

**TOTAL-SYSTEM PERFORMANCE
ASSESSMENT (TPA) VERSION 5.1
MODULE DESCRIPTIONS
AND USER GUIDE**

Prepared for

**U.S. Nuclear Regulatory Commission
Contract NRC-02-07-006**

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**September 2007
Revised November 2007**

Attachment A	
Title: TOTAL-SYSTEM PERFORMANCE ASSESSMENT (TPA) VERSION 5.1 MODULE DESCRIPTIONS AND USER GUIDE	Revision 1 November 2007
Summary of Changes for Revision 1	
Title Page Modified to reflect 2008 new NRC contract number, revision number, and expand list of coordinators	
Acknowledgements – Page xx Modified to reflect 2008 new NRC contract number	
Page 11-28 Updated reference information in remarks column for MatrixKD_TSw_Nb[m3/kg] and MatrixKD_CHnv_Nb[m3/kg] parameters	
Page 11-29 Revised parameter values for MatrixKD_CHnz_Nb[m3/kg], MatrixKD_PPw_Nb[m3/kg], and MatrixKD_UCF_Nb[m3/kg]; updated reference information for these parameters in remarks column	
Page 11-30 Revised parameter value for MatrixKD_BFw_Nb[m3/kg]; updated reference information for this parameter and for MatrixKD_UFZ_Nb[m3/kg] in remarks column	
Page 12-22 Revised parameter value for ImmobileRd_STFF_Nb; updated reference information for this parameter in remarks column	

ABSTRACT

The Total-system Performance Assessment (TPA) Version 5.1 computer code was developed through a joint effort between the U.S. Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA) staff. TPA Version 5.1 is a review tool developed to assist staff in precicensing activities and reviewing a potential U.S. Department of Energy license application.

TPA Version 5.1 includes several changes since the last user guide was published for TPA Version 4.0. Some major changes include the following: (i) drift degradation processes and associated effects of rubble accumulation are considered, including a potential failure mechanism for drip shields and waste packages under rock loads increased by seismic activity; (ii) the waste package localized corrosion model was revised to be more consistent with experimental data, including separate consideration of corrosion on waste package welded areas; (iii) potential sources and transport of radionuclides reversibly and irreversibly sorbed to colloids are now included; (iv) the inventory source was modified to include a fraction of glass waste form; (v) the potential repository footprint geometry was revised to incorporate a more recent design layout; (vi) a tephra redistribution model was implemented to provide improved representation of volcanic eruption consequences; and (vii) dose coefficients were updated to be consistent with the International Commission on Radiological Protection Publication 72.

TPA Version 5.1 is designed to run on desktop personal computers with Microsoft® Windows®-based operating systems (e.g., Windows 2000, Windows XP) and a minimum of 2Gb of RAM (or RAM plus virtual memory). This User Guide describes the code installation and execution procedures; the underlying conceptual and mathematical models; contents of the various input and output files; input data and parameter values for a reference case; and explanation of options for generating various intermediate and summary outputs.

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UNIT CONVERSIONS				
International System of Units (SI)	SI Abbreviation	X (1 SI unit = X OC units)	Other Common Units Used in Document (OC)	OC Abbreviation
becquerel	Bq	2.70270e-11	curie	Ci
centimeter	cm	0.3937	inch	in
cubic meter	m ³	8.107144e-4	acre-foot	acre-foot
cubic meter	m ³	264.1719	gallon	gal
cubic meter per second	m ³ /s	264.1719	gallon per second	gal/s
gram	g	2.2046e-3	pound	lb
kelvins	K	subtract 273.15	degrees Celsius	°C
kelvins	K	subtract 273.15; multiply 0.555555; add 32	degrees Fahrenheit	°F
kilogram	kg	0.001	metric ton (tonne)	MT (t)
kilometer	km	0.621371	mile	mi
kilopascal	kPa	8.247228	millimeter of mercury	mmHg
kilowatt	kW	0.9481819	Btu per second	Btu/s
liter	L	0.2641719	gallon	gal
megagram	Mg	1.0	metric ton (tonne)	MT (t)
megapascal	MPa	9.86923	atmosphere	atm
megapascal	MPa	145.0377	pound-force per square inch	psi
meter	m	3.28083	feet	ft
meter per second	m/s	3.28084	foot per second	ft/s

UNIT CONVERSIONS (continued)				
International System of Units (SI)	SI Abbreviation	X (1 SI unit = X OC units)	Other Common Units Used in Document (OC)	OC Abbreviation
micrometer	μm	3.937e-5	inch	in
millimeter	mm	3.937e-2	inch	in
mole	mol	6.022e+23	atom	atom
mole per cubic meter	mol/m ³	1.0e-3	mole per liter	M
mole per cubic meter	mol/m ³	1.0	mole per liter	mol/L
radian	rad	57.2958	degree (angular)	deg
second	s	1.1574e-5	day	d
second	s	3.1688e-8	year (365.25 d)	yr (a)
sievert	Sv	100.0	rem	rem
square kilometer	km ²	247.105	acre	acre
square meter	m ²	2.471e-4	acre	acre

ACKNOWLEDGMENTS

This User Guide for TPA Version 5.1 documents work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC-02-07-006. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of High-Level Waste Repository Safety. This User Guide is an independent product of the CNWRA and does not necessarily reflect the view or regulatory position of the NRC. The NRC staff views expressed herein are preliminary and do not constitute a final judgment or determination of the matters addressed or of the acceptability of a license application for a geologic repository at Yucca Mountain.

The contributions of Bret Leslie and James Durham, who served as the central coordinators for this entire document, and Christopher Grossman, who assisted in coordination, are greatly appreciated. Technical and programmatic reviews performed by Bret Leslie, Christopher Grossman, Andrew Campbell, Keith Compton, and Albert Wong contributed to the overall consistency and quality of this document. The administrative support provided by Beverly Street, Leona Selvey, and Nora Naukam, and the editorial reviews by Lauren Mulverhill were essential to the timely completion of this document. Appreciation is also given to Bret Leslie, Christopher Grossman, James Durham, Patrick Laplante, Ron Janetzke, Femi Osidele, and Ali Simpkins for their service on the TPA User Guide Committee, which provided guidance to authors and reviews to ensure consistency in content and level of detail. The authors gratefully acknowledge benefitting from the foundation of the user guide previously developed for TPA Version 4.0 (Mohanty, et al., 2000).

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: No original CNWRA-generated data are contained in this report.

ANALYSES AND CODES: No original technical analyses are presented in this user guide. This report documents the technical basis for and use of TPA Version 5.1, which has been developed and fully validated in accordance with CNWRA Technical Operating Procedure TOP-018.

REFERENCE:

Mohanty, S., T.J. McCartin, and D.W. Esh. "Total-system Performance Assessment (TPA) Version 4.0 Code: Module Descriptions and User's Guide." San Antonio, Texas: CNWRA. 2000.

1 INTRODUCTION

1.1 Background

To more effectively fulfill its statutory responsibilities for the licensing of the potential high-level waste repository at the Yucca Mountain site, the U.S. Nuclear Regulatory Commission (NRC) has focused its high-level waste program on resolving issues most critical to overall system performance. The core objective of the NRC high-level waste program is to review a potential license application for a possible future geologic repository at Yucca Mountain, Nevada. In preparation for this objective, the NRC has undertaken prelicensing activities to ensure sufficient information is submitted for a high-quality license application, including

- Interactions with the U.S. Department of Energy (DOE) repository program to gain clarification of potential designs, performance assessments, and supporting information
- Prioritization of NRC activities to focus on key aspects of potential repository performance
- Enhancement of NRC staff understanding and review capabilities
- Development of a regulatory framework, including NRC regulations and staff guidance

To support these activities, NRC staff has developed a generalized computer code specifically tailored for evaluating the total system performance for the potential repository at the Yucca Mountain site. Although NRC previously developed computer codes (Codell, et al., 1992; Wescott, et al., 1995; Mohanty, et al., 2002) to analyze potential repository performance, an updated performance assessment code was developed as an aid in the development of regulatory risk insights that can help to focus a licensing review of the potential geologic repository at Yucca Mountain, Nevada.

This user guide facilitates the effective use of the Total-system Performance Assessment (TPA) Version 5.1 computer code, which was developed through a joint effort between NRC and the Center for Nuclear Waste Regulatory Analyses (CNWRA) staff. This report describes the conceptual and mathematical models; instructions for preparing input files; code installation and execution; explanation of options for generating various intermediate and summary outputs; and example input files for the reference case.

1.1.1 Purpose of TPA Version 5.1 Development

One of the purposes for using TPA Version 5.1 is to simulate a range of potential performance outcomes of the potential repository and secure a detailed and quantitative understanding of the overall risk significance of key factors that control the (i) degradation of the engineered barrier system; (ii) release of contaminants from the potential repository; (iii) subsequent transport of contaminants through various environmental pathways; and (iv) possible human exposure at the locations of the designated receptor. To achieve this understanding, the potential repository system is modeled in a probabilistic manner (Thompson and Sagar, 1993) that considers significant physical and chemical processes, phenomenological interactions and

couplings, and possible disruptive events and processes. This probabilistic approach yields a range of potential future evolutions of the potential repository system. In addition, this approach is favored because it avoids limitations associated with completely deterministic scenario-based assessments, such as the inability to account for uncertainty in model parameter and site characterization data (Thompson, 1988).

1.1.2 Description of the Potential Repository Site

The conceptual and mathematical models included in TPA Version 5.1 were largely selected to be specific to the characteristics and conditions of the Yucca Mountain site. Accordingly, a brief description of the Yucca Mountain site geology, hydrology, climatology, and current potential repository design are presented in this section.

Located in Nye County, the Yucca Mountain site (Figure 1-1) is approximately 120 km [75 mi] northwest of Las Vegas in southern Nevada. The site is entirely on federal land controlled by DOE, the Bureau of Land Management, and the Nellis Air Force Range. The current climate at the site is generally arid to semiarid, with an average precipitation of about 185 mm/yr [7.29 in/yr] in the form of winter rains and snow and summer thunderstorms.

Yucca Mountain is bounded by Crater Flat on the west, by Jackass Flat–Fortymile Wash on the east and southeast, by the Amargosa Basin to the south, and by the Timber Mountain Caldera complex to the north. The stratigraphy at Yucca Mountain is composed of a gently dipping sequence of Miocene ash-flow tuffs, lavas, and volcanic breccias more than 1,800 m [1.12 mi] thick. The rock unit being considered for the potential repository facility is a densely welded ash-flow tuff of the Topopah Spring Member of the Paintbrush Tuff. The potential repository horizon is in the unsaturated zone (UZ)¹ approximately 350 m [1,148 ft] below ground surface and 350 m [1,148 ft] above the water table. There are considerable data for the hydraulic and transport properties of the UZ in Wittwer, et al. (1995); Rautman, et al. (1995); Schenker, et al. (1995); and Civilian Radioactive Waste Management System, Management and Operating Contractor (1998).

The saturated zone (SZ)² in the Yucca Mountain region of interest to possible radionuclide transport can be divided into two major aquifer systems: a fractured tuff aquifer below the potential repository location extending approximately 5–20 km [3.1–12.4 mi] downgradient and an alluvial aquifer extending southward from the terminus of the tuff aquifer to the Amargosa Basin. Patterns of groundwater flow in the tuff aquifer appear to be determined by the combined effects of hydraulic boundary conditions, dipping layers, and the presence of fault zones and laterally extensive shear fracture zones (Geldon, 1993). In contrast, groundwater flow in the alluvial aquifer is likely controlled by the interrelationship of recharge and discharge areas, interbasin transfers, and water-well pumping in the Amargosa Desert area.

¹The unsaturated zone is referenced frequently throughout this chapter. The abbreviation UZ will be used.

²The saturated zone is referenced frequently throughout this chapter. The abbreviation SZ will be used.

