SOFTWARE REQUIREMENTS DESCRIPTION FOR TOTAL-SYSTEM PERFORMANCE ASSESSMENT (TPA) VERSION 5.1

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ABSTRACT

The Total-system Performance Assessment (TPA) code is being developed as a tool to help evaluate any license application that the U.S. Department of Energy may prepare for a potential nuclear waste repository at Yucca Mountain. The code is a joint product of the Center for Nuclear Waste Regulatory Analyses (CNWRA) and the U.S. Nuclear Regulatory Commission. The code development activities are guided by quality assurance procedures in place at CNWRA. This software requirements description is part of the software development life cycle presented in CNWRA Technical Operating Procedure–018, Rev. 10, Development and Control of Scientific and Engineering Software. A software requirements description is required when the scope of the planned code changes is significant. Previous software requirements descriptions were prepared for TPA Versions 3.0, 3.2, 4.0, and 5.0.

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: No CNWRA-generated data are contained in this report. No analyses are presented. This report documents plans for code development, but no codes are used or developed in this report.

1 INTRODUCTION

The Total-system Performance Assessment (TPA) code is being developed as a tool to help evaluate the safety case for a potential nuclear waste repository at Yucca Mountain. TPA Version 5.1 is a joint product of the Center for Nuclear Waste Regulatory Analyses (CNWRA) and the U.S. Nuclear Regulatory Commission (NRC). The code will be used as needed by the NRC and CNWRA staffs in their independent analyses to identify those aspects of natural and engineered repository components that may significantly affect repository performance. During TPA code development, numerous changes have been made to implement modifications to the potential repository design or improvements to the conceptual understanding of natural or engineered system responses. Code development activities are guided by the CNWRA quality assurance procedures in Technical Operating Procedure (TOP)–018, Development and Control of Scientific and Engineering Software. TOP–018 requires the preparation of a software requirements description for all CNWRA-developed software. Once a code is developed, minor changes and maintenance can be documented using software change reports. Significant modifications, however, may necessitate preparation of a new software requirements description.

Changes implemented since the last software requirements description that was prepared for TPA Version 5.0 have been documented via software change reports. These code changes, combined with identified needs for additional code changes, were significant enough to warrant the development of a new software requirements description. Accordingly, this software requirements description documents the features and functional requirements for TPA Version 5.1. Chapter 2 of this document briefly describes the major code changes since TPA Version 4.1j, which is the last version of the code that was adequately described by a user's guide (Mohanty, et al., 2002), leading up to TPA Version 5.0.1betaH. Chapter 3 documents the proposed changes to the current code that are planned to be implemented in the update to Version 5.1. The changes described in this chapter are based on agreements reached between the NRC and CNWRA staffs after a process of deliberation. Chapter 4 provides documentation of the technical bases for methodology and models to be implemented in TPA Version 5.1. Chapter 5 provides information on the computational approach (e.g., hardware and operating system requirements) and requirements for software validation.

2 SOFTWARE DESCRIPTION

TPA Version 5.1 will evaluate potential repository system and subsystem performance for a simulation period of up to 1 million years. TPA Version 5.1 is written in the FORTRAN programming language and can be compiled to execute in either the UNIX environment (FORTRAN 77, Version 5.0) or a personal computer with Windows® environments (Lahey FORTRAN, LF95 Version 7.10.02).

For purposes of this software requirements description, the requirements and capabilities described in Mohanty, et al. (2002) for TPA Version 4.0 are maintained except as indicated by the descriptions of additional or revised conceptual or modeling approaches in the following subsections. For example, since TPA Version 4.1j, capabilities for modeling several significant revisions have been made to consider additional physical phenomena, including

- A glass wasteform source term
- Colloidal transport of radionuclides
- Localized corrosion of the waste package body and welded areas
- Mechanical failure of drip shields under static or seismically enhanced rock load
- Mechanical breaching of waste packages caused by loads transferred to the waste package body from drip shields
- Fluvial and aeolian redistribution of volcanic ash deposits

This software requirements description considers 18 separate modules that are linked during the compiling process. Each of the 18 modules serves a distinct computational function, as described in the following subsections. Each of the following section headings includes a descriptive title for the module and, in parentheses, the name of the file that contains the module source code. Note that a user guide for TPA Version 5.1 is currently under preparation; the following descriptions will be superseded by the more detailed descriptions that will be provided in the user guide.

2.1 Executive Input (*reader.f*)

The TPA executive, EXEC, is responsible for the flow of major data streams throughout the code and the scheduling of the various process models to be executed.

One of the major executive functions is reading the user-supplied data in *tpa.inp*. This file specifies many types of parameter values and is read via the READER subroutine.

Newly implemented parameter types or types that exhibit a behavior different from that described in the last complete documentation in the user's guide (Mohanty, et al., 2002) are described briefly in the following bullets. A unique keyword is associated with each parameter type. For a complete description of other parameter types refer to Mohanty, et al. (2002).

- The <u>colloidalnuclides</u> keyword introduces the specification of irreversible colloidal form for seven radionuclides (Am-241, Am-243, Cm-245, Cm-246, Pu-239, Pu-240, Th-230). These will be identified in the input file with an initial letter "J" and a second character borrowed from the first character in the noncolloidal radionuclide name as follows: Ja-241, Ja-243, Jc-245, Jc-246, Jp-239, Jp-240, and Jt-230, respectively.

- The userdiscreteempirical keyword specifies a uniform distribution with a set of parameter values that will be sampled and associated with the parameter name. For example, in a list of values such as 4, 1.0, 3.0, 5.0, and 6.0, the first value indicates the number of values to follow, and the remaining numbers are the discrete values for Monte Carlo sampling.

- The usersupplieddiscrete keyword specifies a probability distribution function in the form of discrete values that will be sampled.

- The usersuppliedpwisecdf keyword specifies a piecewise cumulative distribution function that will be associated with the parameter named.

- The subarea keyword permits the specification of repository subareas in conjunction with the repository design specification data file, *repdes.dat*. The placement of the waste packages is calculated in the drifts subroutine in *reader.f* using a multipanel layout scheme similar to the repository design specifications used by the U.S. Department of Energy (DOE). Waste package and drift spacing parameters, as well as the spent nuclear fuel and glass payload parameters, are used for this calculation and are specified in *tpa.inp*. The coordinates for the endpoints of the resulting drifts are written to *drifts.dat*. These drifts are used as uniform line heat source elements for the near-field temperature calculations. The heat load in watts per metric ton of uranium is located in *burnup.dat*, and the inventory for a waste package in curies per metric ton of uranium, for both spent fuel and glass, is located in *nuclides.dat*.

