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Contract No. NRC-02-97-009
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U.S. Nuclear Regulatory Commission
ATTN: Mr. James Firth
Office of Nuclear Material Safety and Safeguards
Division of Waste Management
Environmental and Performance Assessment Branch
Mail Stop 7K-02
Washington, DC 20555

Subject: Transmittal of the Software Requirements Description for the TPA Version 5.0 Code

Dear Mr. Firth:

Attached herewith is the Software Requirements Description for the Total-system Performance Assessment (TPA) Version 5.0 Code which fulfills IM 20.01402.762.200, Technical Specifications for TPA Version 5.0 Code—Software Requirements Description. This software requirements description describes the process-level and system-level modifications that were agreed to during meetings between U.S. Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analyses (CNWRA) technical staff. After you have reviewed and approved the software requirements description, CNWRA staff will prepare the software development plan and begin development of the code. The current schedule calls for the TPA Version 5.0 Beta Code to be delivered to you on September 27, 2002. If you have any questions regarding the content of the software requirements description please contact Mr. Ron Janetzke at (210) 522-3318.

Sincerely,

Gordon Wittmeyer

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SOFTWARE REQUIREMENTS DESCRIPTION FOR THE TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 5.0 CODE

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–97–009

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The data presented in Appendix A have been included in several reports and have been reviewed several times for those reports.

1 INTRODUCTION

This software requirements description documents the modifications to be made in updating the Total-system Performance Assessment (TPA) code to version 5.0. The modifications to the TPA code described in this software requirements description were identified using information in an external peer review (Weldy and Peckenpaugh, 2001), the Total System Performance Assessment for the Site Recommendation [Civilian Radioactive Waste Management System Management and Operating Contractor (CRWMS M&O), 2000], Supplemental Science and Performance Analyses (CRWMS M&O, 2001), and discussions with key technical issue leads to improve the capability of the TPA code as a review tool. In the period between the software requirements description for version 4.0 and this software requirements description for version 5.0, some minor modifications were made to the TPA code. These modifications were documented in a series of software change requests, which are maintained in the quality assurance folder at the Center for Nuclear Waste Regulatory Analyses (CNWRA).

Two general categories of modifications are outlined in Chapters 2 and 3 of this software requirements description for version 5.0 as proposed by the U.S. Nuclear Regulatory Commission (NRC) and CNWRA staffs. Chapter 2 includes modifications to the TPA code that are intended to reflect new data, increased knowledge of the repository system, and conceptual model improvements. Chapter 3 of the software requirements description outlines TPA code system-level enhancements. The specific changes in each chapter are identified with a software requirements identification. This identification is a software engineering tool that enables individual requirements to be tracked through the life cycle of the code to the point of delivery of the new version. Appendix B contains changes to the nominal case input file. Although the changes to the input file do not affect any of the modifications discussed in this software requirements description, they are included here as a documentation aid.

2 PROCESS-LEVEL MODIFICATIONS

Four new physical phenomena are to be implemented in the TPA Version 5.0 code.

- Glass waste form source term: this will be included in the release model in addition to the currently modeled spent nuclear fuel source term as part of the nominal scenario.
- Diffusive release of radionuclides from the waste package: this feature will consider diffusive release in the near field.
- Contaminant transport by colloids.
- Weld corrosion of the waste package: this will be considered as a waste package degradation process in addition to the localized and general corrosion processes already a part of the model. The following sections describe the introduction of these new processes as well as modifications to existing models.

2.1 Climate and Infiltration

Climate and infiltration data are provided to the UZFLOW module by the ITYM preprocessor in files prepared before the execution of the TPA code. Some of the changes listed here apply to the ITYM preprocessor code. These changes will provide a more realistic representation of the shallow infiltration and associated uncertainty.

C1 Runoff effect on shallow infiltration

The UZFLOW module presently incorporates data from one-dimensional simulations. Runoff and runon are not included in the one-dimensional model. Watershed simulations will provide abstractions to the ITYM code for the amounts and locations where additional water from runon leads to increased shallow infiltration. These simulations will be implemented in the ITYM preprocessor as an adjustment of precipitation amount for pixels identified by an external file. The new external file will identify geomorphic categories of pixels. Equations will be included in the ITYM preprocessor that identify the amount of additional water available for each particular geomorphic category. The equations will be a function of upslope length and cumulative soil depths. This change does not affect the current format of the *maidtbl.dat* or the *climato2.dat* files.

C2 Modify shallow infiltration estimates to account for vegetation

Vegetation is heuristically included in the shallow infiltration estimates calculated in the ITYM preprocessor. The results of BREATH (Stothoff, 1995) simulations that include vegetation can be included in the ITYM preprocessor by modifying the equations coded into the ITYM preprocessor used to estimate shallow infiltration. This change does not affect the current format of the *maidtbl.dat* or the *climato2.dat* files.

C3 Add shallow infiltration variance factor in UZFLOW

Currently, mean values of shallow infiltration for each 30-m [98.4 ft] pixel are passed from the ITYM preprocessor to the UZFLOW module. The mean values reflect the Monte Carlo analysis performed in the ITYM preprocessor. It is desired to have all stochastic elements of the TPA code controlled by the LHS sampling module used by the executive module in preparing the internal sampled parameter database. This control permits the efficient correlation of all stochastic parameters in the TPA system.

To create a consistent sampling system throughout the TPA system, a new file containing the variance of each 30-m [98.4 ft] pixel will be passed to UZFLOW and a new sampled parameter will be created in the UZFLOW module with a range of −1.0 to 1.0 to determine the shallow infiltration estimate from a distribution defined by files containing the mean and variance. The sampled parameter will be applied consistently across the spatial domain for any particular realization, but will vary between realizations.