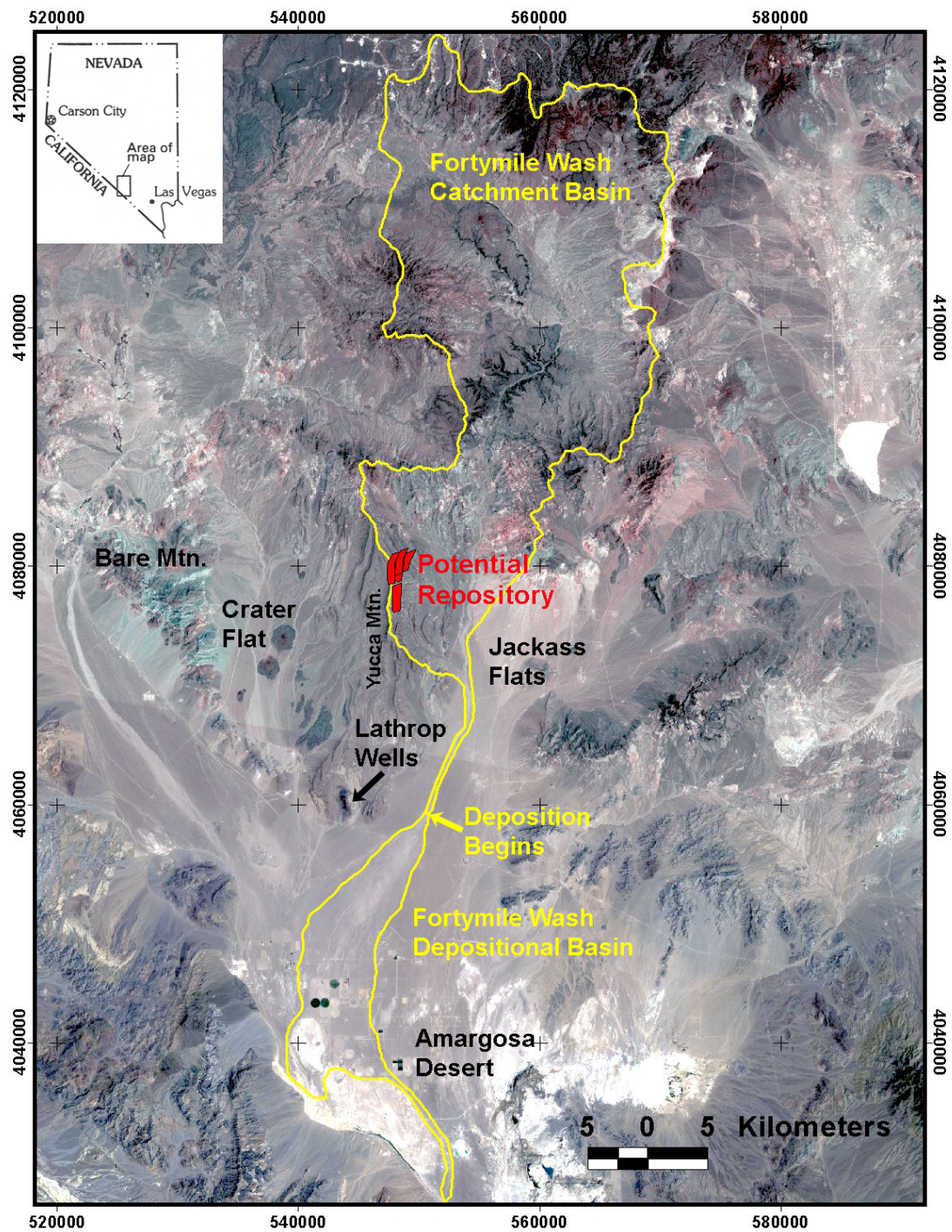


Figure 1-1. Map Location of Yucca Mountain Region

The potential repository at Yucca Mountain is an underground facility designed to accommodate 70,000 metric tons of high-level waste. The waste disposed in the potential repository is expected to consist of commercial spent fuel (~90 percent), vitrified and defense waste, and other DOE high-level waste (~10 percent), with an age between 5 and 50 years. Through a thermal loading strategy that includes an 81-m [266-ft] drift spacing, DOE intends to limit the heating of rock between drifts (i.e., pillars) so that a significant portion of the pillars remain below the boiling temperature of water. Thus, infiltrating and thermally driven water above the potential repository may flow through the cool pillars. The rock in the immediate vicinity of the drifts may be heated above boiling, which may reduce seepage into the drift during the thermal period. DOE intends to create cool pillars and dry drifts using wide drift spacing, close waste package spacing, proper blending of the high-level waste to reduce variation in waste package heat outputs, and active ventilation from the time of waste emplacement through the 50–150 year period before closure (DOE, 2002).

The DOE potential engineered barrier system is expected to include waste packages and drip shields. The waste package design for high-level waste disposal consists of a large cylinder {i.e., approximately 1.8-m diameter and 5.6-m length [5.9-ft diameter and 18.4-ft length]} that includes a 20-mm [0.79-in]-thick Alloy 22 outer container and a 50-mm [2-in]-thick stainless steel type 316NG inner container. The purpose of the outer container is to resist corrosion. The waste package is expected to be emplaced in the drift on a V-shaped support pallet. A drip shield with a thickness of 15 mm [0.59 in] and made of Titanium Grade 7, covers the top and side of the waste package and extends over the length of the emplacement drift. The drip shield is intended to protect the waste package from groundwater dripping onto the waste package surface, especially during the thermal reflux period when the environmental conditions are expected to be conducive to crevice corrosion of the Alloy 22 outer container. Prior to the repository closure, the potential design relies on active ventilation of the loaded emplacement drifts to remove a substantial fraction of the heat emitted by the waste and thus limit temperature-induced cladding failure. Ventilation may also control the relative humidity during the preclosure period (DOE, 2002).

1.2 Overview of TPA Version 5.1 Development

Several versions of TPA have been released since its inception. The history of TPA development is discussed in the last published user guide (Mohanty, et al., 2002) for TPA Version 4.0.

The main motivation behind the creation of TPA Version 5.1 is to reflect updated understanding of processes (e.g., processes related to drift degradation, near-field environment, corrosion of metallic materials potential to construct drip shields and waste packages, and redistribution of tephra following a volcanic eruption).

Consistent with the recommendations of Iterative Performance Assessment Phase 2 (Wescott, et al., 1995), TPA Version 5.1 was developed to include

- Most recent site data and knowledge base for conceptual models
- Most recent potential repository design specifications
- Updated abstractions for features, events, and processes

- Streamlined data transfers between executive and consequence modules
- Improved computational algorithms permitting more detailed analyses
- Improved presentation of results for transparency and traceability

Federal radiation protection standards and regulations for high-level waste disposal in a potential geologic repository are being revised by the U.S. Environmental Protection Agency and NRC, respectively. Site data continue to be acquired, and potential repository and waste package designs continue to evolve. Therefore, it was deemed important to enhance TPA Version 5.1 by increasing its flexibility to evaluate alternative potential repository and design features, analyze the effect of different areal mass loadings for igneous scenarios, and assess performance for periods longer than 10,000 years.

TPA Version 5.1 was developed using technical contributions from staff responsible for reviewing DOE performance assessment model abstractions (NRC, 2003). In addition to contributing to the development of TPA Version 5.1, the technical staff members tested and documented TPA Version 5.1 and prepared the input data set for the reference case.

1.3 Summary of TPA Version 5.1 Changes Since the Previous User Guide

TPA Version 4 was updated to Version 5.1 in response to recommendations from the Risk Analysis for Risk Insights report (Mohanty, et al., 2005); recommendations from the Integrated Issue Resolution Status Report (NRC, 2005); insights from sensitivity analyses with TPA Version 4; new information from site characterization, updated potential repository designs, and updated understanding of processes; and consideration of drift degradation and its associated effects on engineered components. A summary of the major changes implemented in TPA Version 5.1 is provided in the following paragraphs.

Treatment of drift degradation has been added to TPA Version 5.1. Drift degradation may be caused by thermal stresses and seismic events. Various engineered barrier system models have been updated to include the drift degradation process. For example, the thermal model to compute drip shield, waste package, and drift wall temperatures has been revised to reflect the potential accumulation of rubble on drip shields as time elapses. The seepage model also has been revised to add flexibility to account for the relationship between seepage and drift temperature and to characterize seepage diversion by partially degraded structures of the engineered barrier system. A possible consequence of drift degradation is drip shield collapse with the subsequent transfer of rock loads to the waste package. A model has been added to evaluate consequences of drip shield collapse and waste package breaching based on considerations of strength and stiffness of materials. The model for seismic events in TPA Version 4 has been superseded. In the new model, seismic events can cause (i) rockfall from drift walls, (ii) rubble consolidation, and (iii) breaching of drip shields and waste packages due to the transient amplification of rock loads during the events. Chapters 6, 9, and 10 contain additional details.

Corrosion models of drip shield and waste package materials have been updated to reflect current understanding of processes. The Alloy 22 localized corrosion model has been revised to be more consistent with experimental data. In the update, welded regions on the waste package are allowed to be more susceptible to localized corrosion than mill-annealed regions. Also, the action of chemical species in water that promote (e.g., chloride) and inhibit (e.g., nitrate and bicarbonate) localized corrosion has been incorporated in the model. A new near-field environment abstraction has been implemented to provide chemical inputs to the localized corrosion model, enhancing the flexibility to incorporate ranges of concentrations of ionic species. In contrast, TPA Version 4 concentrations were provided via static lookup tables. Chapters 7 and 8 contain additional details.

An updated approach to determine the number of failed waste packages contributing to release has been implemented. The approach considers the likelihood of water contacting waste forms beneath compromised drip shields and waste packages and the initiation of localized corrosion on the waste package. The approach to determine the amount of water contacting waste forms in waste packages contributing to release also has been revised. User-defined parameters consider partial water diversion by compromised drip shields and waste packages. In TPA Version 4, a single parameter was used to represent the combined water diversion by the drift wall, drip shield, and waste package. TPA Version 5.1 allows for a flexible evaluation of release consequences for various waste package breaching mechanisms. Chapter 10 contains additional details.

Actinides transported in colloidal form may be a relevant source of radionuclide migration in a potential repository. Accordingly, a new colloidal source and transport model has been developed for TPA Version 5.1. Radionuclides irreversibly sorbed to colloids (referred to as intrinsic colloids) are tracked as unique species. A model for the source of intrinsic colloids has been developed based on the concept of radionuclide competition for available sorption sites. Also, the geosphere radionuclide transport model has been adjusted to simulate transport of both intrinsic colloids and species that are reversibly sorbed to colloids. Chapters 10, 11, and 12 contain additional details.

The source term model has been extended to consider high-level waste glass. The glass inventory is small compared to the spent fuel inventory in the potential repository system. However, the volume occupied by the glass is significant. TPA Version 5.1 considers waste packages enclosing high-level waste glass. Chapter 10 contains additional details.

The discretization of the potential repository footprint into subareas has been revised to incorporate the latest available DOE potential repository design layout, patterns of present-day net surface infiltration, and UZ rock properties beneath the potential repository footprint. Chapter 11 contains additional details.

A tephra redistribution model has been implemented to provide alternate estimates of volcanic eruption consequences by accounting for wind-field variations along the height of the eruption column and first-order processes affecting fluvial and eolian redistribution of tephra. Chapter 16 contains additional details. In contrast, the model in TPA Version 4 implemented a single wind direction and a single wind speed for calculating the atmospheric transport and deposition of tephra. In TPA Version 5.1, redistribution of tephra is modeled explicitly.

Revised dose coefficients from the International Commission on Radiological Protection Publication 72 (International Commission on Radiological Protection, 1996) have been incorporated into TPA Version 5.1 to enhance dosimetry capabilities. While the dosimetry capabilities implemented in TPA Version 4, based on International Commission on Radiological Protection Publication 30 (International Commission on Radiological Protection, 1979), are maintained as a user-selectable option in TPA Version 5.1, the coefficients based on more recent data and models are used for the reference case. Some of these revised dose coefficients differ significantly from the prior values. Additional details are provided in Chapter 17.

In summary, revisions included in TPA Version 5.1 address uncertainties, enhance the technical basis of models, add flexibility to evaluate processes, and reflect updated understanding of processes.

1.4 Organization of User Guide Conventions

1.4.1 User Guide Chapters

This user guide was prepared as the reference document for TPA Version 5.1 and provides information on the system parameters, conceptual models, input parameters, and code outputs essential to interpreting calculational results. Additionally, this user guide presents the major assumptions, input parameters, and model implementations. Each chapter title identifies the conceptual model described therein as well as the module name in parentheses. The chapter order approximates the sequential flow of nominal (i.e., expected) scenario processes at the potential repository, with the disruptive scenario modules placed toward the end.