There are no specific source code changes planned that would change the overall operation of READER of TPA Version 5.1. However, because this module executes and passes input to several other modules, it is likely that changes will be made, as necessary, to accommodate the code changes planned for several other modules.

Other possible changes to READER of TPA Version 5.1 may be made as part of the efforts to streamline the set of input parameters considered in the *tpa.inp*. For example, some input parameters that are not important to performance or that have insufficient technical bases may be eliminated from the TPA Version 5.1 input file. New parameters may be added in order to improve realism or consideration of spatial variability between or within subareas.

Other changes to TPA Version 5.1 input data may be made that will not likely require any changes to READER. Such possible changes could include

- Revision of repository subarea coordinates

- Addition of new subarea-dependent parameters for any new subareas

- Revision to input parameter values or probability distributions, which may result from updated technical bases and parameter justifications

- Revised header information to input data files to improve transparency

2.2 Executive Output (*exec.f*)

The TPA executive manages the progression of a TPA simulation and makes calls to the various modules and subroutines at the appropriate time. The executive function also organizes the dose (rem/yr) output for display in the standard output (screen output) and the TPA Version 5.1 output files (**.tpa*). Additional TPA Version 5.1 output files provide dose by individual groundwater exposure pathways, including drinking water, animal, milk, plant, inhalation, and external pathways.

EXEC will be modified for TPA Version 5.1 to implement the following additional model outputs:

- Output file *infilper.res* will be modified to report consistent (subarea weighted) averages of net infiltration rates.

- The file *wpsfail.res* will include initial waste package failures.

- Write statements and output file header information will be revised to improve, as time permits, the transparency and traceability of the information contained in each file.

- Subroutine libraries accessed by the executive and other modules will be reviewed to ensure there are no copyrighted routines used without permission. Where such items are found, routines will be rewritten or the necessary permissions will be obtained.

2.3 Climate and Infiltration (*uzflow.f*)

Climate and infiltration data are provided to UZFLOW by the Infiltration Tabulator for Yucca Mountain (ITYM) preprocessor in files prepared before the execution of TPA Version 5.1. Some of the functionality described in this section applies to the ITYM preprocessor code. All existing functionalities of both ITYM and UZFLOW will be maintained.

Results of offline watershed process model simulations provide abstracted input to the ITYM code for the amounts and locations where additional water from runon leads to increased shallow infiltration. These simulations are implemented in the ITYM preprocessor as an adjustment of precipitation identified through an external file. The external file identifies geomorphic categories for areas within the model boundaries. The ITYM preprocessor contains equations that calculate the amount of additional water available for each particular geomorphic category. The equations are a function of upslope length and cumulative soil depths.

Mean values of shallow infiltration for each 120 × 120-m [394 × 394-ft] pixel are passed from the ITYM preprocessor to UZFLOW. The mean values reflect the Monte Carlo analysis performed in the ITYM preprocessor. A file containing the variance of each pixel is passed to UZFLOW, and a sampled parameter with a range of −1.0 to 1.0 is used in UZFLOW to determine the shallow infiltration estimate from a distribution defined by files containing the mean and variance. The sampled parameter is applied consistently across all subareas for any particular realization, but varies between realizations. An algorithm in ITYM calculates the stochastic value of shallow infiltration prior to UZFLOW averaging the values within subarea boundaries.

TPA Version 5.1 will contain modifications to UZFLOW that will permit users to implement a constant net infiltration after the simulation time exceeds 10,000 years. This modification will accommodate anticipated revisions to 10 CFR Part 63 that, if implemented, would require an assumption of specific constant net infiltration conditions after 10,000 years. This revision will not limit the existing capability to treat climate as variable throughout the entire simulation period.

2.4 Near-Field Environment—Chemistry (*nfenv.f*)

NFENV delineates the three possible moist chemical environments and one dry chemical environment in contact with the waste package. The assignment of these environments considers the effects of temperature, relative humidity, drip shield failure time, and the availability of liquid water. The effect of inhibiting oxyanions (i.e., nitrate, sulfate, and carbonate) on the waste package and the effect of fluoride on the drip shield are also included in NFENV.

The three near-field environments with moisture represent environmental conditions composed of (i) deliquescence, (ii) direct seepage contact and evaporation, and (iii) rewetting. In Environment 1, there is no contact between seepage water and the waste package, but the relative humidity (RH) is high enough for salt mixtures to cause deliquescence. Seepage is assumed to occur only when the drift wall temperature (T_{dw}) is below a threshold value. Without seepage contacting the waste package, aqueous solutions on the waste package may form by the deliquescence of dust particles or mixing dust with condensed water. This environment is assumed to prevail if either of the following conditions hold

$$(\mathrm{RH} > \mathrm{RH}_c)$$
$$\text{and}$$
$$[(T_{dw} > \text{seepage threshold temperature}) \text{ or } (\text{time} < \text{drip shield failure time})]$$

where RH_c is the critical relative humidity for aqueous corrosion.

Environment 2 exists when seepage contacts the waste package during the thermal period. In the presence of seepage and evaporation, concentrated brines may develop on the waste package. Deliquescence of salt mixtures also is possible. Dilution may occur if condensed water on the drift wall or drip shield drips on brines formed on the waste package surface. As a conservative approach, this dilution process is neglected in the abstraction. Environment 2 is assumed to prevail if the following three conditions hold

$$(\mathrm{RH} < \text{rewetting humidity})$$
$$\text{and}$$
$$(T_{dw} < \text{seepage threshold temperature})$$
$$\text{and}$$
$$(\mathrm{RH} > \mathrm{RH}_c)$$
$$\text{and}$$
$$(\text{time} > \text{drip shield failure time})$$

where rewetting humidity is a value of the relative humidity at which the seepage rate exceeds the evaporation rate.

In Environment 3, seepage contacts the waste package after the thermal period (negligible evaporation). In the absence of evaporation, solutions in contact with the waste package should reflect the composition of seepage waters. Environment 3 is assumed to prevail if the following conditions hold

$$
\begin{gathered}
(\text{RH} > \text{rewetting humidity}) \\
\text{and} \\
(T_{dw} < \text{seepage threshold temperature}) \\
\text{and} \\
(\text{RH} > \text{RH}_c) \\
\text{and} \\
(\text{time} > \text{drip shield failure time})
\end{gathered}
$$

NFENV also accounts for the effect of inhibiting oxyanions (i.e., nitrate, carbonate, and sulfate) on localized corrosion. An effective inhibitor concentration, which is a linear combination of the relevant inhibiting oxyanion concentrations, is used.

