureRD_CHnzCm	–	Fracture retardation coefficient for curium in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1114
FractureRD_PPw_Cm	–	Fracture retardation coefficient for curium in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1115
FractureRD_UCF_Cm	–	Fracture retardation coefficient for curium in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1116
FractureRD_BFw_Cm	–	Fracture retardation coefficient for curium in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1117
FractureRD_UFZ_Cm	–	Fracture retardation coefficient for curium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1118

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
FractureRD_TSw_Ra	–	Fracture retardation coefficient for radium in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1119
FractureRD_CHnvRa	–	Fracture retardation coefficient for radium in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1120
FractureRD_CHnzRa	–	Fracture retardation coefficient for radium in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1121
FractureRD_PPw_Ra	–	Fracture retardation coefficient for radium in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1122
FractureRD_UCF_Ra	–	Fracture retardation coefficient for radium in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1123
FractureRD_BFw_Ra	–	Fracture retardation coefficient for radium in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1124
FractureRD_UFZ_Ra	–	Fracture retardation coefficient for radium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1125
FractureRD_TSw_Pb	–	Fracture retardation coefficient for lead in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1126
FractureRD_CHnvPb	–	Fracture retardation coefficient for lead in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1127
FractureRD_CHnzPb	–	Fracture retardation coefficient for lead in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1128
FractureRD_PPw_Pb	–	Fracture retardation coefficient for lead in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1129
FractureRD_UCF_Pb	–	Fracture retardation coefficient for lead in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1130
FractureRD_BFw_Pb	–	Fracture retardation coefficient for lead in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1131
FractureRD_UFZ_Pb	–	Fracture retardation coefficient for lead in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1132
FractureRD_TSw-Cs	–	Fracture retardation coefficient for cesium in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1133
FractureRD_CHnvCs	–	Fracture retardation coefficient for cesium in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1134
FractureRD_CHnzCs	–	Fracture retardation coefficient for cesium in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1135

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
FractureRD_PPw_Cs	–	Fracture retardation coefficient for cesium in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1136
FractureRD_UCF_Cs	–	Fracture retardation coefficient for cesium in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1137
FractureRD_BFw_Cs	–	Fracture retardation coefficient for cesium in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1138
FractureRD_UFZ_Cs	–	Fracture retardation coefficient for cesium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1139
FractureRD_TSw_Ni	–	Fracture retardation coefficient for nickel in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1140
FractureRD_CHnvNi	–	Fracture retardation coefficient for nickel in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1141
FractureRD_CHnzNi	–	Fracture retardation coefficient for nickel in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1142
FractureRD_PPw_Ni	–	Fracture retardation coefficient for nickel in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1143
FractureRD_UCF_Ni	–	Fracture retardation coefficient for nickel in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1144
FractureRD_BFw_Ni	–	Fracture retardation coefficient for nickel in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1145
FractureRD_UFZ_Ni	–	Fracture retardation coefficient for cesium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1146
FractureRD_TSw_C	–	Fracture retardation coefficient for carbon in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1147
FractureRD_CHnvC	–	Fracture retardation coefficient for carbon in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1148
FractureRD_CHnzC	–	Fracture retardation coefficient for carbon in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1149
FractureRD_PPw_C	–	Fracture retardation coefficient for carbon in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1150
FractureRD_UCF_C	–	Fracture retardation coefficient for carbon in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1151
FractureRD_BFw_C	–	Fracture retardation coefficient for carbon in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1152

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
FractureRD_UFZ_C	–	Fracture retardation coefficient for cesium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1153
FractureRD_TSw_Se	–	Fracture retardation coefficient for selenium in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1154
FractureRD_CHnvSe	–	Fracture retardation coefficient for selenium in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1155
FractureRD_CHnzSe	–	Fracture retardation coefficient for selenium in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1156
FractureRD_PPw_Se	–	Fracture retardation coefficient for selenium in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1157
FractureRD_UCF_Se	–	Fracture retardation coefficient for selenium in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1158
FractureRD_BFw_Se	–	Fracture retardation coefficient for selenium in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1159
FractureRD_UFZ_Se	–	Fracture retardation coefficient for cesium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1160
FractureRD_TSw_Nb	–	Fracture retardation coefficient for niobium in TSw	constant	1.0	Same as for FractureRD_TSw_I.	1161
FractureRD_CHnvNb	–	Fracture retardation coefficient for niobium in CHnv	constant	1.0	Same as for FractureRD_TSw_I.	1162
FractureRD_CHnzNb	–	Fracture retardation coefficient for niobium in CHnz	constant	1.0	Same as for FractureRD_TSw_I.	1163
FractureRD_PPw_Nb	–	Fracture retardation coefficient for niobium in PPw	constant	1.0	Same as for FractureRD_TSw_I.	1164
FractureRD_UCF_Nb	–	Fracture retardation coefficient for niobium in UCF	constant	1.0	Same as for FractureRD_TSw_I.	1165
FractureRD_BFw_Nb	–	Fracture retardation coefficient for niobium in BFw	constant	1.0	Same as for FractureRD_TSw_I.	1166
FractureRD_UFZ_Nb	–	Fracture retardation coefficient for cesium in UFZ	constant	1.0	Same as for FractureRD_TSw_I.	1167
Other Fracture Properties						
UZFractureForceFactorForKdtoRd	–	Program control switch to turn sorption in fractures on/off for Am, Np, Pu, Th, U.	user-supplied	0.0, 1.0	Default value is 0 (no sorption). If UZFFKTR = 1, Rd for actinides will be calculated from surface response function.	1004