Chapter 2 provides an overview to the overall modeling approach and describes the primary conceptual models and their interrelationships. It describes the conceptualization of the potential repository and the geologic setting. It also summarizes the major abstracted processes for the nominal TPA Version 5.1 scenarios and the alternative and disruptive scenarios.

Chapter 3 provides instructions for installing and running TPA Version 5.1, including instructions for the first-time user. Chapter 3 also describes the input file structure. It discusses the types of probability distributions that can be sampled using Latin Hypercube Sampling and Monte Carlo Sampling.

Chapter 4 describes the execution of TPA Version 5.1, explaining how data are read, how consequence modules are invoked, and how various utility modules (e.g., parameter sampling and radionuclide inventory calculations) are used. Chapter 4 also serves as an introduction to the consequence modules presented in the 13 subsequent chapters.

Chapters 5 through 17 describe the conceptual and mathematical models implemented in the TPA Version 5.1 consequence modules. These chapters also delineate the major assumptions of and model support for each module. These chapters are intended to be structured similarly according to the convention described in the following paragraphs.

The beginning of each chapter briefly describes the consequence module in its simplest form. Typically the description is one or two paragraphs. The intended audience for this introduction is a user who wants a very general overview of the purpose of the consequence model.

Section 1 is titled Conceptual Model, and it qualitatively describes the model at the conceptual level of detail. This section describes the model domain (e.g., temporal and spatial scope), the basic elements modeled (i.e., key features, events, and processes that are included) and important interactions between these key features, events, and processes. The intended audience for this section is a new user who is trying to understand TPA Version 5.1 for the first time.

Section 2, Model Support and Assumptions, briefly describes why the approach taken in the module is believed to be appropriate for regulatory review purposes. This section is not intended to justify the input parameters; instead, it provides justification for the models used. This section also lists and describes any assumptions that underlie the consequence model. This section is also intended for a new user who is trying to understand TPA Version 5.1 for the first time and as a reference for the more experienced user.

Section 3 is titled Implementation of Conceptual Model in TPA Version 5.1. This section explains how the models are implemented in the module. This includes the mathematical representations of key features, events, and processes that are part of the module and the information flow and logic regarding how the module executes these mathematical representations. Included are key equations that are incorporated into TPA Version 5.1. The intended audience for this section is a user who is interested in a detailed description of the module.

Section 4, Input Parameters in *tpa.inp*,³ is composed primarily of a table that lists the input parameters associated with the module. In TPA Version 5.1, input parameters are those parameters defined in *tpa.inp*. Narrative in this section typically further describes those parameters that are highly abstracted. The table contains (i) the name of the input block in *tpa.inp* in which the parameter is defined; (ii) the parameter name as it appears in TPA Version 5.1 and in *tpa.inp*; (iii) the parameter description, including the symbol used to describe the parameter in any equations using the parameter; (iv) the distribution type (i.e., constant, integer constant, probability distribution, etc.); (v) the value of the parameter for the reference case; and (vi) remarks on the parameter, including justification of the reference case value. Note that the listed input parameter distributions and values are provided for the release of TPA Version 5.1 and are subject to change in subsequent versions of TPA Version 5.1 or updates to the input data.

Section 5 is titled Auxiliary Input Data and External Process Models and describes any auxiliary input data files or external process models the module uses. An external process model is a model or code that is run to generate auxiliary input data for TPA Version 5.1. External process models typically are executed once to generate data that is used for multiple realizations. This section describes the output of the external process model without detailing how the model produces the data. Auxiliary input data files, which are listed in this section, are files other than *tpa.inp* that supply input data to TPA Version 5.1 and are contained in the

³Italics represent the name of files that are created by the user or generated by TPA Version 5.1.

\data subfolder distributed with the code. Standalone codes that are executed during a simulation are discussed in their respective chapters.

Section 6, Intermediate Outputs and Information Passed to Other Abstractions, describes the contents of intermediate output files that the module produces.

The final section in Chapters 5 to 17, Section 7, is titled Techniques for Understanding Module Performance. This section informs the user about how to take advantage of specific code capabilities and analysis techniques to better understand how the module works. This section defines techniques that can provide insight into the models used in the module.

Finally, Chapter 18 describes the input files for TPA Version 5.1 and Chapter 19 describes the full set of code output files. Appendix A describes the external process model Infiltration Tabulator for Yucca Mountain. Appendix B provides a detailed description of the models used for heat transfer in the near-field environment module.

1.4.2 Conventions Used in the Text

Several conventions have been adopted for use in the TPA Version 5.1 User Guide. This section describes the conventions and provides justification for their use when appropriate.

The first convention involves file names, module names, and subroutine names. File names are highlighted using italics and lowercase letters (e.g., *tpa.inp*); abbreviations or acronyms for module names are written in all capital letters (e.g., NFENV). When a module name is mentioned for the first time in a chapter, the full name of the module is provided, followed by the abbreviation or acronym [e.g., the Near-Field Environment module (NFENV)]. Subsequent references to the module use only the abbreviation or acronym, including in figures and tables. When a chapter references a module, only the abbreviation or acronym is mentioned, even if the module appears after the chapter in which it is referenced. This convention was adopted to minimize confusion when referencing various modules (see Chapter 4 for module names).

The next convention involves using the terms scenario and case. Scenarios consider a sequence of features, events, or processes. The nominal scenario, the igneous disruptive scenario, the seismic disruptive scenario, and the faulting disruptive scenario are included in TPA Version 5.1. The nominal scenario considers a progression of features, events, and processes that are expected to occur at the potential repository, while disruptive scenarios consider features, events, and processes with lower probabilities. For a given scenario, different cases can be simulated. The reference case for a given scenario indicates using *tpa.inp* data that is included with TPA Version 5.1. Nonreference cases incorporate user-supplied input parameters.

Code that was incorporated in TPA Version 4 or earlier may have been superseded in TPA Version 5.1, and the superseded code is no longer supported. However, for certain modules, the legacy code was not removed from TPA Version 5.1, and it can be invoked by changing the reference case parameter values in *tpa.inp*. In the user guide, the superseded portions of TPA Version 5.1 are mentioned (but not described), and the parameters that need to be changed to invoke the legacy code are discussed in the chapters. The user's guide for TPA Version 4.0 (Mohanty, et al., 2002) presents a more thorough discussion of the superseded code.

The values of input parameters in *tpa.inp* must be entered using the correct system of units (typically Système Internationale). For this reason, dual units are not supplied when a *tpa.inp* parameter is described in the user guide, including figures and tables. A list of unit conversions is provided at the front of this user guide.

When an input parameter is used in an equation or mentioned in the text, both the symbol for the parameter and the parameter name are listed consecutively. This convention was adopted to help the user understand how the input parameters related to the equations in Section 3 of Chapter 5 through 17.

Finally, the user guide describes TPA Version 5.1 and helps the user execute it. The features, events, and processes included in the user guide describe the models in TPA Version 5.1. During the long development history of TPA Version 5.1, understanding many of the features, events, and processes discussed in this guide was considered to enhance the staff's review capability for a potential license application for a potential repository at Yucca Mountain. However, including the features, events, and processes in TPA Version 5.1 and in this user guide does not necessarily represent any conclusions regarding actual present or future conditions at Yucca Mountain or any position regarding the expected disposition of features, events, or processes in any future performance assessment conducted for Yucca Mountain. Furthermore, the DOE is responsible for developing and documenting the case for licensing the potential repository; the sole purpose of the TPA Version 5.1 is to provide a tool to enhance staff understanding and assist the review of any such case presented to the NRC.

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2 OVERVIEW OF TPA VERSION 5.1 CONCEPTUAL MODELS

A key part in developing TPA Version 5.1 is determining the level of detail in the processes, design, and attributes of the potential repository site that are necessary to produce a credible analysis that provides meaningful performance insights without an unreasonable computational burden. TPA Version 5.1 includes the potential repository system description (e.g., representation of the site and potential repository design), conceptual models, and parameter values. The potential repository system description and conceptual models are presented in this section to provide a general overview of TPA Version 5.1.

2.1 Conceptualization of Potential Repository Design and Geologic Setting

2.1.1 Potential Repository Design

The Yucca Mountain site is briefly described in Section 1.1.2. A list of some of the potential repository design characteristics considered in TPA Version 5.1 is provided in Table 2-1.

Table 2-1. TPA Version 5.1 Reference Case Configuration	
Design Characteristics	TPA Version 5.1
Areal mass loading	53.9 MTU/acre [13,300 MTU/km ²]
Emplacement area	1,299 acres [5.257 km ²]
Drift spacing	81 m (center to center)
Drift diameter	5.5 m
Invert	Crushed tuff
Number of waste packages	12,177
Total length of emplacement drifts	64.537 km [40.110 mi]
Waste package materials	2-cm Alloy 22 over 5-cm Stainless Steel 316NG
Maximum waste package capacity	21 pressurized water reactor assemblies
Drip shield	1.5 cm Ti-7
Backfill	None (optional)
Waste package heat output at emplacement	13,400 W/MTU
Preclosure period	100 years

2.1.2 Potential Repository Setting

TPA Version 5.1 approximates the intricate potential repository layout and the complex geologic setting using simplified conceptual representations. The potential repository layout, for example, is represented by an idealized planar feature discretized into a set of discrete homogeneous subareas, while the geology is replaced by a sequence of homogenous layers. Except for the influence of the thermal load, flow and transport processes in and below a given

subarea are modeled to be independent of those processes in other subareas. Flow in the unsaturated zone (UZ)¹ (i.e., geologic media between the land surface and the water table) is treated as vertical within each subarea; lateral flow is not considered.

As illustrated in Figure 2-1, quadrilateral subareas of uniform thickness are used to represent individual subregions of the potential repository. In the current reference case, the potential repository is divided into 10 subareas; however, TPA Version 5.1 can use much finer discretizations of both the potential repository and the geologic setting beneath it. The number of waste packages in each subarea is proportional to the fraction of the total potential repository area represented. Radionuclide releases from the engineered barrier system are calculated by modeling a single representative waste package for each subarea and for each failure type. Performance characteristics of the waste package in each subarea are calculated by considering the evolution of such characteristics as water flux, thermal and chemical conditions, and geologic processes (e.g., seismicity, fault displacement, and igneous activity).

Dividing the potential repository footprint area into subareas allows consideration of spatial variability in the behavior of the engineered and natural systems in TPA Version 5.1. In the reference case, dividing the design footprint into subareas is based solely on natural system considerations (e.g., patterns of present-day net surface infiltration and UZ rock properties beneath the potential repository footprint).

The geologic setting is composed of the UZ and the saturated zone (SZ)² (i.e., the groundwater aquifer beneath the potential repository and extending to the location of the receptor). For simplicity, the stratigraphy is assumed to be laterally continuous and uniform within a subarea to represent the UZ in a separate hydrostratigraphic sequence for each subarea. The geologic setting also includes disruptive features, events, and processes such as seismicity, faulting, and volcanism that affect the performance of the potential repository. The TPA Version 5.1 conceptual model of flow and transport in the SZ consists of three distinct streamtubes over the width of the potential repository footprint that are normal to UZ flow (Chapter 12 contains a detailed description and illustration). Each of the 10 subareas in the UZ is connected to 1 of the 3 streamtubes in the SZ.

2.2 Summary of Major Abstracted Processes for the Nominal Scenario

The following discussion provides a general overview of the key aspects of the major conceptual models in the nominal scenario implemented in TPA Version 5.1 through the use of several different modules. More detailed descriptions of these modules, including the mathematical basis, assumptions, and calculational methodologies, are presented in Chapters 5 through 17.

¹The unsaturated zone is referenced frequently throughout this chapter. The abbreviation UZ will be used.

²The saturated zone is referenced frequently throughout this chapter. The abbreviation SZ will be used.