Concentrations of chloride, oxyanions (i.e., nitrate, carbonate, and sulfate), and pH for Environments 1, 2, and 3 are defined as input parameters in *tpa.inp*. For example, probability distribution functions for concentrations and pH of Environment 2 have been derived from thermodynamic simulations of evaporative processes.

2.5 Near-Field Environment—Temperature (*nfenv.f*)

TPA Version 5.1 has two thermal models that are used to calculate the temperature of various engineered and natural components, including the waste package, backfill, and drift wall. A thermal model is selected in *tpa.inp*. The first thermal model is the basecase cross-sectional drift thermal model. This model accounts for three parallel heat transfer pathways: (i) through the invert, (ii) through the drip shield and backfill in the upper portion of the drift, and (iii) through the drip shield, backfill, and sides of the drift. The thermal conductivity of the backfill is an effective thermal conductivity that accounts for the various heat transfer modes through the backfill. The backfill material can be changed from the basecase type of natural to engineered through the selection of a nonzero value for the EmplacementBackfillThickness parameter in *tpa.inp*.

The second thermal model includes iterative calculations for two parallel heat transfer pathways: (i) through the invert and (ii) through the drip shield and backfill (engineered or natural). In this model, convective heat transfer through the backfill is calculated directly as a function of the backfill material characteristics (e.g., permeability). There are two mutually exclusive alternatives within this second thermal model that affect the permeability and are selected via *tpa.inp*. In the first alternative, the permeability is derived from the statistics of the particle size distribution for the backfill material. In the second alternative, the permeability is calculated using the coefficient of variation and the skewness of the particle size distribution; both of the latter values are input directly into the permeability calculation.

End of Ventilation and Repository Closure

TPA Version 5.1 will contain input parameters to define the end of the ventilation period independent of the time of repository closure. Previously, the end of ventilation and the time of repository closure were equivalent. Flexibility is needed to account for a lag between the end of active ventilation (50 years after emplacement) and repository closure (possibly 100 years after emplacement). During this period, a passive heat loss term will be used for temperature calculations.

Thermal Seepage (Reflux)

Consistency in handling the intact drift and degraded drift scenarios will be enhanced in TPA Version 5.1. Drift degradation effects on temperature are well accounted for in the current version of the TPA code. Drift degradation also affects reflux and seepage. To account for such effects, two *dryout.dat* (dryout zone thickness as a function of time) files will be developed: one for the intact drift scenario and one for the degraded drift scenario. Using flags in the TPA input file, one of the files will be selected for a realization.

2.6 Mechanical Failure (*seismo2.f*)

DRIFTFAIL and MECHFAIL will evaluate drift degradation and drip shield and waste package mechanical failures resulting from rubble accumulation in TPA Version 5.1.

DRIFTFAIL is a standalone module that evaluates drift degradation for thermally induced and seismically induced drift degradation. These calculations are evaluated as a function of time and rock type for each subarea. DRIFTFAIL evaluates the accumulation of rubble, the resulting vertical load on top of the drip shields and waste packages, the equivalent diameter (i.e., radial geometry diameter) for the rubble accumulated, and an equivalent diameter for the degraded drift. DRIFTFAIL is controlled by parameters associated with rock properties (e.g., rock mass density and rock bulking factor) and repository geometry (e.g., drift radius). TPA Version 5.1 can consider user-specified rates of drift degradation.

MECHFAIL is a standalone module that evaluates the fraction of drip shields and waste packages that have mechanically failed as a function of time. MECHFAIL is controlled by parameters associated with drip shield and waste package structural designs (e.g., waste package outer barrier thickness). Mechanical failure of drip shields and waste packages is coupled to environmental chemistry through the impact of corrosion thinning of the drip shield and waste package outer barrier.

A subroutine called by the executive module will generate seismic events. Seismic events will be described by event time, mean annual frequency of exceedance, peak ground velocity, peak ground acceleration, and rubble compaction factors.

The abstraction of mechanical interaction between waste packages and drip shields in TPA Version 5.1 will be updated from the previous TPA Version 5.0 code to be consistent with more recent drip shield and waste package design information. To the extent practical, the abstraction will be adaptable to future design changes and improved understanding of processes (e.g., understanding of seismic event probabilities and magnitudes may change over time; materials of different geometries or different material strengths may be incorporated into the drip shield and waste package designs).

Additionally, the mechanical failure abstractions for drip shields and waste packages in TPA Version 5.1 will be integrated with corrosion abstractions this will allow changes in waste package and drip shield thickness due to corrosion to be passed to the mechanical failure abstraction so that appropriate failure criteria are considered in mechanical interaction calculations.

TPA Version 5.1 will include an update to permit consideration of the potentially significant waste package and drip shield barrier capabilities that might persist following mechanical failure. This capability will consider both a reduction in the number of mechanically failed waste packages in which the damaged region is contacted by water and a reduction in the amount of water that enters those waste packages in which the damaged region is contacted by water. This update requires a more complex linkage between the mechanical failure abstraction, corrosion failure abstraction, and drift seepage abstraction (Sections 2.8 and 3.11).

The mechanical failure abstraction will also be integrated to account for the effects of increased loads that may occur during seismic events. TPA Version 5.1 will contain algorithms to account for both seismic event frequency and the magnitude of seismic acceleration. The seismic model will only consider the larger seismic events with probabilities less than 10^{-4} per year. The seismic abstraction will be structured to facilitate easy updating of the seismic frequency and magnitude input.

2.7 Drip Shield Lifetime (*dsfail.f*, *dsfailt.f*)

The drip shield failure module calculates the time for corrosion failure of the drip shield for each subarea. As part of generating a drip shield failure time, the module also calculates the thickness of the drip shield versus time. TPA Version 5.1 can include an enhancement factor in the corrosion rate as a function of fluoride concentration if the mass of fluoride consumed from anodic dissolution is disregarded.