Table A-1. Sorption-Related Input Parameters for Unsaturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
FractureAperture_TSw_	m	Fracture width (opening); used to estimate surface area for sorption in fractures	constant	1.0E-4	Representative of Topopah Spring welded tuff (0.1-0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003c).	1228
FractureAperture_CHnv	m	Fracture width (opening); used to estimate surface area for sorption in fractures	constant	2.0E-4	Representative of Calico Hills nonwelded vitric tuff (0.2-0.3 mm), as estimated from Bechtel SAIC Company, LLC (2003c).	1225
FractureAperture_CHnz	m	Fracture width (opening); used to estimate surface area for sorption in fractures	constant	2.0E-4	Within range of fracture widths in Calico Hills nonwelded zeolitic tuff (0.2-0.3 mm), as estimated from Bechtel SAIC Company, LLC (2003c).	1226
FractureAperture_PPw_	m	Fracture width (opening); used to estimate surface area for sorption in fractures	constant	1.0E-4	Representative of Prow Pass welded tuff (0.1-0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003c).	1227
FractureAperture_UCF_	m	Fracture width (opening); used to estimate surface area for sorption in fractures	constant	1.0E-4	Representative of Upper Crater Flat tuffs in general (0.1-0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003c).	1229
FractureAperture_BFw_	m	Fracture width (opening); used to estimate surface area for sorption in fractures	constant	1.0E-4	Representative of Bullfrog welded tuff (0.1-0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003c).	1224
FractureAperture_UFZ_	m	Fracture width (opening); used to estimate surface area for sorption in fractures	constant	1.0E-4	Hypothetical unit to model transport through a fault zone. Parameter value retained from TPA Version 4.0 for consistency.	1230

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Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
Matrix Rds						
ImmobileRd_STFF_I	--	Retardation coefficient for iodine in saturated tuff (via matrix diffusion)	constant	1.0	No retardation assumed. Experimental evidence (DOE) using I and alluvium shows that sorption not significantly different than zero (e.g., Bechtel SAIC Company, LLC, 2003a).	1444
ImmobileRd_STFF_Tc	-	Retardation coefficient for technetium in saturated tuff (via matrix diffusion)	constant	1.0	Conservative assumption of $K_d=0$. Confirmed by DOE and CNWRA experimental results (e.g., Bechtel SAIC Company, LLC, 2003a). No retardation.	1445
ImmobileRd_STFF_Cl	-	Retardation coefficient for chlorine in saturated tuff (via matrix diffusion)	constant	1.0	No retardation. Field evidence indicates Cl behaves conservatively (chemically) in the SZ (e.g., Bechtel SAIC Company, LLC, 2004).	1446
ImmobileRd_STFF_Cm	-	Retardation coefficient for curium in saturated tuff (via matrix diffusion)	constant	10400.0	Using an analogy between expected trivalent species Cm^{3+} and Am^{3+} , the Am retardation factor is substituted for Cm. Values in Bechtel SAIC Company, LLC (2003b) for Am sorption in saturated tuff are 1.0 to 10.0 m^3/kg with a truncated normal distribution (mean = 5.5, stdev = 1.5). Bechtel SAIC Company, LLC (2003c) lists K_d s for Am in devitrified layers as 0.1 to 2.0 m^3/kg (uniform distribution). The mean (expected) K_d value of 1.05 m^3/kg for the devitrified layers has been selected and is converted to a retardation factor of 10,400 assuming a bulk density of 1976 kg/m^3 and porosity of 0.20 for the saturated tuff unit.	1447
ImmobileRd_STFF_Ra	-	Retardation coefficient for radium in saturated tuff (via matrix diffusion)	constant	5400.0	Values in Bechtel SAIC Company, LLC (2003b) for Ra sorption in saturated tuff are 0.1 to 1 m^3/kg with a uniform distribution. The mean or expected value of 0.55 m^3/kg has been selected and is converted to a retardation factor of 5400 using a porosity of 0.20 and bulk density of 1976 kg/m^3 for the STFF layer.	1448

Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures (continued)						
Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
ImmobileRd_STFF_Pb	–	Retardation coefficient for lead in saturated tuff (via matrix diffusion)	constant	3000.0	Pb sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates Pb K_d s in SZ ranging from 0.1 to 0.5 m ³ /kg with a uniform distribution. (An assumption is made that devitrified tuff is an adequate analog to the saturated tuff unit and alluvium.) The mean or expected value of 0.3 m ³ /kg has been selected and is converted to a retardation factor of 3,000 using an the saturated tuff unit porosity of 0.20 and bulk density of 1976 kg/m ³ .	1449
ImmobileRd_STFF_Cs	–	Retardation coefficient for cesium in saturated tuff (via matrix diffusion)	constant	7200.0	Based on Cs sorption values from Bechtel SAIC Company, LLC (2003b) for alluvium as there should be little difference between alluvium and devitrified tuff for Cs retention. The range for alluvium is 0.1 to 1 m ³ /kg with a mean value of 0.728 m ³ /kg. Conversion to Rd using a porosity of 0.20 and a bulk density of 1976 kg/m ³ produces a value of 7200.	1450
ImmobileRd_STFF_Ni	–	Retardation coefficient for nickel in saturated tuff (via matrix diffusion)	constant	990.0	Ni sorption value taken from Bechtel SAIC Company, LLC (2001), in which saturated-zone K_d s for Ni range from 0 to 0.2 m ³ /kg with a uniform distribution. (An assumption is made that devitrified tuff is an adequate analog to saturated tuff and alluvium.) The mean or expected value of 0.1 m ³ /kg has been selected and is converted to a retardation factor of 990 using an STFF porosity of 0.20 and bulk density of 1976 kg/m ³ .	1451
ImmobileRd_STFF_C	–	Retardation coefficient for carbon in saturated tuff (via matrix diffusion)	constant	0.0	Assume no retardation for C in UZ or SZ. Carbon is subject to more exchange and sorption reactions than other anions but assumption is conservative (e.g., Bechtel SAIC Company, LLC, 2001).	1452

Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
ImmobileRd_STFF_Se	–	Retardation coefficient for iodine in saturated tuff (via matrix diffusion)	constant	2.0	Se sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates Se K_d s in SZ ranging from 0 to 0.001 m ³ /kg with a beta distribution. (An assumption is made that devitrified tuff is an adequate analog to saturated tuff and alluvium). The mean or expected value of 0.0001 m ³ /kg has been selected and is converted to a retardation factor of 1.98 (rounded to 2) using an STFF porosity of 0.20 and bulk density of 1976 kg/m ³ .	1453
ImmobileRd_STFF_Nb	–	Retardation coefficient for niobium in saturated tuff (via matrix diffusion)	constant	10400.0	Using an analogy between expected trivalent species Nb ³⁺ and Am ³⁺ , the Am retardation factor is substituted for Nb. Values in Bechtel SAIC Company, LLC (2003b) for Am sorption in the saturated tuff unit are 1.0 to 10.0 m ³ /kg with a truncated normal distribution (mean = 5.5, stdev = 1.5). Bechtel SAIC Company, LLC (2003c) lists K_d s for Am in devitrified layers as 0.1 to 2.0 m ³ /kg (uniform distribution). The mean (expected) K_d value of 1.05 m ³ /kg for the devitrified layers has been selected and is converted to a retardation factor of 10,400 assuming a bulk density of 1976 kg/m ³ and porosity of 0.20 for the the saturated tuff unit.	1454
AlluviumMatrixRD_SAV_I	–	Retardation coefficient for iodine in saturated alluvium	constant	1.0	Experimental evidence (DOE) using alluvium shows that sorption not significantly different than zero (e.g., Bechtel SAIC Company, LLC, 2003a). No retardation.	1410
AlluviumMatrixRD_SAV_Tc	–	Retardation coefficient for technetium in saturated alluvium	constant	1.0	Conservative assumption of $K_d = 0$. Confirmed by experimental results (e.g., Bechtel SAIC Company, LLC, 2003a).	1412
AlluviumMatrixRD_SAV_Cl	–	Retardation coefficient for chlorine in saturated alluvium	constant	1.0	No retardation. Field evidence indicates Cl behaves conservatively (chemically) in the saturated zone (e.g., Bechtel SAIC Company, LLC, 2004).	1414

Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures (continued)

Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
AlluviumMatrixRD_SAV_Cm	–	Retardation coefficient for curium in saturated alluvium	constant	35800.0	Using an analogy between expected trivalent species Cm ³⁺ and Am ³⁺ , the Am retardation factor (Rd) is substituted for Cm. Values in Bechtel SAIC Company, LLC (2003b) for Am sorption in saturated alluvium are 1.0 to 10.0 m ³ /kg with a truncated normal distribution (mean = 5.5, stdev = 1.5). The mean or expected value of 5.5 m ³ /kg has been selected and is converted to a retardation factor of 35,800 using an alluvium porosity of 0.30 and bulk density of 1950 kg/m ³ .	1416
AlluviumMatrixRD_SAV_Ra	–	Retardation coefficient for radium in saturated alluvium	constant	3580.0	Values in Bechtel SAIC Company, LLC (2003b) for Ra sorption in saturated alluvium are 0.1 to 1 m ³ /kg with a uniform distribution. The mean or expected value of 0.55 m ³ /kg has been selected and is converted to a retardation factor of 3,580 using an alluvium porosity of 0.30 and bulk density of 1950 kg/m ³ .	1418
AlluviumMatrixRD_SAV_Pb	–	Retardation coefficient for lead in saturated alluvium	constant	1950.0	Pb sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates Pb K _d s in SZ ranging from 0.1 to 0.5 m ³ /kg with a uniform distribution. (An assumption is made that devitrified tuff is an adequate analog to saturated tuff and alluvium.) The mean or expected value of 0.3 m ³ /kg has been selected and is converted to a retardation factor of 1,950 using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .	1420
AlluviumMatrixRD_SAV_Cs	–	Retardation coefficient for cesium in saturated alluvium	constant	4730.0	Values in Bechtel SAIC Company, LLC (2003b) for Cs sorption in saturated alluvium are 0.1 to 1 m ³ /kg with a truncated normal distribution (mean = 0.728). The mean or expected value of 0.728 m ³ /kg has been selected and is converted to a retardation factor of 4,730 using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .	1422

Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures (continued)						
Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
AlluviumMatrixRD_SAV_Ni	–	Retardation coefficient for nickel in saturated alluvium	constant	650.0	Ni sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates Ni K_d s in SZ ranging from 0 to 0.2 m ³ /kg with a uniform distribution. (An assumption is made that devitrified tuff is an adequate analog to saturated tuff and alluvium.) The mean or expected value of 0.1 m ³ /kg has been selected and is converted to a retardation factor of 650 using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .	1424
AlluviumMatrixRD_SAV_C	–	Retardation coefficient for carbon in saturated alluvium	constant	1.0	Assume no retardation for C. Carbon is subject to more exchange and sorption reactions than other anions but assumption is conservative (e.g., Bechtel SAIC Company, LLC, 2001).	1426
AlluviumMatrixRD_SAV_Se	–	Retardation coefficient for selenium in saturated alluvium	constant	2.0	Se sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates Se K_d s in SZ ranging from 0 to 0.001 m ³ /kg with a beta distribution. (An assumption is made that devitrified tuff is an adequate analog to saturated tuff and alluvium.) The mean or expected value of 0.0001 m ³ /kg has been selected and is converted to a retardation factor of 1.65 (rounded to 2) using an alluvium porosity of 0.30 and bulk density of 1950 kg/m ³ .	1428
AlluviumMatrixRD_SAV_Nb	–	Retardation coefficient for niobium in saturated alluvium	constant	35800.0	Using an analogy between expected trivalent species Nb ³⁺ and Am ³⁺ , the Am retardation factor is substituted for Nb. Values in Bechtel SAIC Company, LLC (2003b) for Am sorption in saturated alluvium are 1.0 to 10.0 m ³ /kg with a truncated normal distribution (mean = 5.5, stdev = 1.5). The mean or expected value of 5.5 m ³ /kg has been selected and is converted to a retardation factor of 35800 using an alluvium porosity of 0.30 and bulk density of 1950 kg/m ³ .	1430

Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures (continued)						
Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
Other Matrix Properties						
AlluviumMatrixGrainDensity_SAV	kg/m ³	Grain density of alluvial sediments	constant	2520.0	DOE measured grain density values for alluvium in Bechtel SAIC Company, LLC (2003b) have small range, 2,490 to 2550 kg/m ³ . Mean value of 2,520 kg/m ³ is used.	1439
AlluviumMatrixPorosity_SAV	–	Effective porosity of saturated alluvium	uniform	1.0E-1, 1.5E-1	Current DOE range in SZFT AMR is truncated normal with min = 0.0, mean = 0.18, and max = 0.30, std dev = 0.051. Field measured value at well 19D is 0.10. Best estimate of TPA saturated zone flow modelers, using Walker and Eakin (1963) and Fischer (1992), is to use a uniformly distributed range of 0.10 to 0.15.	1440
AlluviumTotalPorosity_SAV	–	Total porosity of saturated alluvium. Used for calculating retardation factor for radionuclides in the saturated alluvium layer.	uniform	0.15, 0.3	Range based on alluvium porosity data from Bechtel SAIC Company, LLC (2003b).	1441
AlluviumMatrixSpecificSurfaceArea	m ² /kg	Specific surface area of alluvium. Used for calculating retardation factor for radionuclides in the saturated alluvium layer.	uniform	0.9E3, 3.1E3	Range based on analysis of surface area data from Fortymile Wash wells (Bertetti, et al., 2004) using mesopore and micropore analysis (BET method) to attempt to differentiate between clay and non-clay mineral contribution. Subsequent statistical analyses and experimental evidence suggest 10% effective range should be applied with little or no contribution from other minerals (report in preparation).	1442
ImmobileGrainDensity_STFF	kg/m ³	Matrix grain density of saturated tuff	constant	2470.0	DOE data in Bechtel SAIC Company, LLC (2003b) indicate that average grain density of layers that would make up the saturated tuff unit are not significantly different from 2,470 kg/m ³ .	1455
ImmobilePorosity_STFF	–	Matrix porosity in saturated tuff	constant	0.2	Average matrix porosity used by DOE in Bechtel SAIC Company, LLC (2003b) is 0.22. A small range is evident but not likely to have significant effects.	1456

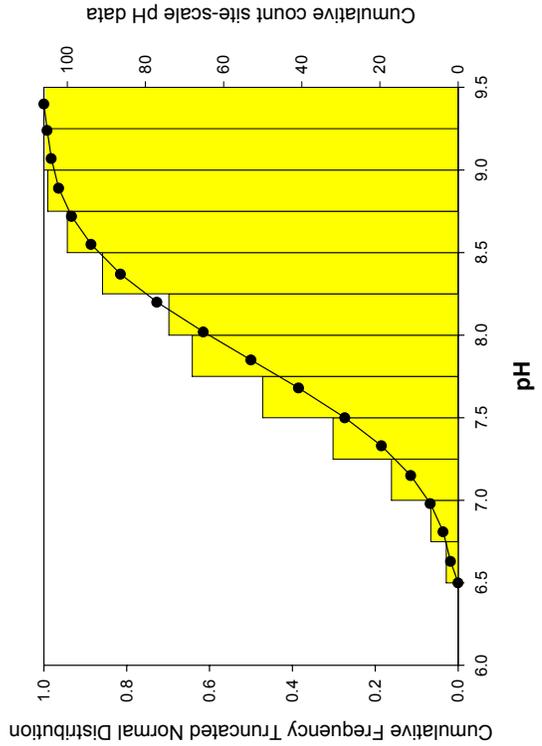
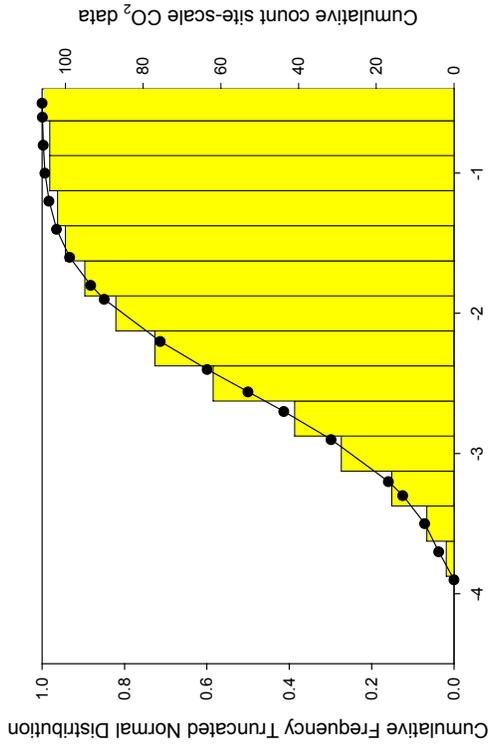
Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures (continued)						
Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
ImmobilePoreRadius_STFF	m	Estimated average pore radius of STFF matrix	constant	5.0E-8	Pore radius is used along with porosity and density to calculate surface area for each hydrostratigraphic layer. The constant value of 5E-8 is consistent with median value based on moisture retention curves used by DOE, from work by Travis and Nuttall (1987). Bechtel SAIC Company, LLC (2003d) indicates a more complex distribution of pore sizes for various rock units (see comments for other hydrostratigraphic layers, below), but there is a general agreement with the 5E-8 m value. To minimize surface area uncertainties, the 5E-8 value is retained pending more detailed characterization.	1457
Rds in Fractures (Tuff Only)						
FractureRD_STFF_I	–	Retardation coefficient for iodine in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1409
FractureRD_STFF_Tc	–	Retardation coefficient for technetium in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1411
FractureRD_STFF_Cl	–	Retardation coefficient for chlorine in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1413
FractureRD_STFF_Cm	–	Retardation coefficient for curium in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1415
FractureRD_STFF_Ra	–	Retardation coefficient for radium in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1417
FractureRD_STFF_Pb	–	Retardation coefficient for lead in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1419
FractureRD_STFF_Cs	–	Retardation coefficient for cesium in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1421
FractureRD_STFF_Ni	–	Retardation coefficient for nickel in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1423
FractureRD_STFF_C	–	Retardation coefficient for carbon in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1425