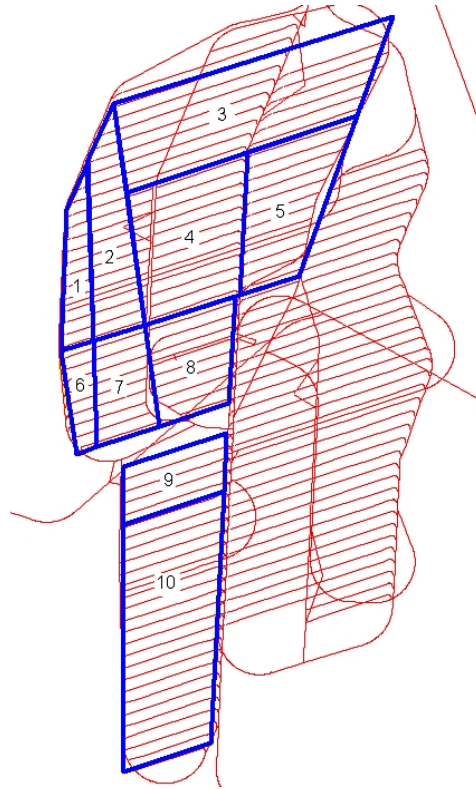


Figure 2-1. Potential Repository Drifts and TPA Version 5.1 Reference Case Subarea Quadrilaterals

In TPA Version 5.1, the performance of a representative waste package and drip shield is modeled for each potential repository subarea. The waste package is conceptualized as two concentric hollow cylinders, denoted as the outer container and the inner container. The waste package rests on an invert, and a drip shield serves as a cover over the entire length of the waste package and invert. The drip shield material is titanium alloy, the waste package outer container material is Alloy 22, and the waste package inner container material is 316NG stainless steel. The performance of the inner container as a barrier is not explicitly considered in TPA Version 5.1, although its structural contribution is included. In TPA Version 5.1, waste package failure occurs when the outer container is breached. Because the outer container is expected to contain numerous welds, it is modeled as having two different regions: mill-annealed and welded Alloy 22. Although the two materials are similar chemically, the welding process is expected to change the metallurgical properties of the welded region that affect localized corrosion.

In the nominal scenario, waste package failures are grouped into four basic categories: (i) localized corrosion failure, (ii) mechanical failure, (iii) general corrosion failure, and (iv) initially defective waste package failures. Waste package contents are modeled as either spent nuclear fuel or high-level waste glass, both waste packages are differentiated only by initial inventories, and both waste packages are modeled as having identical geometries. The following discussion is applicable to a single realization for the reference case.

2.2.1 Infiltration and Deep Percolation

For each realization, the Climate and Infiltration module (UZFLOW)³ (Chapter 5) calculates the areal-average flux of downward-moving water immediately above the potential repository horizon (deep percolation) within each subarea without considering heat generated by the waste packages. Other modules use this water flux to establish the potential repository near-field environment, and the water flux is available for waste package corrosion, dissolution of material in the waste package, and transport of material released from waste packages. UZFLOW considers the history of climatic change and ground surface and subsurface characteristics and performs two main functions. It provides subarea-average percolation fluxes to the Near-Field Environment module (NFENV)⁴ (Chapter 7) to estimate water fluxes that enter the drifts and subarea-average percolation fluxes to the Unsaturated Zone Flow and Transport module (UZFT)⁵ (Chapter 11) for transport of radionuclides through the UZ.

2.2.2 Near-Field Environment

Physical and chemical processes in the near field of the potential repository, such as heat transfer, water–rock geochemical interactions, and refluxing of condensate water, are expected to affect waste package performance. NFENV calculates (i) the heat transfer and temperature on a mountain and drift scale, (ii) the relative humidity in the drift, (iii) the thermally driven refluxing of groundwater, and (iv) the chemical composition of seepage water in the vicinity of the potential repository drift. The movement of fluids in the vicinity of the potential repository is conceptualized as a coupled process of heat transfer (convection, conduction, and radiation), fluid movement (evaporation, condensation, and reflux), and chemistry (dissolution, precipitation, and deliquescence). The heat from radioactive decay causes dry out in the near-field and in-drift components during the peak thermal pulse. The dryout zone above the drift keeps water from entering the drift and contacting the waste package except by preferential flow along fractures that breach the dryout zone. NFENV provides the temperature and relative humidity to the Waste Package Corrosion Failure module (EBSFAIL)⁶ (Chapter 8), the water flow rate and temperature to the Engineered Barrier System Radionuclide Release module (EBSREL)⁷ (Chapter 10), and in-drift heat transfer information and temperature to the Drift Degradation module (DRIFTFAIL)⁸ (Chapter 6).

³The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

⁴The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

⁵The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

⁶The Waste Package Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

⁷The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

⁸The Drift Degradation module is referenced frequently throughout this chapter. The abbreviation DRIFTFAIL will be used.

2.2.3 Engineered Barrier System Failure and Radionuclide Release

In TPA Version 5.1, mechanical failure of the engineered barrier system requires failure of the drip shield and subsequent failure of the waste package caused by waste package–drip shield interactions under rock loads. Mechanical failure of the drip shield is modeled as a result of the combination of corrosion and accumulation of rubble on the drip shield. The Drip Shield Corrosion Failure module (DSFAIL)⁹ (Chapter 8) calculates the thickness of the drip shield as a function of time since emplacement. The thickness of the drip shield is modeled to decrease as a result of general (uniform) corrosion of the drip shield. DSFAIL provides the drip shield thickness as a function of time and the time of corrosive failure to the Drip Shield and Waste Package Mechanical Failure module (MECHFAIL)¹⁰ (Chapter 9).

In the nominal scenario, rubble from rockfall accumulates on the drip shield due to spallation of the drift wall (static loading), which occurs due to the heat of the waste packages. For the seismic disruptive scenario, dynamic loading events are determined using the SAMPLER utility module (Chapter 4), which probabilistically determines the timing and peak ground acceleration of each seismic event for the entire duration of the realization. Static loading is calculated in DRIFTFAIL. For each timestep in the realization, MECHFAIL calculates the combined static (for nominal and seismic scenarios) and dynamic loading (for seismic scenarios) applied to the drip shield (demand).

MECHFAIL also calculates the strength (vertical-load-carrying capacity) of the drip shield taking into account the mechanical properties of the drip shield. The drip shield vertical-load-carrying capacity is expected to decrease due to creep processes, temperature (supplied by NFENV), and corrosion of the drip shield (supplied by DSFAIL). To account for these effects, MECHFAIL applies multiplicative factors to decrease the drip shield load-carrying capacity. MECHFAIL compares the demand to the modified vertical-load-carrying capacity; when the computed demand exceeds the vertical-load-carrying capacity, the drip shield is considered failed. When the drip shield does not undergo mechanical failure by the time that the drip shield thickness becomes zero, the drip shield undergoes corrosive failure.

After drip shield failure, EBSFAIL uses a corrosion rate to determine the thickness of the waste package outer container as a function of the time after emplacement and the time of waste package failure for both general corrosion and for localized (crevice) corrosion. Through the choice of input parameters, three corrosion modes are activated: dry-air oxidation, humid-air oxidation, and aqueous corrosion either as general corrosion or localized corrosion. The corrosion mode (and subsequent corrosion rate) is determined by the relative humidity of the near-field environment, which is provided by NFENV, and the deep percolation flux provided by UZFLOW. EBSFAIL calculates the uncorroded thicknesses (initial thickness minus corroded depth) of the mill-annealed Alloy 22 waste package surface excluding localized corrosion, the mill-annealed Alloy 22 waste package surface including localized corrosion, and the welded areas of the waste package. When the penetrated depth exceeds user-defined fractions either in the mill-annealed or welded areas of the waste package, the waste package is breached.

⁹The Drip Shield Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation DSFAIL will be used.

¹⁰The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAIL will be used.

The time of failure is passed to EBSREL. The uncorroded outer container thickness as a function of emplacement time is passed to MECHFAIL.

When the drip shield has failed, MECHFAIL calculates the vertical-load-carrying capacity of the waste package (including the structural contribution from the inner container), taking into account the corroded outer container thickness from EBSFAIL and the temperature of the near-field environment from NFENV. When the computed demand exceeds the ultimate tensile strength, the waste package is considered to be mechanically failed. When the thickness of the outer container reaches zero before mechanical failure, the waste package is considered failed by corrosion.

2.2.4 Radionuclide Release

Once the waste package is failed, EBSREL calculates the time-dependent release rate of radionuclides from the engineered barrier system. EBSREL computes water delivery to waste forms inside breached waste packages, waste form dissolution, dissolved and colloid-facilitated radionuclide release from waste packages, and transport to the UZ. EBSREL uses time-dependent seepage water flow rates and waste package temperatures from NFENV, the breach time from DSFAIL, and the number of breached waste packages and waste package and mechanical drip shield breach times for various failure modes from EBSFAIL and MECHFAIL to calculate subarea radionuclide release rates as a function of time, which are passed to UZFT.

EBSREL computes the release rate by accounting for the following four model elements: (i) estimates of the amount of water flowing into and out of the waste package, (ii) mass balance of radionuclides in water inside the waste package, (iii) a source term for colloidal releases, and (iv) upscaling of radionuclide release rates from a representative waste package to a subarea for each of several failure modes.

Scaled water flow rates are used to calculate dissolution of radionuclides in water accumulated inside breached waste packages. Radionuclide concentration computations account for (i) decay and ingrowth of inventories; (ii) inventories inside the waste package including waste forms, radionuclides in solution, and radionuclides in precipitated phases; (iii) solubilities of radionuclide-bearing solid phases; (iv) different waste form dissolution rates for spent fuel and high-level waste glass; and (v) radionuclides carried by flowing water away from the waste package (i.e., advective release).

Advective radionuclide releases are adjusted to simulate the release of colloids with irreversibly adsorbed radionuclides. The source-term colloidal model is based on the concept of competitive sorption, under which radionuclides compete for available sorption sites on colloids according to element-dependent affinity factors (i.e., elements with higher affinities more readily occupy sorption sites in colloids).

2.2.5 Flow and Transport of Radionuclides

UZFT calculates the release rate of radionuclides into the SZ below the potential repository footprint by simulating transport of radionuclides in the UZ between the potential repository and the water table using a one-dimensional flow model. In the abstracted conceptual model for TPA Version 5.1, the 10 potential repository subareas extend as vertical prisms through the UZ

from beneath the potential repository to the water table. The rocks in the UZ are represented as a set of layered hydrostratigraphic units with specified hydrogeological properties that affect flow and transport. The layer properties are the same in every subarea, except that the thickness of each layer differs from one subarea to another to represent spatial variation in stratigraphy.

The Saturated Zone Flow and Transport module (SZFT)¹¹ (Chapter 12) describes radionuclide transport in the SZ beginning from the location where flow paths from the UZ reach the water table below the potential repository and ending at a user-specified distance downstream from the potential repository area.

Radionuclide transport processes included in both UZFT and SZFT include (i) advective transport with longitudinal dispersion, (ii) sorption of radionuclides to host rock, (iii) migration of radionuclides reversibly or irreversibly attached to colloids, and (iv) radionuclide decay and ingrowth of progeny products. Matrix diffusion, the movement of radionuclides from flowing fractures into the rock matrix, is only considered for the tuff aquifer portion of the SZFT calculations.

2.2.6 Exposure Pathways and Reference Biosphere

Dose calculations are performed in TPA Version 5.1 by exposure pathways that consider releases to the geosphere and atmosphere followed by transport of released material by various processes to an offsite human receptor. In the reference case, the receptor is an individual adult member of a rural residential farming community located south of the potential repository site in an arid or semiarid climate zone. The biosphere includes those features and processes of the region surrounding Yucca Mountain that can contribute to human exposure to released radionuclides.

The Dose Conversion Analysis for Groundwater module (DCAGW)¹² (Chapter 17) executes pathway and dose conversion calculations. In the reference case, DCAGW calculates doses from groundwater releases.

The biosphere pathway and dose calculations are consistent with the characteristics of the physical environment surrounding Yucca Mountain and the characteristics of the receptor that can be exposed to releases from the potential repository. Regulations in 10 CFR 63.312 define specific characteristics of the receptor (the reasonably maximally exposed individual), and 10 CFR 63.305 addresses the surrounding environment of the receptor (reference biosphere). These characteristics define the exposure pathways for TPA Version 5.1 calculations.

¹¹The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

¹²The Dose Conversion Analysis for Groundwater module is referenced frequently throughout this chapter. The abbreviation DCAGW will be used.