2.8 Waste Package Lifetime (*ebsfail.f*)

<u>Corrosion Potential and Time-Varying In-Drift pH</u>

EBSFAIL calculates the corrosion potential by accounting for the variation of pH with time. The corrosion potential as a function of the time-varying pH is based on experimental data that indicate that there is a transition in the corrosion potential with pH and corrosion potential decreases with increasing pH values. The transition in the corrosion potential is modeled by specifying two sets of kinetic parameters: one set corresponds to the low-pH regime, and the second set corresponds to the high-pH regime. The transition in pH occurs around a value of 6.0. The in-drift pH as a function of time is constructed from distribution functions defined in *tpa.inp* for Environments 1, 2, and 3 (see Section 2.4 for descriptions of these environments).

Weld Corrosion

The extent of corrosion penetration of weld areas is computed in the FAILT standalone code and is used to calculate the waste package outer barrier weld failure time. Corrosion parameters for the welds are included in *tpa.inp*. The geometry of weld corrosion limits the amount of water available for radionuclide release in case of weld failure. The fraction of the weld area in relation to the waste package area is used to determine water infiltration parameters employed in the release calculations.

Localized Corrosion Correction Term

A correction term to the critical potential for localized corrosion of Alloy 22 calculated in EBSFAIL allows the user to consider various aspects that could affect corrosion, including microbial effects. Presently, however, there is no information available that permits the specification of this correction term. The correction term is only intended to allow flexibility in the analytical capability of TPA Version 5.1. The correction term as a function of time is constructed from probability distribution functions defined in *tpa.inp* for Environments 1, 2, and 3.

Passive Current Density as a Function of Temperature

EBSFAIL accounts for the relationship between temperature and passive current density. The current density is an Arrhenius function of the temperature. Estimates of the corrosion potential are improved by accounting for this temperature dependence.

Localized Corrosion Inhibitors

The effect of inhibitors (i.e., nitrate, carbonate, and sulfate) on localized corrosion is included in EBSFAIL. Localized corrosion is assumed to initiate if (i) the chloride concentration is greater than a minimum value, (ii) corrosion potential is greater than the repassivation potential, and (iii) the inhibitor-to-chloride ratio is less than a threshold value. Localized corrosion will not occur unless all three of these conditions are satisfied.

2.9 Faulting (*faulto.f*)

FAULTO determines the location, time, and fraction of waste package failures from direct fault disruption on a subarea basis. A complete description of the current model can be found in the TPA Version 4.0 Module Description and User's Guide (Mohanty, et al., 2002). No changes have been made to this module since TPA Version 4.1j. No additional modifications are proposed for FAULTO for TPA Version 5.1 beyond the capabilities previously described in Section 2.9 of this software requirements description.

2.10 Igneous Activity (*volcano.f*)

The key igneous activity processes are simulated in VOLCANO. VOLCANO selects the event time, the conduit size and location, and the number of waste packages affected by intrusions extending laterally into the drifts from the conduit. The quantities that VOLCANO returns to the TPA Version 5.1 executive are (i) the total metric tons of uranium contained in the waste packages failed by intrusion, (ii) the total metric tons of uranium ejected by the extrusive event, and (iii) the percent of subarea waste packages affected by volcanism.

There are two mutually exclusive models for intrusive failures that can be selected in *tpa.inp*: a geometric model and a distribution model. For the geometric model, the event is constrained to be centered on one of the drift center lines. Each point on all the drift center lines is considered equally likely to be the event location. A dike of the sampled length and angle is considered centered at the event location. Each drift is tested against the subarea boundaries to determine the relevance to the subarea and is tested for dike intersection. All waste packages in an intersected drift are assumed failed by intrusion. The total amount of uranium in the failed waste packages for a subarea is calculated assuming an average payload based on the fraction of uranium in glass form. The extrusive failures are independent of the in-drift failures and are based on the conduit diameter and the waste package spacing. This independence permits the extrusive failures to be assigned to any subarea regardless of the intrusive event location. The same average payload that is used for intrusion is used for the average payload of ejected waste packages.

The intrusive failure distribution model uses one sampled parameter to determine the occurrence of an extrusive event, another to determine the fraction of waste packages entrained by the extrusive event, and a third to determine the fraction of waste packages failed in drift. This fraction of failed waste packages is assigned to each subarea. For this model, the waste packages failed in drift are independent of the event subarea, which is associated only with the extrusive event.

No additional modifications are proposed for VOLCANO for TPA Version 5.1.

2.11 Source Term (*ebsrel.f*)

Consideration of radionuclide releases from the engineered barrier system to groundwater pathways in TPA Version 5.1 has been improved to consider the dependence of radionuclide release rates on waste package failure mode. This dependence is accommodated by the definition of six waste package classes. The waste package classes are sets of waste packages experiencing similar degradation mechanisms and are designated as (i) initially defective, (ii) mechanical, (iii) faulting, (iv) intrusive igneous, (v) localized corrosion, and (vi) general corrosion. The classes are used to track the number of waste packages affected, and select appropriate wasteform water contact modes (either bathtub or flow through) and values of the wasteform wetted fraction parameter. Waste packages in a class may undergo more than one degradation process (e.g., mechanical waste packages may experience early localized corrosion followed by later general corrosion) by considering changes in water contact rates as additional failure modes are realized.

Wasteform Dissolution Models

TPA Version 5.1 will include the capability to consider four alternative models for spent nuclear fuel dissolution rates, as described by Mohanty, et al. (2002). Model 1 reflects the behavior of spent nuclear fuel in pure carbonate solutions under specified chemical conditions. Model 2 is based on an Arrhenius dependence on temperature of the spent fuel dissolution rate, derived from tests in groundwater containing calcium and silica. Model 3 allows direct user input of a constant rate, and Model 4 invokes dissolution control by schoepite solubility. The spent fuel specific surface area is also a term calculated in RELEASET. Model 2 will be the default model for the reference data set; the other three models are considered exploratory.

Addition of a Glass Wasteform Source Term

TPA Version 5.1 will account for release of radionuclides from the glass wasteform in addition to spent nuclear fuel. The glass wasteform behaves differently from spent uranium dioxide fuel. Estimates of high-level waste glass dissolution rates will be based on forward rate measurements on a five-component glass (e.g., Knauss, et al., 1990). Note that the dissolution rate of glass wasteform decreases in the presence of various dissolved ions; however, this effect will not be included explicitly in the model. Consideration of the glass wasteform will be included in the TPA Version 5.1 reference data set.