The UZFLOW module, besides needing a new sampled parameter, will need to be read in a new external file. Currently, it reads in multiple sets of mean shallow infiltration values contained in a single file covering the range of climatic conditions expected for the repository. A corresponding external file of variance will also need to be read by the UZFLOW module. An algorithm will be added to the UZFLOW module to calculate the stochastic value of shallow infiltration for each pixel prior to aggregating the pixel values to subarea averages.

2.2 Near-Field Environment

NF1 Update Thermal Model

A new semianalytical thermal model will be used for predicting repository temperature. The new model is expected to compute temperatures more accurately in the vicinity of the waste package. Two approaches will be investigated. The first approach will be an improvement to the existing semianalytical solution. It appears that the two-dimensional repository-layout assumption in the model is currently contributing to the loss of accuracy in the temperature prediction within the drift, especially in determining the impact of backfill on temperature, by not appropriately accounting for the drift geometry. The second approach is an ellipsoidal approximation of the waste package and the surrounding medium. The ellipsoidal model is expected to resolve the near-waste package descriptions more accurately than the fist approach. However, the computational needs are not obvious. Therefore, one of these two models will be selected on the basis of accuracy of the results and computation time to replace the existing thermal model.

Attempts will be made to better capture temperature distribution within a subarea. Because in the nominal case TPA run, the temperature tends to have a dominant influence on the spent nuclear fuel dissolution rate, spatial dependency of temperature will be carried through the TPA code for computing the spent nuclear fuel dissolution rate. Temperatures will be calculated for either individual waste packages or for a group of waste packages. A source term will be calculated for each of these temperatures within a subarea. This approach will require changes to the current thermal model and the executive code.

2.3 Drip Shield Lifetime

DS1 Drip shield failure model

Currently, the drip shield model is limited to the specification of a single failure time. It is desired to have a parametric model that considers general corrosion rates and fluoride concentration and allows flexibility to consider mechanical failure modes (such as those due to rockfall). The new parametric model will be coded in a new TPA module called DSFAIL. It will interface to the TPA executive in a manner similar to the other modules; that is, DSFAIL will receive near-field chemistry information in a manner similar to the EBSFAIL module and return drip shield failure times to the executive. The drip shield failure times will affect water contacting the waste package and the near-field chloride concentration. The module will be designed so that mechanical failures of the drip shield and waste package are treated consistently.

2.4 Waste Package Lifetime

The following modifications to be made to the TPA code will affect the calculation of the waste package lifetime:

WP1 Variable pH

The pH value is used to compute the corrosion potential of the waste package. The pH value is currently hard coded in the FAILT auxiliary code as a constant equal to 9. A time dependent value will be specified in an input data file. The equations for the computation of the corrosion potential will be modified to account for the variation of pH versus time.

WP2 Weld corrosion

The extent of corrosion penetration of weld areas will be computed in the FAILT auxiliary code and used to calculate the waste package failure time. Corrosion parameters for the welds will be added to the *tpa.inp* input file. The corrosion of welds is not currently evaluated in the TPA code. The geometry of weld corrosion should limit the amount of water available for radionuclide release, in case of weld failure. Consideration of the geometry of the weld area will be accomplished to modify water infiltration parameters.

WP3 Microbial induced corrosion

Microbial induced corrosion is not currently considered in the TPA code. A correction term to the critical potential for localized corrosion of Alloy 22 will be added. This correction term will be defined as a function of time in a look-up table. This correction is intended to allow the user to consider those aspects that could affect the critical potential for localized corrosion, with microbial induced corrosion among them. It must be noted that at present, there is no information to define this correction term. This change is only intended to allow flexibility in the analyses that can be performed with the TPA code.

2.5 Source Term

The following modifications to be made to the TPA code will affect the calculation of the spent nuclear fuel and glass release:

SF1 Glass source term

Currently, the TPA code does not consider a glass source term for the release of radionuclides from the glass waste form. There will be substantial waste packages containing vitrified glass waste forms. These waste forms will behave differently from spent uranium dioxide fuel, which makes up most of the inventory of the repository. The glass waste form is different in several respects, including

- The waste form does not produce substantial heat, but can be heated by surrounding waste packages containing spent nuclear fuel.

- The glass waste form will have a different exposed surface area than an equivalent quantity of spent nuclear fuel.
- The glass waste form will contain a different mix of radionuclides than spent nuclear fuel.
- The glass waste form degrades at a different rate than spent nuclear fuel.

The TPA code will include a model that takes into account the differences in spent nuclear fuel by modifying the equations to simulate glass waste forms. This model will be included directly into the existing EBSREL module.

SF2 Colloid source term

The release of radionuclides that become associated with colloids has not been considered in previous versions of the TPA code. Colloidal consideration can be separated into two parts, reversible and irreversible colloid attachment. The release model will be modified to account for irreversible colloid attachment of radionuclides released from the engineered barrier subsystem. Irreversible attachment can be simulated by specifying a fraction of the release for a particular radionuclide that will represent the colloidal release. This fraction will be assigned to a set of new (artificial) radionuclides that will possess transport properties appropriate for colloids. The elements considered for irreversible attachment are plutonium, americium, thorium, and curium. The new radionuclides will populate new decay chains that will be developed for colloids to the point where an aqueous daughter product is generated. At that point, ingrowth to the aqueous phase daughter is assumed.