2.3 Summary of Alternative Models and Disruptive Scenarios

Not all disruptive events that can be simulated by TPA Version 5.1 are selected in the nominal scenario. In particular, the faulting, seismic, and igneous activity simulations are not enabled. In addition, several of the numerical models have two or more modes of operation. Some of the modes maintain the ability to compare results from previous versions, while others permit the comparison of two different, but viable, approaches to modeling a given physical phenomenon. Selecting the models that are executed for a simulation is controlled in *tpa.inp*.

The *tpa.inp* file has two parameter types (iflag and iconstant) that are used to control the execution of alternative models, model modes, and disruptive scenarios. The parameter values for the reference case do not execute all of the models or all of the disruptive scenarios. While the disruptive scenario flags and the models they control are not mutually exclusive, other flags control parts of some models that are mutually exclusive, and as such, only one modeling approach from a set of two or more can be executed in a simulation.

The simulation features whose execution can be controlled in this way are volcanism, faulting, seismic activity, drift degradation, invert radionuclide transport, and irreversible colloids. The operational modes that are controlled by flags or constants are sampling mode (Chapter 3); UZFLOW sample mode, annual infiltration loss, and climate perturbation; NFENV thermal model, particle model, temperature reference point, usage of tabular temperature and relative humidity, water contact modes, number of weights for Legendre integration; EBSREL release model selection, control for using the seepage threshold, partial protection from seepage; DCAGW plume capture model selection, present-day dilution model, age and dosimetry model, groundwater protection output; the Igneous Disruptive Event Involving Magma module (VOLCANO)¹³ (Chapter 14) extrusive event mode; the Igneous Activity Deposition and Evolution of Ash module (ASHRMOVO)¹⁴ (Chapter 16) ash evolution mode, direct release only mode; UZFT usage of the Network Flow and Transport in Time-Dependent Velocity Fields code (NEFMKS)¹⁵ (Chapter 11), adopted from the code NEFTRAN II (Olague, et al., 1991) velocity file; and SZFT selection of separate runs of NEFMKS for the tuff and alluvium layers in the SZ.

2.3.1 Seismicity

Seismicity is one of the disruptive processes that TPA Version 5.1 can simulate. Seismicity is not considered in the nominal scenario, but can be activated by the SeismicDisruptiveScenarioFlag(yes=1,no=0) input control flag.

The characteristics of seismic events are associated with the seismic hazard curve specified in *tpa.inp*. The sampling is controlled with an independent random number generator rather than

¹³The Igneous Disruptive Event Involving Magma module is referenced frequently throughout this chapter. The abbreviation VOLCANO will be used.

¹⁴The Igneous Activity Deposition and Evolution of Ash module is referenced frequently throughout this chapter. The abbreviation ASHRMOVO will be used.

¹⁵The Network Flow and Transport in Time-Dependent Velocity Fields code is referenced frequently throughout this chapter. The abbreviation NEFMKS will be used.

the Sandia National Laboratory Latin Hypercube Sampling standalone code. Characteristics associated with the seismic hazard curve are the mean annual frequency of exceedance, peak ground velocity, peak ground acceleration, and rubble compaction factor.

The impact of seismicity on the potential repository performance is assessed through two main processes. The first is an increase in rubble accumulation computed by DRIFTFAIL for static load calculations where a linear relationship is used to compute rubble accumulation resulting from ground motion. It is noted that thermally induced drift degradation (either independently or in conjunction with seismicity) can also be considered. The second is the effect of seismic motion for dynamic load calculations. The dynamic load as a fraction of peak ground acceleration and static rubble load is computed by MECHFAIL.

2.3.2 Faulting

The Direct Faulting Disruptive Event module (FAULTO)¹⁶ (Chapter 13) calculates the fraction of the waste packages failed in each subarea and the time of their failure due to a direct fault disruption following a one-time faulting event. The analysis is conditional in that faulting occurs in each realization of the faulting scenario. Thus, results need to be weighted by an occurrence probability in a postprocessing calculation. For the nominal scenario, FAULTO is not activated.

FAULTO models faults as near-vertical planar deformation zones with a constant displacement rate and a constant length and width within which all waste packages that are intersected are breached at the time of the critical displacement. To cause damage to the waste package, the total fault slip (constant displacement plus event displacement) must exceed a user-defined threshold displacement value. Because waste packages in the current drift layout design are set back from two major faults, the Solitario Canyon fault to the west and the Ghost Dance fault to the east, the current conceptual model in FAULTO evaluates the impact of new or undiscovered faults that become active within the drift layout footprint.

2.3.3 Igneous Activity

Igneous activity involving magma interaction with waste packages is a disruptive scenario with a relatively low annual probability of occurrence but potentially high radiological dose consequence. Models of igneous disruptive events at the potential repository involve the intersection of ascending basaltic magma by way of a dike or conduit with one or more drifts; the advancement of magma into drifts; the interaction between magma and waste packages; and the eruption, dispersal, and deposition pattern of tephra. Based on large uncertainties in the behavior of engineered barriers during a volcanic event, all waste packages that are exposed to basaltic magma are assumed to fail and release waste in TPA Version 5.1.

Two types of volcanic event consequence modules, extrusive and intrusive, result in waste package failures and waste releases by way of two different pathways. Extrusive events involve the continued ascent of magma subsequent to intersection with a drift and an eruption at the surface. During its rise, magma can disrupt waste packages and directly transport

¹⁶The Direct Faulting Disruptive Event module is referenced frequently throughout this chapter. The abbreviation FAULTO will be used.

high-level waste into the accessible environment via the airborne pathway. Intrusive events are defined as subsurface igneous activity in which flowing magma penetrates drifts and enhances waste package degradation but does not breach the ground surface. After intrusive events, waste is transported from failed waste packages via the groundwater pathway.

VOLCANO simulates key potentially disruptive igneous processes related to the intrusion of basaltic magma rising along a dike or conduit within the potential repository footprint and possibly erupting at the surface. It determines (i) the timing of possible igneous events, (ii) the type of igneous event, (iii) the location and number of failed waste packages using either a geometric or user-specified distribution model, and (iv) the mass of waste released via airborne and groundwater pathways.

The geometric model assumes a simplified geometric relationship exists between ascending magma and the potential repository and therefore uses geometric constraints to calculate the number of waste package failures. To account for a range of alternative igneous scenarios, a second method was developed that incorporates composite statistical parameters to evaluate waste package disruption through a user-defined distribution. After the amount of waste released to the groundwater and airborne pathways is calculated, the amount due to intrusion is provided to the groundwater release module in EBSREL, and the amount due to extrusion is provided to one of two direct release modules described next.

The extrusive consequence modules assume that the magma intercepts waste packages, moves upward to the land surface, and then ejects the tephra and spent fuel mixture into the atmosphere. The physical characteristics of each simulated eruption (e.g., conduit size, event power, and event duration) and atmospheric conditions are treated as statistical parameters in calculations of tephra dispersal and deposition patterns, tephra deposit thickness, and radionuclide soil concentrations. Three primary factors determining the tephra plume geometry and transport rates include

- Power and duration of the eruption
- Wind speed and direction
- Spent fuel particle sizes

Following an extrusive event, the mobilization of contaminated ash to the receptor can be considered using one of two approaches as described in the following two sections.

2.3.3.1 Ash Remobilization Consequence Module

The igneous scenario reference case uses the Igneous Activity Ash Remobilization module (ASHREMOB)¹⁷ (Chapter 15) to calculate the evolution of airborne concentration of high-level waste at the receptor location following a volcanic eruption. In ASHREMOB, an ash remobilization model accounts 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.

¹⁷The Igneous Activity Ash Remobilization module is referenced frequently throughout this chapter. The abbreviation ASHREMOB will be used.

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 calculates doses from the inhalation pathway, which is the dominant pathway in direct releases. There are no dose calculations for other pathways such as external dose from contaminated soil or ingestion.

2.3.3.2 Direct Deposition Consequence Module

The alternate consequence modules, retained from TPA Version 4.0 (Mohanty, et al., 2002), invoke the Igneous Activity Airborne Transport module (ASHPLUMO),¹⁸ ASHRMOVO, and the Dose Conversion Analysis for Ground Surface module (DCAGS).¹⁹ ASHPLUMO calculates the areal density of spent fuel on the ground surface at the receptor location after an extrusive volcanic event. The spent fuel concentration from the deposition is provided to ASHRMOVO, which redistributes the spent fuel over time. The redistributed spent fuel is subsequently provided to DCAGS for dose calculation.

2.4 References

Mohanty, S., T.J. McCartin, and D.W. Esh. "Total-system Performance Assessment (TPA) Version 4.0 Code: Module Descriptions and User's Guide." San Antonio, Texas: CNWRA. 2002.

Olague, N.E., D.E. Longsine, J.E. Campbell, and C.D. Leigh. NUREG/CR-5618, "User's Manual for the NEFTRAN II Computer Code." Washington, DC: NRC. February 1991.

¹⁸The Igneous Activity Airborne Transport module is referenced frequently throughout this chapter. The abbreviation ASHPLUMO will be used.

¹⁹The Dose Conversion Analysis for Ground Surface module is referenced frequently throughout this chapter. The abbreviation DCAGS will be used.

3 INSTALLING AND EXECUTING TPA VERSION 5.1

This chapter provides TPA Version 5.1 user information on installation, execution, and input file preparation. The first section provides installation instructions for the first-time user. The structure of *tpa.inp* is then described, followed by a description of the various probability density functions (PDFs)¹ that are available for sampled parameters. The fourth section describes sampling of the seismic hazard curve to determine seismic parameters, and the final section describes key output information generated by TPA Version 5.1.

3.1 First-Time User Instructions

The following instructions are for executing TPA Version 5.1 in the Microsoft® Windows® environment using the command prompt. TPA Version 5.1 requires 2 GB of combined memory and virtual memory on the host machine. The user will receive TPA Version 5.1 as one folder entitled TPA5.1. This folder contains a directory tree as depicted in Figure 3-1. All files and subdirectories should be copied onto the target computer or, using Windows copy and paste commands, into a folder on a hard drive. For the purpose of this example, this will be TPA5.1 on the hard drive designated d:\.

Once the folder has been copied onto the machine, access the command prompt using the Start Menu.

```
d:\>
```

Change directories using the following command

```
d:\>cd tpa5.1
```

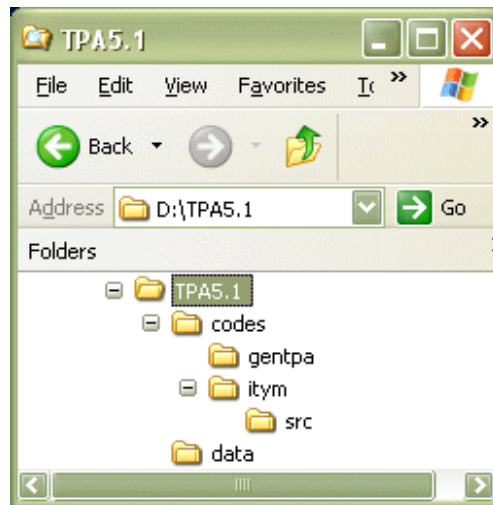


Figure 3-1. TPA5.1 Folder and Subfolder Structure

¹Probability Density Functions are referenced frequently throughout this chapter. The abbreviation PDFs will be used.

and the command prompt should now reflect

```
d:\tpa5.1>
```

Now make a new directory called `tparun` (or another name of the user's choosing) using the command

```
mkdir tparun
```

and change to that directory using

```
cd tparun
```

The command prompt should now say

```
d:\tpa5.1\tparun>
```

Environmental variables must be set, which requires the following statements to be entered:

```
SET TPA_TEST=d:\tpa5.1
SET TPA_DATA=d:\tpa5.1
```

Note that the path following the “=” must reflect the location where the user has copied the folder `TPA5.1`, which in this example is `d:\tpa5.1`. The path name string length for either environment variable cannot contain a space and cannot exceed 35 characters.

Next the user must copy the input file into the folder in which the simulation will be executed and in which all output files will be written—in this example, the `\tparun` folder—using the following command:

```
copy ..\tpa5.1\tpa.inp
```

Make any necessary changes to *tpa.inp* (see Section 3.2 for the structure of the file) within the `\tparun` folder. Note *tpa.inp* that is contained within the `\tpa5.1` folder is NOT accessed during execution. Changes to the file can be made using any standard text editor.

Other input files are discussed in Chapter 18 and do not need to be relocated to the `\tparun` folder.