Colloid Source Term

The release of radionuclides associated with colloids is considered in EBSREL. Colloidal consideration can be separated into two parts: reversible and irreversible colloid attachment. The release model accounts 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. This fraction is assigned to a set of new (artificial) radionuclides representing colloidal species that possesses transport properties appropriate for colloids. The four elements allowed to bind irreversibly to colloids are plutonium, americium, thorium, and curium. The new species will populate new decay chains developed for colloids to the point where an aqueous daughter product is generated. At that point, ingrowth to the aqueous phase daughter is assumed.

The source term abstraction for radionuclides irreversibly attached to colloids will be modified to assign radionuclide mass to colloids until the finite sorption capacity is reached. This approach could also account for competitive sorption among released radionuclides (e.g., uranium), which may further limit the sorption capacity for species such as plutonium.

Diffusive Release

The RELEASET code module permits consideration of diffusive transport through cracks in the welds of those waste packages. In general, the diffusive release conceptual model assumes the presence of a continuous water film between the wasteform, a crack in the waste package, and the exterior of the waste package. For TPA Version 5.1, the diffusive release abstraction will be turned off in the reference case in favor of an advective release model; however, the ability to utilize the diffusive release model will be retained.

Cladding Protection

In TPA Version 5.1, it will be assumed for the reference case that spent nuclear fuel cladding instantaneously degrades up to an extent defined by a cladding correction factor and remains fixed at that level for the entire simulation period. As an exploratory alternative model, TPA Version 5.1 also will allow consideration of gradual cladding degradation (e.g., unzipping) simply by modifying input parameters. This approach will permit consideration of differing concepts for degrees and rates of waste exposure due to cladding failure. The exploratory cladding degradation model will be consistent with a cladding unzipping concept that may occur as a result of processes such as alteration or spent fuel to secondary phases with higher molar volumes or, as studies at Argonne National Laboratory have shown, unzipping may be caused by Zircaloy oxidation-generated stress (Bechtel SAIC Company, LLC, 2004).

Abstraction of Water Contacting Waste

In TPA Version 5.1, EBSREL will compute the amount of water available for contacting the wasteform according to

$$q_{in} = Q_R \, F_{FMF} \, F_{ow} \, F_{mult} \, F_r \, F_d \, F_{WP}$$

where

q_{in}	—	water flow rate into the waste package [m^3/yr]
Q_R	—	percolation flow per waste package, from NFENV [m^3/yr]
F_{FMF}	—	factor to account for flow convergence and divergence as specified by the *tpa.inp* input parameter WastePackageFlowMultiplicationFactor
F_{ow}	—	temporal flow focusing factor interpolated from data in *wpflow.def*
F_{mult}	—	near- and in-drift flow diversion factor
F_r	—	rubble flow factor
F_d	—	drip shield flow factor
F_{WP}	—	waste package flow factor

The flow factors F_{FMF}, F_{ow}, F_{mult}, F_r, F_d, and F_{WP} are used to modify flow rates to simulate the action of components of the engineered barrier system (e.g., drift wall, drip shield, waste package). After all of the flow factors are applied, the final result is the flow rate available to mobilize wasteforms, q_{in}.

In EBSREL, damaged drip shields and waste packages partially divert water. The waste package factor, F_{WP}, is selected based on the waste package category or class. F_{WP} = 1 for waste packages in the general corrosion class. Special constructs of the factor F_{WP} are implemented to account for specific or time-varying conditions for (i) initially defective, (ii) mechanical, and (iii) faulting, intrusive igneous, and localized corrosion waste package classes.

Time-dependent values for the flow factors F_{mult}, F_{ow}, F_{wet}, F_r, F_d, F_{wc}, F_{wm1}, F_{wm2}, and F_{id} will be specified in TPA Version 5.1 using the auxiliary input file *wpflow.def*.

2.12 Unsaturated Zone Flow and Transport (*uzft.f*)

An improved method of determining and using partition coefficients (K_d) and retardation factors (R_d) for the unsaturated zone and saturated zone is described in Appendix A of the software requirements description for TPA Version 5.0 (Janetzke, et al., 2002). This method determines these parameters as a function of pCO_2 and pH and is currently used for radionuclides Am, Cm, Np, Pu, Th, and U. This approach permits the removal of many of the K_d or R_d specifications in *tpa.inp* and the addition of sampled correlated parameters for pH and pCO_2. A conversion of K_d to R_d for fractures is performed in UZFT and SZFT as required by the NEFMKS input file.

The calculation of K_d or R_d values is a feature of TPA Version 5.1 that is closely associated with the colloid release considerations mentioned in Section 2.11, Source Term. The additional colloidal radionuclide species are accounted for with all the other radionuclides processed by NEFMKS. A second set of effective retardation factors for colloids is contained in *tpa.inp* for the irreversible attachment radionuclides for which release is coincident with the aqueous phase of the same radionuclide.

In addition to irreversible colloid transport, the transport properties of a subset of the aqueous radionuclides are adjusted to reflect the reversible attachment of colloids. These new properties have been included in the reference data set.

An initial inventory of zero for the irreversible attachment colloid radionuclides is set in *nuclides.dat* and serves as a placeholder for sections of the code that expect all chain members to have an initial inventory specified. The release in Ci/yr is assigned to each irreversible colloid when the release values are calculated for the invert module (EBSFILT). The colloid release values can be adjusted by using a user-specified colloid release 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. Because radionuclides bound to colloids are not affected by the solubility limit, an enhanced solubility limit is calculated to account for the presence of colloids before RELEASET is called. In this way, the aqueous portion of the released radionuclide is still limited by the intended solubility limit.

In the irreversible colloid model, colloid filtration (permanent removal) is applied at stratographic unit boundaries in the unsaturated zone when flow is in matrix units. A colloid retardation factor is sampled and used for all colloid-associated species. The effects of reversible colloids are modeled using equations that calculate an effective retardation factor.

The Calico Hills nonwelded lithologic thickness comprises vitric (CHnv) and zeolitic (CHnz) components. Given any two of the three quantities, the third can then be determined. The overall unsaturated zone CHn thickness is constant for a given subarea, and the uncertainty in the CHnv thickness is reflected by a sampled parameter in *tpa.inp*. The CHnz thickness is calculated from these quantities.

The current dispersivity parameter value for the unsaturated zone transport module has a realistic lower limit of 0.01 m [0.33 ft] for layer thicknesses less than 40 m [131.2 ft].