Table A-2. Sorption-Related Input Parameters for Saturated-Zone Matrix and Fractures (continued)						
Parameter Name	Units	Description	PDF Type	TPA Value	Comments	Order for TPA.INP
FractureRD_STFF_Se	–	Retardation coefficient for selenium in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1427
FractureRD_STFF_Nb	–	Retardation coefficient for niobium in fractures of saturated tuff	constant	1.0	Bounding assumption of no retardation in fractures.	1429
Other Fracture Properties						
SZFractureForceFactorForKdToRd	–	Program control switch to turn sorption in fractures on/off for Am, Np, Pu, Th, and U.	constant	0.0	This user option applies only to retardation in the saturated tuff, not alluvium. Acceptable values are 0 and 1. Default value is 0 (no sorption in fractures). If SZFFFKTR = 1, Rd for actinides will be calculated from surface response function.	1401
FractureAperture_STFF[m]	m	Fracture width; used to estimate surface area for sorption.	constant	1.0E-4	Aperture width is representative of DOE estimates for fracture width in tuff layers (0.1-0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003e).	1438
<p>References</p> <p>Bechtel SAIC Company, LLC. "Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing, and Recharge at Yucca Mountain, Nevada." ANL-NBS-HS-000021. Rev. 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2004.</p> <p>———. "Technical Basis Document No. 11: Saturated Zone Flow and Transport." Rev. 02. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003a.</p> <p>———. "SZ Flow and Transport Model Abstraction." MDL-NBS-HS-000021. Rev. 00. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003b.</p> <p>———. "Radionuclide Transport Models under Ambient Conditions." MDL-NBS-HS-000008. Rev. 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003c.</p> <p>———. "Particle Tracking Model and Abstraction of Transport Processes." MDL-NBS-HS-000020. Rev. 00. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003d.</p> <p>———. "Analysis of Hydrologic Properties Data." MDL-NBS-HS-000014. Rev. 00. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003e.</p> <p>———. "Unsaturated Zone and Saturated Zone Transport Properties." ANL-NBS-HS-000019. Rev 00 ICN 02. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2001.</p> <p>Bertetti, FP., J. Prikryl, and B. Werling. "Development of Updated Total-System Performance Assessment Parameter Distributions for Radionuclide Transport in the Saturated Zone. San Antonio, Texas: CNWRA. September 2004.</p> <p>Fisher, J.M. "Sediment Properties and Water Movement through Shallow Unsaturated Alluvium at an Arid Site for Disposal of Low-Level Radioactive Waste near Beatty, Nye County, Nevada." U.S. Geological Survey Water Resources Investigations Report 97-4243. 1992.</p> <p>Travis, B.J. and H.E. Nuttall. "Two-Dimensional Numerical Simulation of Geochemical Transport in Yucca Mountain." Report No. LA-10532-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. 1987.</p> <p>Walker, G.E. and T.E. Eakin. "Geology and Ground Water of Amargosa Desert, Nevada-California." Ground Water Resources, Reconnaissance Series Report 14. Carson City, Nevada: State of Nevada, Department of Conservation and Natural Resources. 1963.</p>						

APPENDIX B

Table of Values for the User-Specified Piecewise Distributions Used for pH and CO₂ in TPA Updates. Plots Compare the Distributions (Lines) with pH and CO₂ Site-Scale Data (Bars).