To execute TPA Version 5.1, enter the following:

```
d:\tpa5.1\tparun>..\tpa.exe >tpa.out
```

where `>tpa.out` is an optional command that redirects the main screen output to a user-defined file. Depending on the scenario selected and the number of realizations, execution time can vary from seconds to hours or days. Note that each time TPA Version 5.1 is executed, the *tpa.out* and all other output files will be overwritten. To ensure the simulation is preserved, moving the entire `\tparun` folder to an archive location and saving it for each simulation is recommended. This can be accomplished using copy and paste commands within Windows

or using the command prompt. Using a mechanism that removes all files from the \tparun folder is preferred, because any files not removed may remain unaltered even though another simulation is executed. This may occur when the second simulation is executed with different input parameters, causing a different set of output files to be generated. These files can cause confusion during later analysis activities.

3.2 *tpa.inp* Input File Structure

Primary input data are contained within *tpa.inp*, which can be edited using any standard text editor. The file is large and is best navigated by becoming familiar with the general file structure and using the “find” command to locate various modules or parameters.

The file has the following general layout: global parameters, consequence-module-specific parameters, and correlated parameters. Global parameters include those that can affect the overall simulation such as scenario flags, simulation times, and output print options. The user should always check the scenario flags to ensure the intended scenario has been selected. Simulation times should be checked prior to each simulation as well as to ensure the proper time period has been entered.

To reduce the size of *tpa.inp*, a mechanism has been introduced to allow specification of seldom-modified parameters in an auxiliary data file called *tpa_include.inp*. This file is treated as part of *tpa.inp* when its name appears in *tpa.inp* following the “include” keyword. The file is located in the \data subdirectory and does not have to be present in the run directory at the start of a simulation. The format of *tpa_include.inp* is the same as that of *tpa.inp*, and it is processed completely at the point it was specified in *tpa.inp*, before processing of *tpa.inp* is continued.

With the exception of flags and the radionuclide list, every parameter in *tpa.inp* must have a distribution assigned to it. To establish a parameter distribution for each parameter, at least three lines are entered in *tpa.inp*. The first line specifies the distribution type, the second line specifies the parameter name to which the distribution is applied, and the remaining lines specify the required parameters for the distribution type. In the following example, the *tpa.inp* parameter TimeOfNextFaultingEventinRegionOfInterest[yr] is assigned to a finite exponential distribution with a recurrence rate of 2.0×10^{-5} , a lower bound of 100 years, and an upper bound of 10,000 years.

```
finiteexponential
TimeOfNextFaultingEventinRegionOfInterest [yr]
100.0, 10000.0, 2.0e-5
```

More information on the finite exponential distribution is provided in Section 3.3. Note that different distributions require different parameter specifications. **The user should exercise caution when removing or replacing program execution or parameter definition lines in *tpa.inp* as comment lines.** During program execution, each of the parameters is checked to assure it is present and has an acceptable value. Comment lines can be added to the input file by making the first character an asterisk (*). Comment lines should be placed between groups of input data to improve the readability of the input file.

Table 3-1 shows the general order of input parameter sections in *tpa.inp*. Table 3-1 also provides chapter numbers for each consequence module. Information on the specific inputs for each consequence module is provided in the respective chapter. Global parameters are discussed next. It is suggested that the user obtain a printout of *tpa.inp* or have *tpa.inp* in view on a computer screen using a text editor when reading this section.

3.2.1 Global Parameters

3.2.1.1 Disruptive Scenario Flags

This portion of *tpa.inp* determines whether or not certain disruptive processes will be executed. The disruptive processes include volcanism, faulting, seismicity, and drift degradation. It also contains the direct-release-only flag [DirectReleaseOnlyFlag(yes=1,no=0)], which is used for computational efficiency when only atmospheric releases with no groundwater releases are to be considered for the igneous disruptive scenario. Finally, it contains the ash evolution mode flag AshEvolutionMode[0=no_ashremob,1=ashremob], which is used to select the use of ASHPLUMO, ASHRMOVO, and DCAGS or ASHREMOB to treat redistribution of ash.

3.2.1.2 Simulation Times

This section of *tpa.inp* allows the user to enter two distinct simulation time periods and two simulation timesteps. The two timesteps are designed to allow a more detailed simulation at earlier times and to allow the simulation to proceed faster at later times. The two simulation times periods are defined by the *tpa.inp* parameters DurationOfCompliancePeriod[yr] and MaximumTime[yr]. The DurationOfCompliancePeriod[yr] parameter was used in TPA Version 4.0 (Mohanty, et al., 2002) and was retained in TPA Version 5.1 only to stipulate the end time for the first simulation period. The total number of timesteps for two simulation periods is limited to 5,001. The number of timesteps is directly proportional to the execution time of a simulation.

3.2.1.3 Parameter Sampling

This portion of *tpa.inp* contains information on the number of realizations. The number of realizations affects the ability of the Sandia National Laboratory Latin Hypercube Sampling standalone code (SNLLHS),² originally developed by Iman and Shortencarier (1984), to generate correlated parameter values. Correlated values cannot be properly computed unless the number of realizations is set to a value greater than the number of sampled parameters. The number of sampled parameters can be obtained from the output file *sp.tpa*. The number of realizations requested directly affects the execution time required for a simulation. Even though the user can control the first and last realizations for processing (by using the *tpa.inp* parameters StartAtRealization and StopAtRealization), caution should be used when using fewer than the suggested number of realizations. Using fewer than the suggested number of realizations does not allow for adequate coverage of the range of values in the distribution functions and can introduce instability into the simulation. The maximum allowed number of realizations is 1,024.

²The Sandia National Laboratory Latin Hypercube Sampling standalone code is referenced frequently throughout this chapter. The abbreviation SNLLHS will be used.

Table 3-1. Major Headings Within <i>tpa.inp</i>		
Major Headings	Subheadings	Chapter
GLOBAL PARAMETERS	Disruptive Scenario Flags Simulation Times Parameter Sampling Nuclides and Chains Output Print Options Groundwater Protection	3
CONSEQUENCE MODULE PARAMETERS	UZFLOW ¹	5
	DRIFTFAIL ²	6
	NFENV ³	7
	DSFAIL ⁴	8
	EBSFAIL ⁵	8
	MECHFAIL ⁶	9
	EBSREL ⁷	10
	EBSFILT	10
	UZFT ⁸	11
	SZFT ⁹	12
	FAULTO ¹⁰	13
	VOLCANO ¹¹	14
	ASHREMOB ¹²	15
	ASHPLUMO ¹³	16
	ASHRMOVO ¹⁴	16
	DCAGS ¹⁵	17
	MASS LOADING AND OCCUPANCY FACTORS	
	DCAGW ¹⁶	17
	GENTPA	17
CORRELATED PARAMETERS		
¹ Climate and Infiltration ² Drift Degradation ³ Near-Field Environment ⁴ Drip Shield Corrosion Failure ⁵ Waste Package Corrosion Failure ⁶ Drip Shield and Waste Package Mechanical Failure ⁷ Engineered Barrier System Radionuclide Release ⁸ Unsaturated Zone Flow and Transport ⁹ Saturated Zone Flow and Transport ¹⁰ Direct Faulting Disruptive Event ¹¹ Igneous Disruptive Event Involving Magma ¹² Igneous Activity Ash Remobilization ¹³ Igneous Activity Airborne Transport ¹⁴ Igneous Activity Deposition and Evolution of Ash ¹⁵ Dose Conversion Analysis for Ground Surface ¹⁶ Dose Conversion Analysis for Groundwater		

3.2.1.4 Nuclides and Chains

The user specifies the number and names of radionuclides to be considered in the groundwater pathway during the simulation. The nuclide set analyzed for the direct release pathway is always the full complement of 43 (colloids are not a direct release phenomenon in TPA Version 5.1). For more information on the nuclide set, see Chapter 4. The number of nuclides and chains analyzed directly affects the execution time required for a simulation. The user must also identify the decay chains and the order of nuclides in chains. The reference case includes 13 decay chains. If additional radionuclides are added, then radionuclide-specific data must be added for the following parameter classes: R_D s, K_D s, solubility limits, gap fractions, colloid release factors, diffusion correction factors, and parameter correlations.

For computational performance reasons, when using long simulations (greater than 100,000 years), it is recommended that the alternate nuclide set be included by replacing the reference case set with those suggested in the comment section of *tpa.inp*. This can be accomplished by commenting the reference nuclide set and uncommenting the alternative nuclide set in the input file. Instructions for these actions are included in the Nuclides and Chains subsection of the Global Parameters section of *tpa.inp*. Although a suggested set of radionuclides is included in *tpa.inp* for long simulations, the user should carefully consider the radionuclides simulated for the analysis of interest.

3.2.1.5 Output Print Options

The user can choose to generate optional intermediate output files that contain more comprehensive and detailed information. Optional intermediate output files echo other intermediate output files but append the information to the end of the file for each subarea rather than overwriting the file from the previous subarea, as is done for most of the other intermediate output files. Optional intermediate output files can grow very large; the user should make sure there is sufficient disk space to store the complete set of output files. To minimize storage issues, the user can select just one module-specific set of optional intermediate output files rather than generating the full set. There is currently no mechanism to permit the selection of two or more module-specific sets; only the full set can be selected for all modules. If this is desired and if disk space is more limited than processing time, consider executing two or more simulations with different modules selected for optional intermediate output in each simulation. Table 3-2 contains the option codes for the modules.

3.2.1.6 Groundwater Protection

The generation of output files pertaining to the groundwater protection standard is controlled by parameters in this section. See Chapter 17 for details.

3.2.1.7 Correlated Parameters

The user can correlate parameters by specifying the “correlateinputs” keyword and then listing the two parameter names for which the correlation is desired. After the parameter names are listed, the correlation coefficient is specified. The range for the correlation coefficient input is -0.9999 to 0.9999, with -0.9999 indicating a strong negative correlation and 0.9999 indicating a strong positive correlation.

Table 3-2. Optional Intermediate Output File Identification		
Option Code	Files Generated	Chapter With Additional Information
0	append all files	4
1	<i>uzflow.ech</i> and <i>uzflow.rlt</i> only	5
2	<i>nfenv.ech</i> and <i>nfenv.rlt</i> only	7
3	<i>ebsfail.ech</i> and <i>ebsfail.rlt</i> only	8
4	<i>driftfail.ech</i> , <i>driftfail.rlt</i> , <i>mechfail.ech</i> , and <i>mechfail.rlt</i> only	6 and 9
5	<i>faulto.ech</i> and <i>faulto.rlt</i> only	13
6	<i>volcano.ech</i> and <i>volcano.rlt</i> only	14
7	<i>ebsrel.ech</i> , <i>ebsrel.rlt</i> , and <i>ebsrel.cum</i> only	10
8	<i>uzft.ech</i> and <i>uzft.rlt</i> only	11
9	<i>szft.ech</i> and <i>szft.rlt</i> only	12
10	<i>dcagw.ech</i> and <i>dcagw.rlt</i> only	17
11	<i>ashplumo.ech</i> and <i>ashplumo.rlt</i> only	16
12	<i>ashrmovo.ech</i> and <i>ashrmovo.rlt</i> only	16
13	<i>dcags.ech</i> and <i>dcags.rlt</i> only	17
14	<i>ashplume.cum</i> only	16
15	<i>failt.cum</i> only	8
16	<i>nefiuz.cum</i> and <i>nefiisz.cum</i> only when SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 0	11 and 12
16	<i>nefiailuv.cum</i> and <i>nefiituff.cum</i> only when SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 1	11 and 12
17	<i>releaset.cum</i> only	10
18	<i>ggenii.cum</i> only	17
19	<i>genv.cum</i> only	17
20	<i>dcfgw.cum</i> and <i>dcfgs.cum</i> only	17
21	<i>dsfail.ech</i> and <i>dsfail.rlt</i> only	8
22	files needed by the graphical postprocessor (not currently available)	none
23	<i>infilper.cum</i> only	5, 10

When three or more parameters are correlated, the correlation coefficients of all the combinations of the three or more correlated parameters taken two at a time must be supplied. When the correlation coefficient for a combination pair is not supplied, the correlation coefficient for that pair is zero.