<u>Input Data Management</u>

The pH and CO_2 parameter value distributions in TPA Version 5.1 have been carefully tailored to site data, and effective ranges within *coefkdeq.dat* are optimized to this data. Modifying pH or CO_2 distributions would likely produce many realizations where a default K_d of zero is produced. A similar result may also be produced by lack of correlation between pH and CO_2. Because these values are not intended to be modified by an inexperienced user, the pH and CO_2 data will be moved from *tpa.inp* to *tpa_include.inp*.

Consideration of Decay Chains

Previous versions of the TPA code have encountered difficulties in certain realizations that include the Cm-Am-Np decay chain, leading to a suggestion to remove the Cm-Am-Np decay chain from consideration in simulations longer than 100,000 years. To address this issue, *tpa.inp* will be updated to provide guidance on which decay chains to consider for such long simulations. Supporting analyses will be required to justify under which circumstances certain decay chains can be excluded from consideration and what if any compensating changes to radionuclide inventories may be needed (e.g., it could be necessary to increase Np inventory to account for the exclusion of the Cm-Am portion of the Cm-Am-Np decay chain).

Limitations of the External NEFMKS Radionuclide Transport Code

A limitation of the current TPA code is that long run times are often encountered for some realizations because of the NEFMKS transport code must use extremely small timesteps to simulate short travel times. This issue was addressed in the previous TPA versions by bypassing unsaturated zone transport calculations altogether for realizations where the calculated unsaturated zone groundwater travel time is less than 20 years. Complete bypassing of unsaturated zone transport, however, may bias total-system results. Experience has shown that NEFMKS problems are generally associated with realizations in which sampled values of the Calico Hills nonwelded vitric (CHnv) Layer are less than about 2 m [6.6 ft] thick. To address this issue, the *tpa.inp* values for layer thicknesses to UZFT will be updated so that thin layers less than approximately 2 m [6.6 ft] thick for the CHnv unit will be set to zero. If the layer thickness is to be a sampled parameter, the sample distributions will be modified such that samples will be selected from user-specified distributions that use either zero values or values greater than approximately 2 m [6.6 ft].

Colloid Filtration in the Unsaturated Zone

Colloid filtration will be applied in the unsaturated zone as a one-time filtration event. This approach is based on a conceptual model that the fraction of colloid filtration does not increase with distance traveled or the number of layers through which the colloids flow.

2.13 Saturated Zone Flow and Transport (*szft.f*)

The streamtube dimensions of width and length are specified in *strmtube.dat* as a table of constant values used for all realizations. The uncertainty of these data is reflected by representing a streamtube width multiplier as a sampled parameter. This width multiplier is applied to all streamtubes for their entire lengths. The range of this multiplier is consistent with the data values in *strmtube.dat* so that the total streamtube width remains within realistic limits.

TPA Version 5.1 permits the saturated zone flux to change in response to climatic conditions. The change to climatic conditions relative to present-day conditions is available in *climato2.dat* in UZFLOW. This change is contained in a velocity file that reflects the time-dependent flux change at the assigned porosity. The degree of this effect is controlled by the *tpa.inp* input parameter that controls the climatic deviations relative to present-day conditions as applied to the flux rates. The present-day flux rates are specified in *strmtube.dat*.

For the saturated zone transport calculations, TPA Version 5.1 allows users to select running NEFMKS once for the entire saturated zone combining tuff and alluvium legs or twice with separate runs for the tuff and alluvium. When separate transport legs are considered, some realizations may have transport legs in tuff with very short travel times. As discussed in the preceding section, the NEFMKS transport code may fail to run or result in long run times for realizations with fast groundwater travel times. It may therefore be necessary to modify SZFT such that transport legs with short travel times are bypassed in NEFMKS transport simulations.

In TPA Version 5.1 separate probability distributions for the colloid retardation factor will be implemented for fractured tuff and alluvium. The reference data set for TPA Version 5.1 will not consider retardation of dissolved species in tuff fractures; however, the user can consider this process by specifying values greater than 1.0 or probability distributions for fracture retardation factors.

2.14 Determination of Receptor Dose—Groundwater Release (*dcagw.f*)

DCAGW determines the dose to the receptor by considering three controlling parameters: (i) distance to the receptor, (ii) receptor lifestyle, and (iii) climate conditions. The distance to the receptor is a *tpa.inp* parameter that determines the streamtube width at the receptor location. The basecase distance to receptor location is approximately 18 km [11.2 mi]. The receptor lifestyle is a *tpa.inp* parameter used to select the residential or farming library of dose conversion factors to be used in the dose calculations. The biosphere climate conditions select the current biosphere or pluvial biosphere library of dose conversion factors to be used in the dose calculations. The dilution volume is specified in *tpa.inp* as 3,000 acre-ft/yr [3.7×10^6-m^3/yr].

DCAGW also produces the U.S. Environmental Protection Agency groundwater protection output files *gwppktim.res* and *gwp_ave.res* with physical units consistent with the standards (e.g., mrem/yr and pCi/L). Uranium is not included in the output because it is not part of the standard.

No additional modifications have been proposed for DCAGW for TPA Version 5.1 beyond the capabilities previously described in Section 2.14 of this software requirements description. Note, however, that a request is pending for copyright permission to use the input data set for dose conversion factors derived from the International Commission on Radiological Protection, Publication 72. If the International Commission on Radiological Protection refuses copyright permission, dose conversion factors that are derived from a non-copyrighted source, such as Federal Guidance 11, will be implemented.

2.15 Volcanic Ash Remobilization Model 1 (*ashremob.f*)

The ash remobilization model is implemented with two modes of operation. The first mode uses ASHREMOB to calculate the evolution of airborne concentration of high-level waste at the receptor location following a volcanic eruption. In ASHREMOB, results from detailed analytical work and an ash remobilization model account for variations in wind speed and wind direction along the height of the tephra column and for first-order processes affecting fluvial and eolian remobilization of ash. The second mode is consistent with previous abstractions for a single wind speed and direction per realization, which invoke ASHPLUMO, ASHRMOVO, and DCAGS.

The ash remobilization model calculates a time history of airborne concentrations of high-level waste at the receptor location. The concentrations are based on the resuspension of material from three source regions: initial ash deposit at the receptor location, fluvially remobilized ash in Fortymile Wash, and ash deposited in the Yucca Mountain region and remobilized by eolian processes. ASHREMOB accounts for the inhalation pathway, which is a dominant pathway in the direct release scenario, and there are no calculations for other pathways, such as groundshine or ingestion.