Parameter Name	Units	Distribution Type	Values
LogCO2PartialPressure_AIIUZ_SZLayers	Log atm	user-supplied piecewise	-3.9, 0.000 -3.7, 0.037 -3.5, 0.071 -3.3, 0.124 -3.2, 0.159 -2.9, 0.298 -2.7, 0.413 -2.56, 0.500 -2.4, 0.599 -2.2, 0.713 -1.9, 0.849 -1.8, 0.882 -1.6, 0.933 -1.4, 0.965 -1.2, 0.983 -1.0, 0.993 -0.8, 0.997 -0.6, 0.999 -0.5, 1.000
pH_AIIUZ_SZLayers	--	user-supplied piecewise	6.5, 0.000 6.63, 0.018 6.81, 0.036 6.98, 0.067 7.15, 0.114 7.33, 0.185 7.5, 0.273 7.68, 0.385 7.85, 0.500 8.02, 0.615 8.2, 0.727 8.37, 0.815 8.55, 0.886 8.72, 0.933 8.89, 0.964 9.07, 0.982 9.24, 0.992 9.4, 1.000



APPENDIX C

This is a table of response surface function coefficients proposed for use in TPA updates for the actinides americium (Am), neptunium (Np), plutonium (Pu), thorium (Th), and uranium (U). The applicable partial pressure of CO₂ [logP_{CO2} (atm)] and range of pH (pH_{low} to pH_{high}) for each segment of the response surface for each actinide are also listed. The coefficients correspond to the function, $y = a + bx + cx^2 + dx^3 + ex^4 + fx^5$, where x is the sampled pH and y is the K_A value that would be produced by TPA. This coefficient table would be included in TPA updates as the auxiliary file *coefkdeq.dat*.

Table C-1. Table of Response Surface Function Coefficients for the Actinides Americium (Am), Neptunium (Np), Plutonium (Pu), Thorium (Th), and Uranium (U)

Am(III)								
logPCO2 (atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.5	-3488.09627424	2629.51291541	-788.56176251	117.56073070	-8.70093305	0.25541926
-1.0	6.0	8.5	-2773.90316917	2025.80503602	-588.12441063	84.82299722	-6.06673419	0.17183905
-1.5	6.0	8.75	-2570.99868836	1798.94821209	-500.31232997	69.11860003	-4.73305712	0.12824036
-2.0	6.0	9.25	-529.70097000	382.57883000	-109.82740500	15.64244660	-1.09501774	0.02991442
-2.5	6.0	9.25	9.99115550	-19.12208470	8.43510534	-1.57254303	0.14374613	-0.00530121
-3.0	6.0	9.5	207.97473500	-163.91087800	50.26749810	-7.53911613	0.56336067	-0.01690361
-3.5	6.0	9.5	275.22137700	-211.82535300	63.68167270	-9.37809594	0.68606024	-0.02004885
-4.0	6.0	10.0	277.38065700	-210.45818600	62.29763580	-9.01473543	0.64646365	-0.01846756
-4.5	6.0	10.0	130.72585800	-98.62225380	28.50975860	-3.95833162	0.27147852	-0.0074348
-5.0	6.0	10.0	33.74073080	-25.65826470	6.78522964	-0.75797035	0.03813970	-0.00069526

Table C-1. Table of Response Surface Function Coefficients Used in TPA Version 5.0 for the Actinides Americium (Am), Neptunium (Np), Plutonium (Pu), Thorium (Th), and Uranium (U) (continued)

Np(V)								
logPCO2(atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.0	562.54981909	-500.89579959	176.89291310	-31.07712090	2.71862591	-0.09472022
-1.0	6.0	8.25	2093.54379394	-1650.20606982	518.44037026	-81.22795811	6.34997857	-0.19817761
-1.5	6.0	8.5	3360.84305038	-2509.67817430	746.96930394	-110.83848641	8.20266948	-0.24225613
-2.0	6.25	8.75	5795.34019404	-4067.33587609	1138.92231362	-159.10933648	11.09252611	-0.30878820
-2.5	6.5	9.25	4450.35090337	-3040.94202166	829.04301093	-112.76701087	7.65514069	-0.20751759
-3.0	6.75	9.5	6708.93933767	-4381.17145649	1141.77048723	-148.46955823	9.63518289	-0.24968824
-3.5	6.75	9.5	3211.45694881	-2095.04642211	545.01405769	-70.70323196	4.57549503	-0.11818698
-4.0	6.75	9.5	1346.51069701	-890.32073161	234.26972802	-30.69262895	2.00353111	-0.05214334
-4.5	7.0	9.75	1322.21173052	-859.71080915	222.41887757	-28.64267275	1.83707983	-0.04695287
-5.0	7.0	10.0	1106.08206519	-712.38086622	182.41875534	-23.23471499	1.47291641	-0.03717996