3.3 *tpa.inp* Sampled Parameters

The SAMPLER utility module (Chapter 4) dynamically stores and retrieves information for model input parameters with assigned PDFs. PDFs are defined in *tpa.inp* during program execution before any consequence modules are invoked. Although SAMPLER supports both Monte Carlo Sampling (MCS)³ and Latin Hypercube Sampling (LHS),⁴ LHS is the sampling scheme used in

³The sampling method Monte Carlo Sampling is referenced frequently throughout this chapter. The abbreviation MCS will be used.

⁴The sampling method Latin Hypercube Sampling is referenced frequently throughout this chapter. The abbreviation LHS will be used.

the reference case for all sampled parameters other than hazard curve sampling, which is discussed in Section 3.4. The user selects the sampling scheme in *tpa.inp*. When LHS is selected, SNLLHS develops the required random variates using a program modified from Iman and Shortencarier (1984).

The main advantage of LHS over MCS is that the parameter ranges are covered more evenly and, in general, fewer vectors are necessary to achieve statistical convergence in the results when large numbers of parameters are sampled. The output of LHS is written to *sp.tpa* with a size that depends on the number of realizations and the number of sampled values in each realization. For instance, if there are n random variables and N realizations are required, then the output file will contain N realizations, each containing n values.

3.3.1 Statistical Distributions for Sampled Parameters

The statistical distributions included in the SAMPLER utility module are

• Constant	• Normal	• Logtriangular	• Finite exponential
• Uniform	• Lognormal	• Beta	• Integer uniform
• Loguniform	• Triangular	• Exponential	• Logbeta

The mathematical representation of distribution functions available in SAMPLER is described next. Any distribution function that is not available in SAMPLER can be approximated by either the beta distribution or user distribution options in the SNLLHS standalone code.

3.3.1.1 Constant Distribution

A parameter can be specified as a constant such that it remains at a fixed value for the simulation. The constant distribution is treated as a PDF consisting of a Dirac delta function located at the value of the constant [see Boyce and DiPrima (1977) for a discussion of the Dirac delta function].

3.3.1.2 Uniform Distribution

The PDF for the uniform distribution is

$$f(x) = \frac{1}{(B - A)}, \quad A < x < B \quad (3-1)$$

where

A	—	lower bound of distribution
B	—	upper bound of distribution
x	—	independent variable
$f(x)$	—	probability density of x

3.3.1.3 Integer Uniform Distribution

The integer uniform distribution is a variation of the uniform distribution with the following changes: (i) the lower limit is specified to be $A-1$ and (ii) the outputs are rounded up to the next whole number.

These changes assume that both the lower and upper limits, A and B , are included in the distribution.

3.3.1.4 Loguniform Distribution

The loguniform distribution is a variation of the uniform distribution. The actual endpoints of the loguniform distribution are (a, b) . The endpoints passed to the uniform distribution are the logtransformation of the actual endpoints [e.g., $A = \log(a)$, $B = \log(b)$]. The exponential of the sampled value from the uniform distribution is then returned as the value for the loguniform distribution.

3.3.1.5 Normal Distribution

The PDF of the normal distribution is

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], \quad -\infty < x < \infty \quad (3-2)$$

where

μ	—	mean of distribution
σ	—	standard deviation of the distribution
σ^2	—	variance of distribution
x	—	independent variable
$f(x)$	—	probability density of x

SAMPLER generates samples having a truncated standard normal distribution (mean of 0.0 and standard deviation of 1.0) with lower and upper cutoff A and B . SAMPLER requires specification of A and B at the 0.1 and 99.9 percentiles of the normal distribution

$$P(x < A) = 0.001 \quad (3-3)$$

where

A	—	lower bound of distribution
x	—	independent variable
$P(x)$	—	cumulative probability of x

and

$$P(x < B) = 0.999 \quad (3-4)$$

where

B — upper bound of distribution

x — independent variable

$P(x)$ — cumulative probability of x

The mean of the normal distribution is

$$\mu = \frac{A + B}{2} \quad (3-5)$$

where

A — lower bound of distribution

B — upper bound of distribution

μ — mean of distribution

The variance of the normal distribution is

$$\sigma^2 \approx \left(\frac{B - A}{6.180465} \right)^2 \quad (3-6)$$

where

A — lower bound of distribution

B — upper bound of distribution

σ^2 — variance of distribution

3.3.1.6 Lognormal Distribution

The lognormal distribution is a variation of the normal distribution. The actual cutoffs of the lognormal distribution are (a, b) . The cutoffs passed to the normal distribution are the logtransformation of the actual cutoffs [e.g., $A = \log(a)$, $B = \log(b)$] and represent the 0.1 and 99.9 percentiles of the corresponding normal distribution.

3.3.1.7 Triangular Distribution

The triangular distribution is described by a minimum value, maximum value, and a mode or peak value. The PDF of the triangular distribution is

$$f(x) = \begin{cases} \frac{2(x-A)}{(C-A)(B-A)}, & A < x < B \\ \frac{2(C-x)}{(C-A)(C-B)}, & B < x < C \end{cases} \quad (3-7)$$

where

- A — lower bound of distribution
- B — mode of distribution
- C — upper bound of distribution
- x — independent variable
- $f(x)$ — probability density of x

The mean of the triangular distribution is

$$\mu = \left(\frac{A+B+C}{3} \right) \quad (3-8)$$

where

- A — lower bound of distribution
- B — mode of distribution
- C — upper bound of distribution
- μ — mean of distribution

3.3.1.8 Logtriangular Distribution

The logtriangular distribution is a variation of the triangular distribution. The actual endpoints of the logtriangular distribution are (a, c) with a peak at b . The endpoints passed to the triangular distribution are the logtransformation of the actual endpoints [e.g., $A = \log(a)$, $C = \log(c)$]. The samples are then drawn from the triangular distribution. The exponential of this sample is then returned for the logtriangular distribution.

3.3.1.9 Beta Distribution

The PDF of the beta distribution between 0 and 1 (standard beta distribution) is defined as

$$f(x) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1}, \quad 0 < x < 1 \quad (3-9)$$

where

- β — positive shape parameter
- α — positive shape parameter

x	—	independent variable
$\Gamma()$	—	gamma function
$f(x)$	—	probability density of x

The mean of the standard beta distribution is

$$\mu = \frac{\alpha}{\alpha + \beta} \quad (3-10)$$

where

β	—	positive shape parameter
α	—	positive shape parameter
μ	—	mean of distribution

The user supplies A (lower bound), B (upper bound), p (shape parameter β), and q (shape parameter α). The range of the desired distribution from A to B is linearly mapped to the standard beta distribution range (0 to 1).

3.3.1.10 Logbeta Distribution

The logbeta distribution is a variation of the beta distribution. The actual endpoints of the logbeta distribution are (a, b) . The endpoints passed to the beta distribution are the logtransformation of the actual endpoints [e.g., $A = \log(a)$, $B = \log(b)$]. The α and β positive shape parameters are also passed to the beta distribution. The samples are then drawn from the beta distribution. The exponential of this sample is then returned for the logbeta distribution.

3.3.1.11 Exponential Distribution

The PDF of an exponential distribution is

$$f(x) = \lambda e^{-\lambda x}, \quad 0 < x \quad (3-11)$$

where

λ	—	recurrence probability
x	—	independent variable
$f(x)$	—	probability density of x

The exponential distribution is frequently used to describe the time between independent events occurring at a constant average rate. In these cases, λ is the annual recurrence probability that is the reciprocal of the return period.

The mean of the exponential distribution is

$$\mu = \frac{1}{\lambda} \quad (3-12)$$

where

λ — recurrence probability

μ — mean of distribution

A random sample is drawn from the exponential distribution by

$$x = \frac{-\ln(1-u)}{\lambda} \quad (3-13)$$

where

λ — recurrence probability

u — uniform variate between 0 and 1

x — random sample

3.3.1.12 Finite Exponential Distribution

The PDF for the finite exponential distribution is

$$f(x) = \left(\frac{\lambda}{e^{-\lambda A} - e^{-\lambda B}} \right) e^{-\lambda x} \quad 0 \leq A < x < B \quad (3-14)$$

where

A — lower bound of distribution

B — upper bound of distribution

λ — recurrence probability

x — independent variable

$f(x)$ — probability density of x

The PDF is equal to zero outside the range from A to B . When the return period ($1/\lambda$) is long compared to $(B - A)$, the finite exponential is approximately a uniform distribution.

A random sample from the finite exponential is drawn by

$$x = \frac{-\ln[e^{-\lambda A} - (e^{-\lambda A} - e^{-\lambda B})u]}{\lambda} \quad (3-15)$$

where

A	—	lower bound of distribution
B	—	upper bound of distribution
λ	—	recurrence probability
u	—	uniform variate between 0 and 1
x	—	random sample

3.3.1.13 User-Discrete Empirical Distribution

If the information for an input parameter is only available in the form of equiprobable sample data, then the user-discrete empirical distribution can accommodate these data and sample them. This is accomplished by sampling directly from the empirical distribution function formed from available data. For example, suppose there are eight equally probable sample data points: 0.3, 0.7, 1.3, 1.8, 2.0, 2.6, 3.0, and 3.3. The cumulative distribution functions for these example data are shown in Figure 3-2. The step heights (probabilities) are all the same, and in this case, are equal to one-eighth of the total probability. Samples from this distribution will be one of the eight input values, and neither interpolation nor extrapolation of the data is performed. Hence, the cumulative distribution function has a staircase profile. SAMPLER also allows the input of user-supplied data for defining and sampling from a user-supplied discrete distribution and from a user-supplied cumulative distribution.

3.3.1.14 User-Supplied Discrete Distribution

The user provides both the discrete parameter values to be sampled and the corresponding probability for each value. The sum of the probabilities must equal 1.0.

3.3.1.15 User-Supplied Piecewise Cumulative Distribution Function

The user provides a number of parameter value pairs from which the minimum and maximum of the parameter range can be determined. Each parameter value is associated with the corresponding cumulative probability for the value. The first parameter value must have a cumulative probability of 0, and the last value must have a cumulative probability of 1.0.

3.3.2 TPA Version 5.1 Parameter Sampling

Table 3-3 lists the distribution functions available in TPA Version 5.1, along with examples to guide the user to the correct parameter specifications. Many distributions can be also approximately represented by choosing appropriate combinations of p and q for the beta distribution. Figure 3-3 illustrates how various distribution functions can be approximated using the beta distribution.

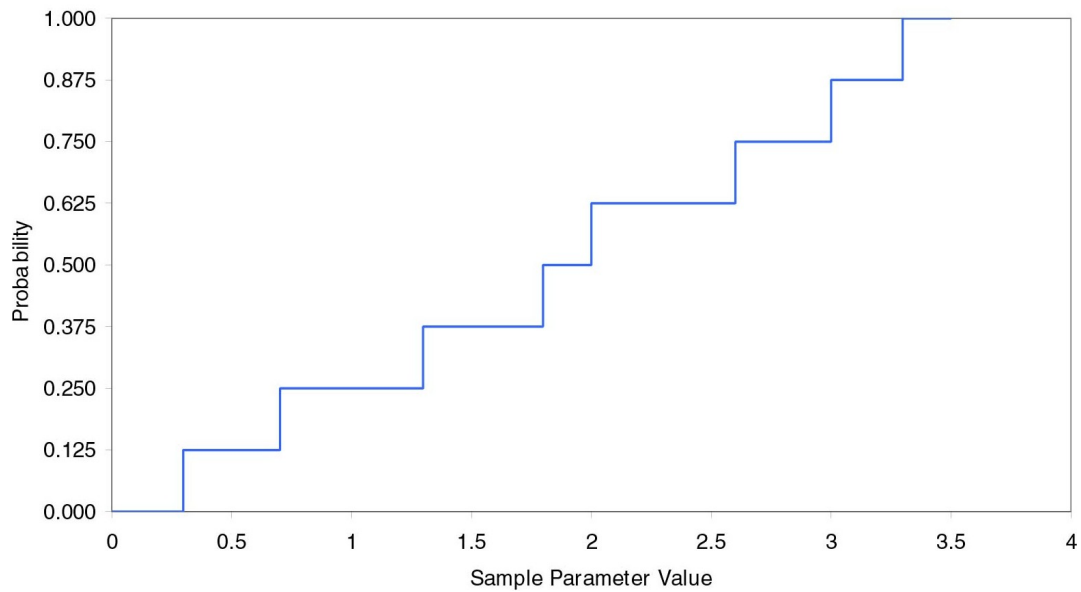


Figure 3-2. User-Discrete Empirical Distribution

Table 3-3. Distribution Functions Available in TPA Version 5.1		
Distribution	Parameter Specifications	Example
beta	A B p q A and B are distribution endpoints; ($A < B$), p , and q are shape parameters	beta RD_Invert_Cm 2001.0, 20001.0, 9.039, 18.079
exponential	λ λ is recurrence rate	exponential TimeOfNextVolcanicEventInRegionOfInterest[yr] 1.0e-7
finite-exponential	A B λ User must specify recurrence rate λ , lower and upper limits A and B ; $A < B$	finiteexponential TimeOfNextFaultingEventInRegionOfInterest[yr] 100.0, 10000.0, 2.0e-5
integer-uniform	A B User must specify endpoints A and B as integers; $A < B$	iuniform SubareaOfVolcanicEvent[] 1, 10
logbeta	A B p q A and B are distribution endpoints; ($A < B$), p , and q are shape parameters; user must specify $A > 0$ and $B > 0$	logbeta RD_Invert_Cm 2001.0, 20001.0, 9.039, 18.079