SF3 Diffusive Release

Currently there is no diffusive release model in the TPA code, although a previous version of TPA contained one. The U.S. Department of Energy (DOE) performance assessment models depend almost entirely on diffusion to release radionuclides from the waste form to the geosphere, whereas TPA relies on advective transport by water flowing through the waste packages. It is possible that advective transport will be small or nonexistent with the advent of the drip shield and corrosion resistant waste packages, so TPA will incorporate a diffusive model to simulate transport in the near field. The diffusive model in TPA will take into account diffusion within the waste package in thin water films on the waste form, support structure, and waste package walls; through cracks and openings in the waste package walls; and along the outside of the waste package. The model should also account for diffusion through the rock on the outside of the waste package, including the invert and any rock fall that comes into contact with the waste package. TPA currently has a model for advective and diffusive transport through the invert, but the assumptions will be reexamined to see if the invert model still applies or needs to be updated.

Most changes would be included in the EBSREL module and its associated code in the executive module. The model would probably use a finite difference approach, similar to past versions of TPA, which proved to be efficient and easily incorporated into the structure of the mixing cell module for the waste package concentration. The EBSFILT module for the invert will be modified as needed to make it consistent with the diffusive release model.

SF4 Time dependent cladding failure

The *tpa.inp* file contains a cladding correction factor that is used in the determination of the wetted area of the spent nuclear fuel. This value is currently set to 1.0, thus indicating no reduction in the wetted area due to cladding. It is desired to accommodate a look-up table that includes a cladding protection factor as a function of time starting at repository closure. It must be noted that there is no information available to define precisely the cladding protection factor as a function of time. This change in the TPA code is proposed to allow flexibility in importance and sensitivity analyses and also to provide the TPA code with flexibility to review the total system performance assessment results by the DOE.

2.6 Unsaturated and Saturated Zones Flow and Transport

Modifications to the TPA code related to the unsaturated zone and saturated zone flow and transport involve the following:

FT1 Represent K_Ds and R_fs for unsaturated zone and saturated zone as a function of geochemistry

An improved method of determining and using K_Ds and R_fs for the unsaturated zone and saturated zone is proposed by the staff associated with the Radionuclide Transport Key Technical Issue. See Appendix A for discussion of the theory. The implications of this method to the TPA code are the removal of many of the K_D or R_d specifications in the *tpa.inp* file and the addition of sampled correlated parameters for pH and PCO_2. Conversion of K_D to R_d for fractures will be performed in UZFT and SZFT as required by the NEFTRAN input file.

FT2 Colloid transport

This is a new feature of the TPA code that is closely associated with the colloid release considerations mentioned in the section on Source Term. The additional radionuclides will be accounted for with all the other radionuclides processed by the NEFTRAN module. This feature will necessitate the implementation of a second set of effective retardation factors for the irreversible attachment radionuclides whose release is coincident with the aqueous phase of the same species. This second set will be specified in the *tpa.inp* input file.

In addition, the transport properties of a subset of the aqueous radionuclides will be adjusted to reflect the reversible attachment of colloids. These new properties will be included in the nominal case data set.

An inventory of zero for the irreversible attachment colloid radionuclides may need to be maintained in the inventory database serving as a place holder for sections of the code that expect all chain members to be specified. The release in Ci/yr can be assigned to each when the release values are calculated for input to the invert module (EBSFILT). The colloid release values can be adjusted by using a user specified colloid fraction and applying it to the input file for EBSFILT. This will apportion the spent nuclear fuel release values between the aqueous radionuclides and the colloid radionuclides.

FT3 Reflect uncertainty in CHnv thickness

Currently, the thickness of the nonwelded vitric CHnv unsaturated zone layer below the repository is a fixed value specified in the *tpa.inp* file. The proposed change will make the CHnv thickness a sampled parameter that reflects the mineralogic and lithologic thickness uncertainty. With the addition of an overall unsaturated zone thickness parameter, the UZFT module will be modified to adjust the CHnz layer thickness to compensate for the variable CHnv thickness to maintain the desired overall unsaturated zone thickness for each subarea.

FT4 Multiple fracture flow and matrix flow epochs

The UZFT module currently restricts the flow media of a given layer to matrix or fracture for the entire simulation time. It is desired to allow the flow to share or switch media types one or more times during a simulation. This condition can be approximated by using two legs for one hydrostratigraphic unit in the NEFTRAN input data set. This feature will be added to the UZFT module to increase the flexibility of the code.

FT5 Variable dispersivity for UZFT

Currently, the dispersivity in the unsaturated zone is limited to a minimum of 0.1 m [0.33 ft] regardless of the layer thickness. To provide a more realistic parameter value for the unsaturated zone transport module this limit will be lowered to 0.01 m [0.33 ft] for layer thicknesses less than 40 m [131.2 ft].

FT6 Reflect uncertainty in streamtube dimensions

The streamtube dimensions of width and length are specified in the *strmtube.dat* file as a constant table used for all realizations. It is desired to reflect the uncertainty of these data by subjecting them to the influence of sampled parameters. This process will require the generation of a new sampled parameter representing a streamtube width multiplier. All routines that read the *strmtube.dat* file to obtain streamtube dimensions will be modified to include the use of the new parameters. This width multiplier will be applied to all streamtubes for their entire lengths. The range of this multiplier will be consistent with the data values in the *strmtube.dat* file so that the total streamtube width remains within realistic limits.

FT7 Update streamtube flux after climate change

Currently, the streamtube flux is implemented as a constant value read from the *strmtube.dat* file. The TPA code should permit the flux to change in response to climatic conditions. The change to climatic conditions relative to present day conditions is currently available in the UZFLOW file called *climato2.dat.* Normally, the saturated zone transport code considers a fixed porosity and fixed velocity for the transport legs. To consider time dependent flow, however, a velocity file will be generated to reflect the time dependent flux change at the assigned porosity. The degree of this effect will be controlled by an input factor which will control the scaling of the climatic deviations relative to present day conditions as applied to the flux rates. The present day flux rates will continue to be specified in the *strmtube.dat* file. This change will be made with time permitting.