Values for TPA Version 5.1 input parameters and data for a lookup table, which accounts for the effect of a stratified wind field on ash dispersion and deposition during modeled eruptions, were generated to accompany the implementation of ASHREMOB. The lookup table is based on TEPHRA code calculations of a three-dimensional deposition of ash with a stratified wind field and provides eight parameters that characterize the tephra deposit.

ASHREMOB will be modified to accept the number of waste packages or mass of high-level waste entrained as determined by VOLCANO. Additionally, header information that includes improved descriptions of output will be added to the output file named *ashremob.out*.

2.16 Volcanic Ash Deposition (*ashplumo.f*)

This module is retained for backward compatibility with previous versions of the TPA code where it was the only module available to model ash deposition. The user may utilize ASHPLUMO by selecting the nonbasecase mode of operation for the volcanic eruption scenario. This mode invokes ASHPLUMO, ASHRMOVO, and DCAGS instead of ASHREMOB. ASHPLUMO is described in more detail in Mohanty, et al. (2002). No changes have been made to this module since the user's guide.

No additional modifications are proposed for ASHPLUMO for TPA Version 5.1 beyond the capabilities previously described in Section 2.16 of this software requirements description.

2.17 Volcanic Ash Remobilization Model 2 (*ashrmovo.f*)

This module is retained for backward compatibility with previous versions of TPA where it was the only module available to model ash remobilization. ASHRMOVO is used in calculations for the nonbasecase mode of operation for the volcanic eruption scenario. This mode invokes ASHPLUMO, ASHRMOVO, and DCAGS instead of ASHREMOB. ASHRMOVO is described in more detail in Mohanty, et al. (2002). No changes have been made to this module since the user's guide.

No additional modifications are proposed for ASHRMOVO for TPA Version 5.1 beyond the capabilities previously described in Section 2.17 of this software requirements description.

2.18 Determination of Receptor Dose—Direct Release (*dcags.f*)

The airborne mass loading model in DCAGS allows an expanded set of airborne mass loading and occupancy fraction parameters to be used. The basecase volcanic eruption scenario, which invokes ASHREMOB, utilizes an inhalation pathway model (i.e., airborne mass loading and occupancy fraction model) that is consistent with the inhalation model in DCAGS to determine the contribution from the initial deposit at the receptor location. The user may utilize the full dose pathway analysis in DCAGS by selecting the nonbasecase mode of operation for the volcanic eruption scenario.

For transparency and traceability, the mass loading and occupancy factors in DCAGS are divided into several inside and outside categories. Five categories of occupancy fractions are used, including one category for time spent offsite. Each airborne mass load parameter corresponds to a specific occupancy fraction parameter. Contributions from the five occupancy fraction categories for inhalation are summed and used to compute a biosphere dose conversion factor for inhalation. After the GENTPA code generates the biosphere dose conversion factors for the noninhalation exposure pathways, DCAGS sums the biosphere dose conversion factors and computes the total dose from all pathways. Biosphere dose conversion factors are computed for each realization. This mechanism is consistent with DCAGW.

No additional modifications are proposed for DCAGS for TPA Version 5.1 beyond the capabilities previously described in Section 2.18 of this software requirements description.

3 TECHNICAL BASIS FOR REQUIREMENTS: PHYSICAL AND MATHEMATICAL MODELS

The technical basis for all models and abstractions in TPA Version 5.1 will be documented in a user guide which is presently being developed. Because the user guide is not yet complete, the following sections summarize documents that contain much of the currently available information that was used as the technical basis for TPA Version 5.1 development. The following information will be superseded upon publication of the TPA Version 5.1 User Guide (expected by September 2007).

3.1 Executive Input (*reader.f*)

The technical basis and basic operation of READER are detailed in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are described in Section 2.1 of this software requirements description. Source references and technical bases for TPA Version 5.1 input parameters and data files have also previously been compiled in Appendix A of Mohanty, et al. (2002). Many new parameters and data inputs have been added to the TPA code that will be included in TPA Version 5.1. Additionally, basecase values or statistical distributions for numerous previously existing parameters have been updated. Effort to provide updated technical bases for all TPA Version 5.1 input parameters is ongoing. A database of updated basecase input parameter justifications, therefore, will be developed in conjunction with the code development.

3.2 Executive Output (*exec.f*)

There are no physical or mathematical models in this module that require a technical basis. The operation of EXEC is described in detail in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are described in Section 2.2 of this software requirements description.

3.3 Climate and Infiltration (*uzflow.f*)

The technical basis and basic operation of UZFLOW are described in detail in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are described in Section 2.3 of this software requirements description.

3.4 Near-Field Environment—Chemistry (*nfenv.f*)

The technical basis and basic operation of NFENV are described in detail in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are described in Section 2.4 of this software requirements description. The methodology and technical basis for the current abstraction is discussed in greater detail by Mohanty, et al. (2005, Chapter 3).

3.5 Drip Shield Lifetime (*dsfail.f*, *dsfailt.f*)

A general summary of DSFAIL and DSFAILT is given in Section 2.5 of this software requirements description. Detailed descriptions of the methodology and technical basis for the current abstraction of drip shield corrosion are provided by Mohanty, et al. (2005, Chapter 13).

3.6 Mechanical Failure (*seismo2.f*)

The abstraction of mechanical failures of waste packages has been modified significantly since TPA Version 4.1j to account for mechanical interaction with drip shields. The technical basis for this abstraction is provided by Ofoegbu, et al. (2007) and Ibarra, et al. (2007).

3.7 Near-Field Environment—Temperature (*nfenv.f*)

The technical basis and basic operation of NFENV are described in detail in TPA Version 4.1j and summarized briefly in Section 2.7 of this software requirements description. The methodology and technical basis for this abstraction are described in greater detail by Mohanty, et al. (2005, Chapter 11). Additional technical bases for parameter selections are provided in Fedors, et al. (2005).

3.8 Waste Package Lifetime (*ebsfail.f*)

The technical basis and basic operation of EBSFAIL are described in detail in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are summarized briefly in Section 2.8 of this software requirements description. The methodology and technical basis for the current abstraction are described in greater detail by Mohanty, et al. (2005, Chapter 3).

3.9 Faulting (*faulto.f*)

A complete description of the technical basis for FAULTO can be found in Mohanty, et al. (2002). No changes have been made to this module since TPA Version 4.1j.

3.10 Igneous Activity (*volcano.f*)

The technical basis and basic operation of VOLCANO are described in detail in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are described in Section 2.10 of this software requirements description. These sources provide sufficient technical bases.