Table C-1. Table of Response Surface Function Coefficients for the Actinides Americium (Am), Neptunium (Np), Plutonium (Pu), Thorium (Th), and Uranium (U) (continued)

Pu(V)								
logPCO2(atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.0	366.75890755	-290.45801925	91.10737170	-14.22926620	1.11534214	-0.03530710
-1.0	6.0	8.25	869.22207223	-636.87831165	185.29514508	-26.82308684	1.94004147	-0.05630215
-1.5	6.0	8.5	427.10428374	-283.30036981	73.83983268	-9.48024499	0.60537760	-0.01557462
-2.0	6.25	8.5	-1427.39393419	1048.62353965	-306.60395427	44.54748036	-3.21024959	0.09168272
-2.5	6.5	9.0	1154.53608473	-699.56871657	166.97348103	-19.60986323	1.13564166	-0.02602837
-3.0	6.75	9.5	5842.89310451	-3657.34302232	911.90899478	-113.24694750	7.01025797	-0.17318426
-3.5	6.5	9.5	-1127.03127420	757.26130875	-202.36042870	26.85098224	-1.76452805	0.04586762
-4.0	6.5	9.75	-1326.95887035	862.80644367	-223.12180648	28.65734115	-1.82389617	0.04594980
-4.5	6.5	9.75	-1500.18897302	954.15744220	-241.28205853	30.30072357	-1.88600354	0.04648962
-5.0	7.0	10.0	-2361.88329888	1437.86286277	-348.42895826	41.99020928	-2.51303984	0.05969658

Table C-1. Table of Response Surface Function Coefficients for the Actinides Americium (Am), Neptunium (Np), Plutonium (Pu), Thorium (Th), and Uranium (U) (continued)

Th(V)								
logPCO2(atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.5	-312.14711523	243.99009612	-73.03800105	10.68670601	-0.76572596	0.02148313
-1.0	6.0	9.0	-178.60426661	137.73479859	-39.62233542	5.50279873	-0.36964490	0.00956996
-1.5	6.0	9.0	-22.15437259	17.78354930	-3.27591815	0.06714595	0.03117773	-0.00208040
-2.0	6.0	9.25	22.19042131	-14.82976722	6.12630097	-1.25638885	0.12171609	-0.00447272
-2.5	6.0	9.25	0.00987343	3.44007829	0.13956325	-0.28092710	0.04270240	-0.00192857
-3.0	6.0	9.5	-30.36665828	27.32153765	-7.32247331	0.87766304	-0.04670166	0.00081467
-3.5	6.0	9.5	-50.36155981	42.99824237	-12.20001276	1.63047122	-0.10434437	0.00256662
-4.0	6.0	10.0	-59.35569634	49.98525001	-14.35431507	1.96006372	-0.12936953	0.00332113
-4.5	6.0	10.0	-62.85636897	52.70342414	-15.19121240	2.08779456	-0.13903535	0.00361134
-5.0	6.0	10.0	-63.80070118	53.43751658	-15.41765407	2.12244405	-0.14166587	0.00369062

Table C-1. Table of Response Surface Function Coefficients for the Actinides Americium (Am), Neptunium (Np), Plutonium (Pu), Thorium (Th), and Uranium (U) (continued)

U (VI)								
logPCO2(atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.5	-109.00613767	120.39993399	-49.95905087	9.92659335	-0.94794423	0.03464480
-1.0	6.0	8.5	-195.74323141	176.71524472	-62.86725608	11.03888628	-0.95124562	0.03184985
-1.5	6.0	9.0	-29.18182775	52.10286104	-24.62789427	5.03783001	-0.47158120	0.01637571
-2.0	6.0	9.0	815.18397479	-512.78403463	126.86426513	-15.34454440	0.90594827	-0.02102466
-2.5	6.5	9.5	3059.73497195	-1924.39125807	481.06384571	-59.69824366	3.67990926	-0.09036028
-3.0	6.25	9.5	-75.43057307	96.37998368	-36.95785740	6.31128400	-0.50069832	0.01494114
-3.5	6.25	9.5	-2943.52020106	1944.83311429	-510.19392904	66.47503413	-4.29924708	0.11026458
-4.0	6.5	9.5	-5184.51971388	3302.21750148	-835.85755021	105.14807966	-6.57156173	0.16311656
-4.5	7.0	9.75	-9215.05453242	5594.86360139	-1351.52037089	162.41121670	-9.70671057	0.23071448
-5.0	7.0	9.75	1382.60890665	-955.33506081	261.50876815	-35.38624263	2.36964433	-0.06292418