2.7 Determination of Receptor Dose

D1 Add plume capture model

Currently, the DCAGW module handles the plume capture due to pumping at 10 km [6.2 mi] differently than at 20 km [12.4 mi]. An option will be provided in the *tpa.inp* file to select a single algorithm to be used for both locations consistent with the rule specification of a pumping rate of 3,000 acre-feet/year.

D2 U.S. Environmental Protection Agency (EPA) groundwater protection output

Currently, the EPA groundwater protection output in files *epapktim.out* and *epa_avg.out* are produced by the DCAGW module. Most of the output is in the form of unitless ratios of dose to their EPA limits. The output files will be reformatted to add data in raw form or in physical units consistent with the standards (e.g., mrem and pCi/L). In addition, uranium will not be included in the output, because it is not part of the standard, and the headings will be clarified to designate fraction of limit and radium where appropriate.

D3 Use 18 km [11.2 mi] as receptor location

The maximally exposed individual will be moved to 18 km [11.2 mi] from the previous value of 20 km [12.4 mi]. This valve is contained in the *tpa.inp* file and would normally not be considered a code change. But since there exists some legacy code that contains confusing variable names for this value, clarifying the variable names is considered a code change. This change will affect several modules of the TPA code in both variable name nomenclature and internal documentation and comments. The data file *strmtube.dat* may also need to be modified to accommodate the change.

D4 Use GENTPA for DCAGS dose conversion factors

Currently, DCAGW uses GENTPA to generate the groundwater dose conversion factors for each realizations, but DCAGS does not. It uses a fixed table look-up scheme instead. An identical dose conversion factor generation mechanism will be introduced using the GENTPA code for the DCAGW dose conversion factor values. This change will be made with time permitting.

2.8 Igneous Activity

IA1 Divide mass loading and occupancy factors into inside and outside components

Currently, only single values for the mass load and occupancy factor are used to determine the dose conversion factors for inhalation in the igneous case. To accommodate the new definition of the lifestyle for the reasonably maximally exposed individual, five categories of disturbance parameters will be used, including one category for offsite time. Each category will have a mass load and an occupancy time. The doses from these five categories for inhalation will be summed and used in the current dose conversion factor expressions. Even if the GENTPA code is used to generate the ground surface dose conversion factors for the other exposure pathways, the dose from the inhalation pathway will continue to be calculated by the TPA code and added to the results of the GENTPA code.

IA2 Modify Igneous Activity source term

The current igneous activity module assumes that spent nuclear fuel would be incorporated into the magma on the basis of an incorporation ratio that assumes that ash particles can incorporate spent nuclear fuel particles smaller than a certain ratio of diameters of the ash particle. There does not appear to be a justification for this choice of conceptual models. An alternative conceptual model of fuel incorporation into ash that takes into account the relative mass of spent nuclear fuel and ash in a range of particle size classes will be considered. The model will make minimum assumptions about the physics of incorporation because little is know about the phenomenon. Instead, the model will assume that the probability of the incorporation of spent nuclear fuel into ash depends only on the relative mass of fuel and ash in each particle size class. This is called the parsimony model by R. Codell because it is the simplest set of assumptions about the physics of the situation and should stand until the time that there is better evidence about actual mechanisms. The intent of this change is to match the grain size with the ash size, and this matching will require a new particle size distribution, uranium solubility in ash, and incorporation ratio in ASHPLUME.

IA3 Add ash redistribution model

Currently, the TPA code considers only the long term ash removal process for tephra deposition directly at the reasonably maximally exposed individual location. A more realistic model will be added that includes a source term for the mobilization of ash that lands in the catchment basin north of Fortymile wash. Input parameters that will be used in support of the model include (i) fraction of redistributable ash that is mobilized each year, (ii) erosion rate of redistributable ash, (iii) density of redistributable ash, (iv) fraction of remobilized ash that stays in reasonably maximally exposed individual area, (v) concentration of spent nuclear fuel in the remobilized tephra, (vi) dilution factor during transport, and (vii) rate of deposition of windblown soil from noncontaminated sources. This change will be made with time permitting.

2.9 Seismic Activity

SA1 Add rockfall effects on drip shield to SEISMO

Currently, the SEISMO module of the TPA code calculates rockfall effects on the waste package only. With the anticipated modification to include a model of the drip shield failure, the SEISMO module will need to be updated to include the effects of rockfall on the drip shield. The SEISMO module will provide the number of drip shield failures and waste package failures for each seismic event.

3 SYSTEM-LEVEL MODIFICATIONS

This section describes the changes to the executive driver to accommodate added flexibility to several consequence modules and the changes to accommodate parameters representing new data that characterize the site. It is intended that all new modules and process implementations have a single point neutralization or removal mechanism available to the user that would permit the execution of the code as if the new feature had not been implemented. This mechanism will aid in testing the code as well as performing the importance analysis studies.

Changes to the nominal scenario data set are not usually considered part of the software development effort. However, because the TPA code has a large set of input parameters that may be adjusted in lieu of implementing certain code modifications, a list of proposed nominal case data changes are included in Appendix B.

3.1 Repository Design

EX1 Limited flexibility will be added to the executive to accommodate variations to the DOE current thermal loading strategy.

3.2 Parameter Sampling

EX2 Update the SNLLHS code with new user discrete distributions.

EX3 Generate the SNLLHS input file such that only the input parameters that will be used during the run will be submitted to the SNLLHS code for sampling. This select submission will reduce the number of sampled parameters when not needed for a particular run.

3.3 Dose Output

EX4 Create a new output file that contains the pathway specific doses.

3.4 Miscellaneous

EX5 Miscellaneous readability, maintenance, and performance items will be addressed as encountered in development of the TPA Version 5.0 code.