3.11 Source Term (*ebsrel.f*)

The abstraction of radionuclide release source term has been modified significantly since TPA Version 4.1j to include a glass source term and a source term for radionuclides that are reversibly and irreversibly attached to colloids. A general summary of the current EBSREL is given in Section 2.11 of this software requirements description. Detailed descriptions of the methodology and technical bases for these modifications, however, have not been prepared. Planned modifications to the colloid source term abstraction are discussed in Section 3.11. An updated technical basis for EBSREL, therefore, will need to be developed.

With regard to the colloid source term abstraction, the following specific tasks have been identified:

- The cited documents (Ebert and Bates, 1992; Finn, et al., 1996; Wilson, 1990a,b) will be reviewed during development of the colloid source term abstraction to ensure that the effects that have been observed (e.g., plating out) can be explained in relation to the adopted abstraction or incorporated into the abstraction, if relevant. These documents will be considered in the development of the technical basis for the colloid abstraction.

- Written documentation of the technical basis for colloids will be developed concurrently with the TPA Version 5.1 abstraction. This documentation should describe both reversible and irreversible colloid abstractions, colloid filtration, the method for calculating J-species radionuclide concentrations, and the method for accounting for limited sorption sites for irreversible sorption to colloids.

3.12 Unsaturated Zone Flow and Transport (*uzft.f*)

The technical basis of UZFT is detailed in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are summarized briefly in Section 2.12 of this software requirements description. A more detailed description of the methodology and technical basis for the current abstraction of radionuclide retardation in the unsaturated zone is provided by Bertetti, et al. (2005). A detailed description of the basis for input parameters to define hydrostratigraphic layers for unsaturated zone transport is provided by Fedors, et al. (2005).

Based on recent discussions, analyses are needed to determine when it may be appropriate to exclude the Cm-Am-Np decay chain from consideration. Depending on the outcome of these analyses, a validated TPA Version 5.1 code may include a comment line in *tpa.inp* input to advise users of when this decay chain may be excluded.

3.13 Saturated Zone Flow and Transport (*szft.f*)

The technical basis and basic operation of SZFT are described in detail in Mohanty, et al. (2002); modifications made since TPA Version 4.1j are summarized briefly in Section 2.13 of this software requirements description. A more detailed description of methodology and technical basis for the current abstraction of radionuclide retardation in the saturated zone is provided by Bertetti, et al. (2005). A detailed description of the basis for the input data file to define one-dimensional streamtubes for saturated zone transport calculations is provided in Fedors, et al. (2005).

3.14 Determination of Receptor Dose—Groundwater Release (*dcagw.f*)

A description of the technical basis for DCAGW can be found in Mohanty, et al. (2002). A summary of the current abstraction is provided in Section 2.14 of this software requirements description. These sources provide sufficient technical bases for the abstraction.

3.15 Volcanic Ash Remobilization Model 1 (*ashremob.f*)

The abstraction of direct release through ash remobilization is a recent addition to TPA Version 5.1 that was not included in Version 4.1j. A general summary of ASHREMOB is given in Section 2.15 of this software requirements description. A detailed description of the methodology technical basis for this abstraction is provided by Mohanty, et al. (2005, Chapter 6).

Based on recent discussions, the following specific tasks have been identified to be completed by the DIRECT2 and DOSE2 project staff to improve the technical basis for this abstraction in conjunction with the TPA Version 5.1 code development:

- Analyses are needed to ensure that this abstraction is consistent with the concept of the reasonably maximally exposed individual and that it does not presume a location of the individual in or directly adjacent to the depositional fan of Fortymile Wash. Analyses on existing TEPHRA code realizations will, therefore, be conducted to estimate the amount of tephra potentially deposited outside the current Fortymile Wash drainage basin.

- Staff need to evaluate the effects of the disconnect of ASHREMOB from VOLCANO. Presently, the TEPHRA code samples from 1 to 10 waste packages entrained, separate from any sampling in the TPA code. The proposal is to conduct all TEPHRA realizations with a single waste package, and then multiply the tephra concentrations by a factor that is the sampled number of waste packages in the TPA code. Because there is only a slight effect of waste entrainment on plume dynamics, this procedure is deemed acceptable. As noted in Section 3.15 of this software requirements description, CNWRA will recast the TEPHRA code results on this basis. Sensitivity studies for other volcanic parameters, such as eruption power or duration, will still need to use realizations from the TEPHRA code.

- A strengthened technical basis or revised model is needed to address the lack of decay related to fluvial remobilization. Checks will be performed in an offline analysis to ensure that deposition in the distal regions of the depositional basin is small by sampling TEPHRA code results at several points. This effort will include continuing reviews of the technical basis for time-dependent processes in the redistribution model.

- A technical basis is needed for the three weighting factors (initial, fluvial, and eolian). As these weighting factors are input data, the development of a technical basis may follow the actual code development.

3.16 Volcanic Ash Deposition (*ashplumo.f*)

The technical basis and basic operation of ASHPLUMO are described in detail in Mohanty, et al. (2002). No changes have been made to this module since TPA Verison 4.1j. A brief summary of the current abstraction is given in Section 2.16 of this software requirements description. These sources provide sufficient technical bases. No additional changes are planned for the update to TPA Version 5.1.

3.17 Volcanic Ash Remobilization Model 2 (*ashrmovo.f*)

The technical basis and basic operation of ASHRMOVO are described in detail in Mohanty, et al. (2002). No changes have been made to this module since TPA Verison 4.1j. A brief summary of the current abstraction is given in Section 2.17 of this software requirements description. These sources provide sufficient technical bases. No additional changes are planned for the update to TPA Version 5.1.

3.18 Determination of Receptor Dose—Direct Release (*dcags.f*)

The technical basis and basic operation of DCAGS are described in detail in Mohanty, et al. (2002). A brief summary of the current abstraction is given in Section 2.18 of this software requirements description. These sources provide sufficient technical bases. No additional changes are planned for the update to TPA Version 5.1.

4 COMPUTATIONAL APPROACH

4.1 Data Flow and User Interface

There are no significant changes required for the data flow or the user interface. Please refer to Mohanty, et al. (2002) for a description of these items.

4.2 Hardware and Software Requirements

Please refer to the discussion in the introduction to Chapter 2.

4.3 Graphics Requirements

None required.

4.4 Pre- and Postprocessors

None required.

4.5 Software Validation

Full software validation of TPA Version 5.1 will be performed in accordance with CNWRA Technical Operating Procedure TOP–018.

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