4 TECHNICAL BASIS: PHYSICAL AND MATHEMATICAL MODEL

Technical bases for the modifications proposed in this site requirements description are in the preceding sections and in Appendix A for changes related to the unsaturated zone transport. These changes have been discussed during several meetings with the key technical issue leads.

5 COMPUTATIONAL APPROACH

Please refer to the discussion in the previous sections.

6 REFERENCES

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APPENDIX A

DETAILS ON PROPOSED MODIFICATIONS TO RADIONUCLIDE TRANSPORT PARAMETERS FOR THE TPA VERSION 5.0 CODE

INTRODUCTION

In the TPA Version 3.2 code, a K_D probability distribution function is assigned to each radionuclide for each hydrostratigraphic unit. For most of the radionuclides, the probability distribution functions are based on expert judgment supported by laboratory sorption data. Experimental data, however, show a link between the aqueous speciation of an actinide and its sorption behavior. Experimental and modeling results indicate that sorption behavior expressed as K_D, at least for actinides, is particularly influenced by physical and chemical parameters such as solution pH, PCO_2, and effective specific surface area A′. In the TPA Version 3.2 code, an effort was made to incorporate indirectly the effects of geochemistry by using site-specific hydrochemical data (Perfect, et al., 1995; Turner and Pabalan, 1999; Turner, et al., 1999) to calculate K_D values for a limited suite of actinides (Am^{3+}, U^{6+}, Np^{5+}, Pu^{5+}, and Th^{4+}). The results of these model calculations provided constraints on K_D probability distribution functions in the hydrologically saturated alluvium (hydrostratigraphic unit SAV). The correlation among the five different actinides is used to condition the Latin hypercube sampling of each probability distribution function and indirectly represents the geochemical link in sorption behavior.

PROPOSED APPROACH FOR DETERMINING SORPTION PARAMETERS

Considering the potentially large number of sorption parameters necessary to represent 16 radionuclides, 9 hydrostratigraphic units, and 2 types (fracture and matrix) of transport, the use of correlation coefficients is a cumbersome means to address the effects of geochemistry. A more efficient means is proposed for implementation in the TPA Version 5.0 code.

The proposed method (Turner, et al., 1998) would involve development of a $K^{A'}$ response surface to represent sorption as a function of critical parameters such as pH and PCO_2. During a given in the TPA Version 5.0 code realization, probability distribution functions for pH and C_T would be sampled and the values used to determine the appropriate value for $K^{A'}$ from the response surface, either through a parametric representation of the surface or through interpolation of a look-up table. To determine the value for K_D used in the transport calculation, the sampled $K^{A'}$ value would be normalized using the specific surface area and the relationship $K_D = K^{A'} \times A'$. The specific surface area A′ can either be determined through sampling a probability distribution function or using empirical relationships between porosity/permeability and surface area.

IMPLEMENTATION OF A K_D RESPONSE SURFACE

Development and implementation of the K_D response surface would occur through several steps:

- Experimental data would be used to calibrate geochemical sorption models. Such calibration has already been performed to a limited extent for Am^{3+}, U^{6+}, Np^{5+}, Pu^{5+}, and Th^{4+}. Additional radioelements (technetium, iodine, and selenium) have also been considered.

- The calibrated geochemical sorption models would be used to calculate radionuclide sorption expressed as KA′ for a broad range in pH and C_T. The proposed approach has been demonstrated using a diffuse-layer surface complexation model to develop a response surface for Np(V) sorption as a function of pH and PCO_2 (Figure A–1). Both a look-up table (Table A–1) and a series of parametric equations (Table A–2) have been used to define this surface.

- Site-specific geochemistry (Figures A–2 and A–3) can be used to constrain probability distribution functions (Table A–3) for sampling hydrochemical parameters such as pH and C_T. Because these parameters are linked through the aqueous carbonate chemistry, correlation will have to be developed for the latin hypercube sampling routine, either explicitly through mass action and mass balance or implicitly through a sample-by-sample comparison.

CONCLUSION

Experimental sorption data for a wide range in chemical conditions is limited for various radionuclides of interest in the TPA Version 5.0 code. Identifying appropriate data sets, calibrating sorption models, applying these to a broad range in conditions to develop the response surfaces, and identifying probability distribution functions for the hydrochemical parameters is time consuming. It is reasonable that this approach could be implemented in the TPA Version 5.0 code as an option for a few select radionuclides. For example, a response surface has been developed for Np(V) sorption (Figure A–1). Testing would be used to ensure that the method is implemented correctly and produces consistent results. Refinement of the approach and extension of the method to other radionuclides would begin in later versions of the TPA code.

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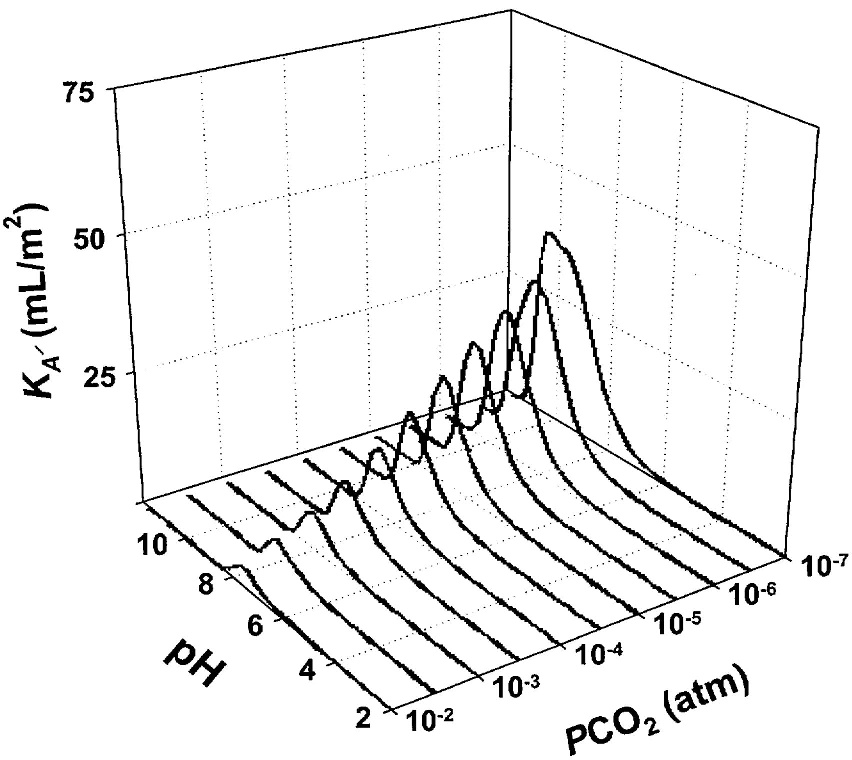

Figure A-1. Sorption Parameter Response Surface Calculated for Np(V) Using a Diffuse-Layer Surface Complexation Model

Table A–1. Sample Look-Up Table for Np(V) Sorption Response Surface (KA′ in mL/m^2); Np(V)total = 10-6 molal, M/V = 4 G/L

pH	Log PCO_2 (atm)											
	no CO_2	-7.00	-6.50	-6.00	-5.50	-5.00	-4.50	-4.00	-3.50	-3.00	-2.50	-2.00
2.00	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407
2.25	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785
2.50	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785
2.75	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785
3.00	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785
3.25	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785
3.50	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785	0.20785
3.75	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407
4.00	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407
4.25	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407	0.23407
4.50	0.26034	0.26034	0.26034	0.26034	0.26034	0.26034	0.26034	0.26034	0.26034	0.26034	0.26034	0.26034
4.75	0.28666	0.28666	0.28666	0.28666	0.28666	0.28666	0.28666	0.28666	0.28666	0.28666	0.28666	0.28666
5.00	0.31303	0.31303	0.31303	0.31303	0.31303	0.31303	0.31303	0.31303	0.31303	0.31303	0.31303	0.31303
5.25	0.36595	0.36595	0.36595	0.36595	0.36595	0.36595	0.36595	0.36595	0.36595	0.36595	0.36595	0.36595
5.50	0.44572	0.44572	0.44572	0.44572	0.44572	0.44572	0.44572	0.44572	0.44572	0.44572	0.44572	0.44572
5.75	0.55285	0.55285	0.55285	0.55285	0.55285	0.55285	0.55285	0.55285	0.55285	0.55285	0.55285	0.55285
6.00	0.68799	0.68799	0.68799	0.68799	0.68799	0.68799	0.68799	0.68799	0.68799	0.68799	0.68799	0.68799
6.25	0.90713	0.90713	0.90713	0.90713	0.90713	0.90713	0.90713	0.90713	0.90713	0.90713	0.90713	0.90713
6.50	1.21444	1.21444	1.21444	1.21444	1.21444	1.21444	1.21444	1.21444	1.21444	1.21444	1.21444	1.18621
6.75	1.64510	1.64510	1.64510	1.64510	1.64510	1.64510	1.64510	1.64510	1.64510	1.64510	1.64510	1.64510
7.00	2.30218	2.30218	2.30218	2.30218	2.30218	2.30218	2.30218	2.30218	2.30218	2.27163	2.27163	2.24115
7.25	3.25067	3.25067	3.25067	3.25067	3.25067	3.25067	3.21803	3.21803	3.21803	3.21803	3.15295	2.99153
7.50	4.58393	4.58393	4.58393	4.58393	4.58393	4.58393	4.58393	4.58393	4.54821	4.47703	4.23052	3.61471
7.75	6.48362	6.48362	6.48362	6.48362	6.48362	6.48362	6.48362	6.44330	6.32294	6.00633	5.12992	3.44811
8.00	9.10258	9.10258	9.10258	9.10258	9.10258	9.05545	9.00844	8.86820	8.36349	7.18486	4.83630	2.21073
8.25	12.46597	12.46597	12.46597	12.46597	12.40932	12.35283	12.12856	11.47131	9.82514	6.68675	3.05588	0.79711
8.50	16.54732	16.54732	16.54732	16.54732	16.40879	16.13444	15.33238	13.15912	8.96157	4.16083	1.10188	0.10351
8.75	21.25818	21.25818	21.17252	21.08716	20.74882	19.68218	16.89766	11.57926	5.42922	1.50003	0.15557	0.00000
9.00	26.08434	25.98021	25.87650	25.46576	24.17486	20.83294	14.37197	6.80986	1.91015	0.20785	0.00000	0.00000
9.25	30.37756	30.13395	29.65303	28.25866	24.56508	17.18213	8.27330	2.36348	0.28666	0.00000	0.00000	0.00000
9.50	33.88698	33.06972	31.62813	27.80933	19.84308	9.77604	2.86369	0.33946	0.02580	0.00000	0.00000	0.00000
9.75	36.78310	34.58558	30.87119	22.67266	11.63347	3.48128	0.44572	0.02580	0.00000	0.00000	0.00000	0.00000
10.00	40.82421	35.30073	27.14918	14.75070	4.65561	0.60674	0.02580	0.00000	0.00000	0.00000	0.00000	0.00000

Table A–2. Equation Parameters and Summary of Fit Results for Model Curves at Discrete PCO_2; Np(V)total = 10-6 molal, M/V = 4 g/L

PCO_2 (atm)	Coefficients [ln (KA′, in mL/m^2) = a + bx + cx2 + dx3 + ex4 + fx5]							
	a	b	c	d	e	f	r2 value	pH range used for fit
10-2.0	-323.7345029	151.4136753	-17.3990293	-1.7541185	0.4728224	-0.0247745	0.9999	6–9.25
10-2.5	-441.4872516	226.8171288	-37.7488848	1.2089255	0.2378357	-0.0167447	0.9999	6–9.25
10-3.0	148.2265595	-173.8278793	69.4791195	-12.8694017	1.1394455	-0.0390727	0.9999	6–9.50
10-3.5	604.4445148	-474.5177627	147.2075461	-22.6668262	1.7364614	-0.0529354	0.9999	6–9.50
10-4.0	847.1361569	-620.1544804	180.5362481	-26.2031203	1.8992944	-0.0549789	0.9999	6–10.00
10-4.5	925.7298724	-652.8079406	183.1897645	-25.6433576	1.7939710	-0.0501685	0.9999	6–10.25
10-5.0	923.2318767	-632.0905821	172.1420527	-23.3803904	1.5872876	-0.0430961	0.9999	6–10.50
10-5.5	672.7843206	-452.9837012	121.1472289	-16.1548188	1.0777544	-0.0287889	0.9999	6–11.00
10-6.0	393.8474607	-258.6708687	67.3400912	-8.7496479	0.5711094	-0.0149989	0.9999	6–11.25
10-6.5	722.6946490	-436.2310889	104.2139278	-12.3723844	0.7340464	-0.0174653	0.9978	6–11.50
10-7.0	2202.1902289	-1290.5774270	299.2738666	-34.3781522	1.9602212	-0.0444424	0.9816	6–11.75
no CO2	1211.3978170	-705.8275247	161.4080394	-18.1364167	1.0036927	-0.0219067	0.9996	6–11.75

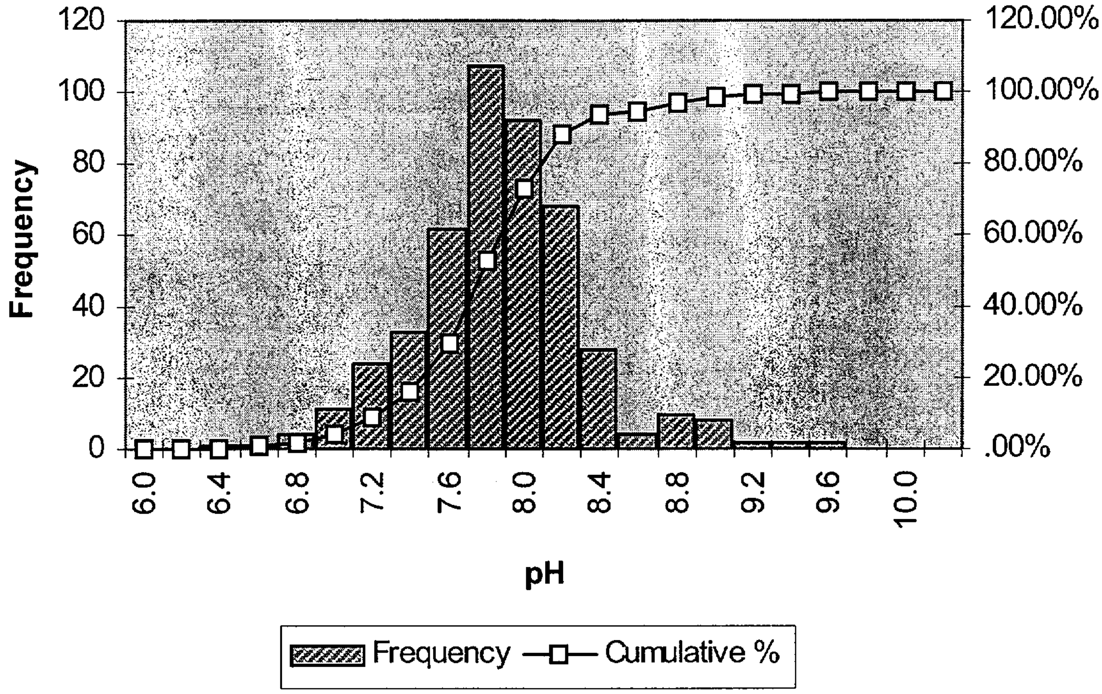

Figure A–2. Distribution of pH for Saturated Zone Regional Groundwaters

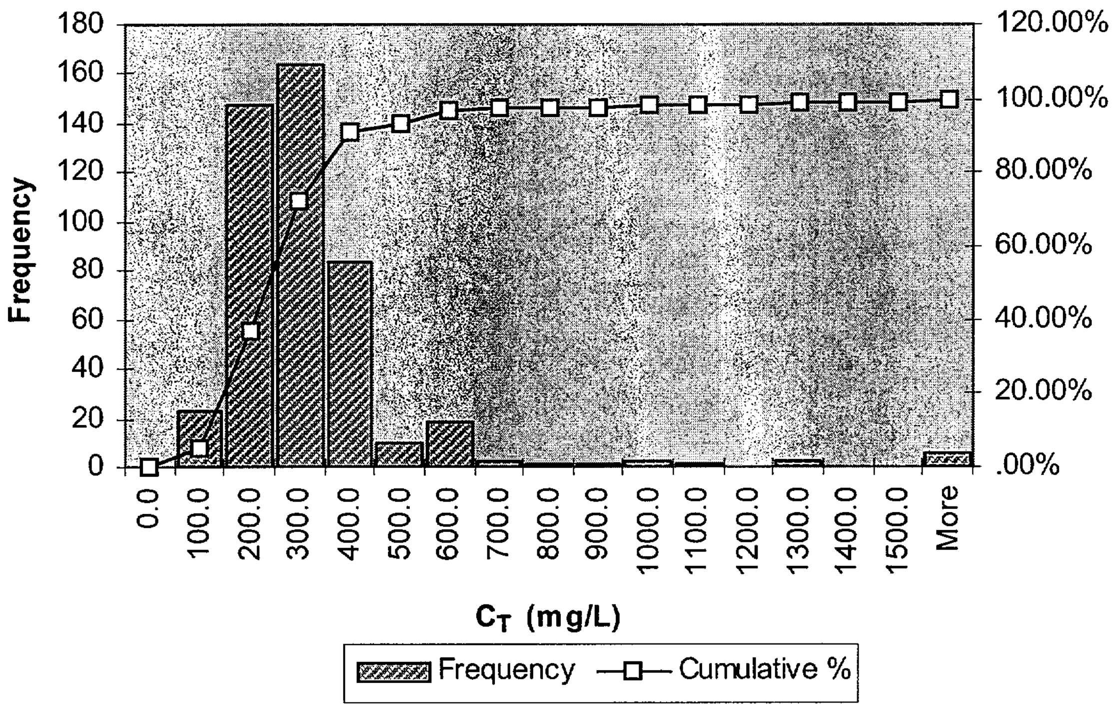

Figure A–3. Distribution of Total Inorganic Carbon (C_T in mg/L) for Saturated Zone Regional Groundwaters

Table A–3. Descriptive Statistics of Saturated Zone Measured Groundwater Chemical Parameters (Perfect, et al., 1995)			
	pH (standard units)	C_T (mg/L)	Log PCO_2 (atm)
Mean	7.83	295.76	-2.50
Median	7.8	245.0	-2.45
Mode	7.8	300.0	-2.34
Standard Deviation	0.45	525.99	0.54
Kurtosis	1.75	270.67	3.73
Skewness	0.43	15.03	-1.30
Range	3.3	10133.20	4.311
Minimum	6.3	6.80	-5.08
Maximum	9.6	10140.00	-0.77
Count	460	460	460

APPENDIX B

SUMMARY OF PROPOSED DATA CHANGES FOR TPA VERSION 5.0 CODE

Table B–1. Data Changes		
Item #	**Proposed Data Changes**	**Description**
DC1	Adjust value of the fracture-to-matrix diffusion parameter, DiffusionRate_STFF, in SZFT section of *tpa.inp*	Impermeable fracture coatings may affect fracture-to-matrix diffusion and sorption. This change will account for the potential presence of impermeable fracture coatings limiting matrix diffusion in the tuff aquifer.
DC2	Adjust parameters in wpflow.def, which are used to derive F_{ow}, to account for the thermal effects on fracture dilation	Fracture dilation may result from thermal-mechanical effect. Dilation may affect fracture flow and could divert flow from the pillar to the drift. Effects of fracture dilation will be accounted for through the F_{ow} factor, which accounts for flow potentially reaching a wetted waste package.
DC3	Revise F-factors, which are used to derive F_{mult}, to be more technically defensible	Need agreement among various technical staff as to the values assigned. F_{mult} is accounted for in the TPA code through use of the WastePackageFlowMultiplicationFactor in the EBSREL section of *tpa.inp*.
DC4	Adjust transfer parameters in *gftrans.def*, which are used in GENTPA module, to address site-specific data as they become available from DOE	These are biosphere transfer coefficients for radionuclides between soil, crops, and animal products. Parameters can be changed to address site-specific data as they become available from DOE.
DC5	Make K_D parameter sampling consistent for biosphere and ASHRMOVO	K_Ds, located in *tpa.inp,* are sampled parameters for biosphere but are constants for ASHRMOVO, thus, an inconsistency.
DC6	Revise/evaluate airborne mass loading factors in DCAGS section of *tpa.inp*	Airborne mass loading factors, AirborneMassLoadAboveFreshAshBlanket and AirborneMassLoadAboveSoil, account for mass of soil suspended in air above surface.

Table B–1. Data Changes (continued)		
Item #	**Proposed Data Changes**	**Description**
DC7	Update and add new parameters to MULTIFLO data file	Currently in the TPA code, information on chloride concentrations, temperature, and saturations as a function of time is accessed for waste package corrosion calculations via the look-up table *multiflo.dat*. For the TPA Version 5.0 code, a new conceptual model will be developed to describe chemical components important to both drip shield and waste package corrosion models. Values of PO_2 and pH, as well as concentrations of total dissolved carbonate, chloride, nitrate, and fluoride will be provided in a new look-up table. In this new abstraction, the performance assessment period will be divided into a few discrete parcels of time characterized by constant chemical conditions in the look-up table. Temperature, saturation, and relative humidity, determined from off-line TPA and MULTIFLO runs, will be used to define time periods be represented in the TPA Version 5.0 code as having similar chemical conditions.
DC8	Continuum approach for fractured tuff; once fracture flow starts, it should continue to layers below (unsaturated zone conceptual model)	The current NEFTRAN simulation of the unsaturated zone water flow assumes that fracture flow in the TSw unit is instantaneously received by the CHnv matrix flow. A more realistic model would have the TSw fracture flow feed the CHnv fracture flow. This approach can be approximated by adjusting the length of the CHnv unit and accomplished with a data change for the CHnv unit thickness in the *tpa.inp* file.
DC9	Correlate conduit diameter to power of the event	The conduit diameter range in previously reported data is seen by some to be too small to infer a correlation, This feature however, can be accommodated using the TPA parameter correlation feature. The parameter names also could be clarified to suggest reference to conduit instead of cone for the controlling parameter in the *tpa.inp* file.

Table B–1. Data Changes (continued)		
Item #	**Proposed Data Changes**	**Description**
DC10	Cool edges of repository	This capability requires another subarea dedicated to cooler temperatures. The subarea geometry can be modified to add a subarea on the edge of important subareas.