Table 3-3. Distribution Functions Available in TPA Version 5.1 (continued)		
Distribution	Parameter Specifications	Example
lognormal	$A \quad B$ User must specify $A > 0$, $B > 0$ such that $P(X < A) = 0.001$ and $P(X < B) = 0.999$	lognormal MatrixPermeability_TSw_[m2] 5.6e-20, 5.6e-18
logtriangular	$A \quad B \quad C$ A and C are endpoints of the range; B is x-coordinate distribution apex; allows for $A < B < C$ or $A = B < C$ or $A < B = C$; user must specify $A > 0$, $B > 0$, and $C > 0$	logtriangular AshMeanParticleLogDiameter[d_in_cm] 0.01, 0.1, 1.0
loguniform	$A \quad B$ User must specify endpoints $A > 0$ and $B > 0$; $A < B$	loguniform SolubilityTh[kg/m3] 5.6e-7, 3.6e-3
normal	$A \quad B$ User must specify A and B such that $P(X < A) = 0.001$ and $P(X < B) = 0.999$; $A < B$	normal ContactAngleSubarea_1[degrees] -30.8, 30.8
triangular	$A \quad B \quad C$ A and C are endpoints of the range; B is x-coordinate of the distribution apex; Allows $A < B < C$ or $A = B < C$ or $A < B = C$	triangular GapFractionForCS135 8.8e-3, 2.5e-2, 5.8e-2
uniform	$A \quad B$ User must specify endpoints A and B ; $A < B$	uniform SFWettedFraction_Initial 0.033, 1.0
user-discrete-empirical	$N \quad x(1), x(2), x(3), \dots, x(N)$ Used for sampling from distribution whose distribution is not built into the program; N is number of sample data points and $x(i)$ are equiprobable sample data	userdiscreteempirical ThresholdDisplacementForFaultDisruptionOf WP[m] 4 0.1 0.2 0.3 0.4

Table 3-3. Distribution Functions Available in TPA Version 5.1 (continued)		
Distribution	Parameter Specifications	Example
user-supplied-discrete	N x(1), y(1), x(2), y(2), x(3), y(3), ..., x(N), y(N) Used for sampling from distribution whose distribution is not built into the program; N is number of data points for which probabilities are supplied, x(i) are permissible values to be sampled for the parameter, and y(i) are the corresponding probabilities	usersupplieddiscrete CHnvThickness_9Subarea[m] 4 4, 0.6 20, 0.1 50, 0.1 70, 0.2
user-supplied-piecewise-cdf	N x(1), y(1), x(2), y(2), x(3), y(3), ..., x(N), y(N) Used for specifying the cumulative distribution function of the probability curve from which samples are made; N is the number of points defining the CDF curve in ascending order; x(1) is the exclusive minimum parameter value and must be associated with a y(1) having a value of 0; x(N) is the maximum parameter value and must be associated with a y(N) having a value of 1	usersuppliedpwisecdf KD_Soil_Se[cm3/g] 11 36.0, 0.0 38.1, 0.184 42.9, 0.274 48.3, 0.382 54.6, 0.500 61.6, 0.618 69.4, 0.726 78.3, 0.816 88.2, 0.885 99.5, 0.933 100.0, 1.0
correlate-inputs	Correlates parameters sampled from two different distributions; correlation value must be greater than or equal to -0.9999 and less than or equal to 0.9999; no more than 50 pairs of correlated inputs can be provided	Correlation inputs EnvironmentII_pH_Subarea_1[] EnvironmentII_C03_Subarea_1[mol/k] 0.9

3.3.3 SNLLHS Standalone Code

SNLLHS (Iman and Shortencarier, 1984) was modified substantially for TPA Version 5.1. This included the addition of a new distribution type—user-supplied piecewise cumulative distribution function—as well as modifications to the user-defined empirical, user-defined discrete, and beta distributions.

When the *tpa.inp* parameter LatinHyperCubeSampling(yes=1,no=0) is set to 1, the stratified sampling scheme is used by the SNLLHS. When the parameter is set to 0, SNLLHS uses Monte Carlo sampling to generate the sample. The SNLLHS code produces two output files, *lhs.out* and *lhse.out*. The main output file is named *lhs.out* and contains all of the sampled parameters for all realizations. The block format of the file enables the efficient reading of the

data in the SAMPLER utility module. All of the parameters for a given realization are grouped into a single block of data values. The second output file, *lhse.out*, captures the output of the SNLLHS standalone code that appears as screen output when SNLLHS is run as a standalone code.

3.4 Sampling of Seismic Hazard Curve

The SAMPLER utility module uses the seismic hazard curve (Bechtel SAIC Company, LLC, 2004) to obtain the timing of seismic events, the mean annual frequency of exceedance, the peak ground velocity, the peak ground acceleration, and the amount of rubble compaction for each event. Because seismic events are expected to affect the entire potential repository, SAMPLER samples the seismic hazard curve once for each realization when seismicity is activated. When sampling the seismic hazard curve, SAMPLER does not use LHS, and it uses a different random number generator than when it samples other PDFs.

Parameter specifications for sampling the hazard curve are

- HazardCurve
- number of lines of input data

Each line of input data contains values for the following five parameters (all on one line)

- mean annual frequency of exceedance [1/yr]
- mean peak ground velocity [m/s]
- median peak ground acceleration [m/s²]
- standard deviation of the natural logarithm of the mean peak ground acceleration [unitless]
- lower boundary of the compaction factor [unitless]
- upper boundary of the compaction factor [unitless]

An example of the use of the seismic hazard curve is given in Chapter 9.

Two processes are used in the seismic hazard curve sampling. First, the timing of the seismic events are selected considering a Poisson process. Then, the type and characteristics of the seismic event are selected using a truncated exponential distribution.

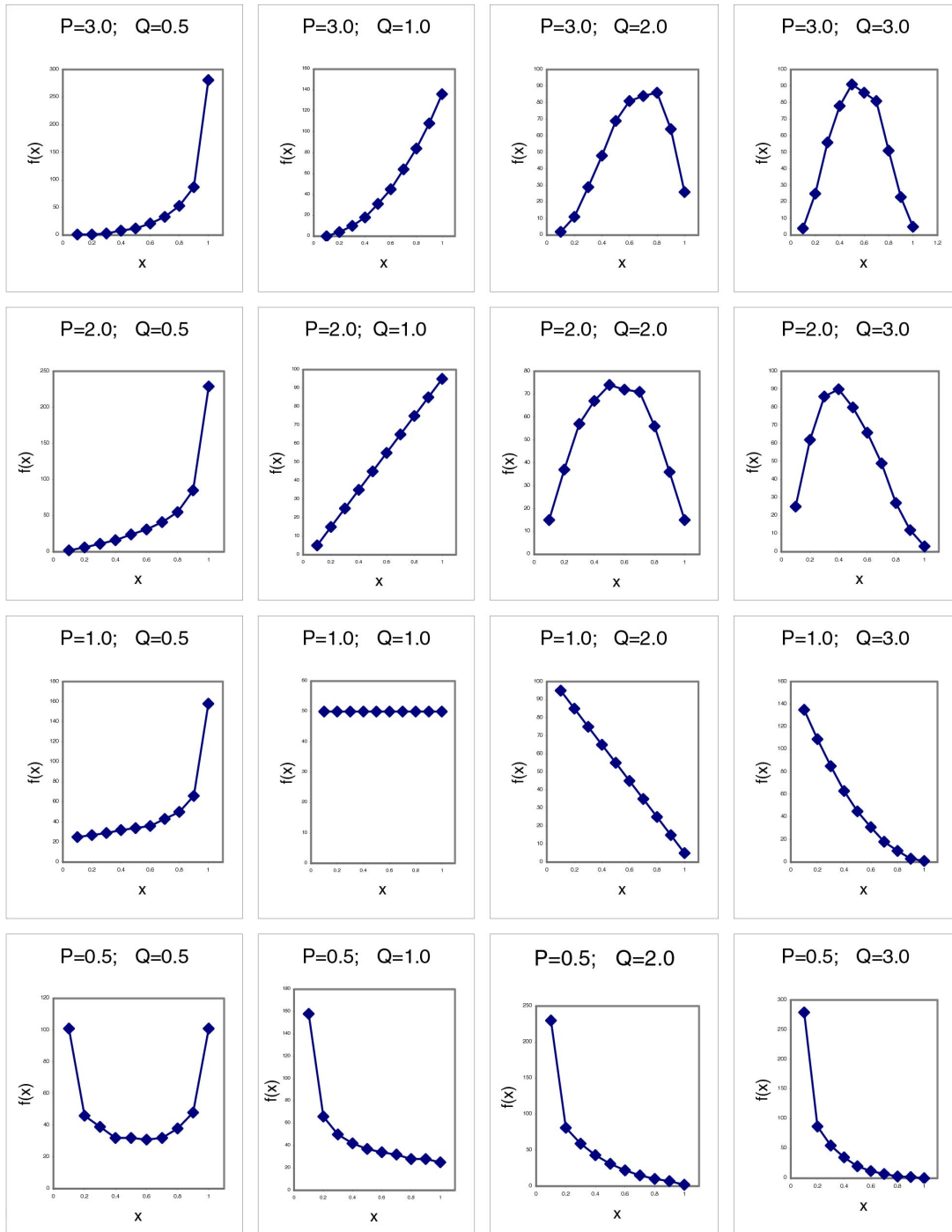


Figure 3-3. An Example Set of Distribution Functions Approximated Using the Beta Distribution

3.4.1 Timing of Seismic Events

Seismic events are modeled as a Poisson process in which discrete events occur with the probability given by

$$P(n) = \frac{(\nu t)^n e^{-\nu t}}{n!} \quad (3-16)$$

where

- $P(n)$ — probability of having n seismic events
- n — random variable representing the number of seismic events
- t — timespan being evaluated as specified by the *tpa.inp* parameter
MaximumTime[yr]
- ν — recurrence rate [yr^{-1}]

The recursion frequency used to evaluate seismicity is the largest mean annual frequency of exceedance supplied in the seismic hazard curve as specified by the MAPE parameter in the *tpa.inp* parameter array

Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_]. For the Poisson process, the interarrival time between seismic events is calculated using an exponential distribution given by

$$f_T(t) = \nu e^{-\nu t} \quad t \geq 0 \quad (3-17)$$

where

- $f_T(t)$ — interarrival time
- ν — event recurrence rate defined by the maximum frequency of exceedance as specified by the MAPE parameter in the *tpa.inp* parameter array
Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_]
- t — the time between events

SAMPLER samples 30,000 seismic events. The time of an individual event is then the sum of the interarrival times of the preceding events plus the interarrival time of the event. SAMPLER determines the target peak ground velocity in the horizontal direction, the peak ground acceleration in the vertical direction, and the rubble compaction factor for each event. The method used by SAMPLER to obtain these values is described below. SAMPLER then compares the seismic event occurrence times with the maximum simulation time, returning the number and characteristics of the seismic events which occur during the simulation time.

3.4.2 Event Probability Distribution

The mean annual frequency of exceedance (MAPE) is determined by sampling from a uniform distribution bounded by the maximum and minimum mean annual frequencies of exceedance (first and last MAPE value in the seismic hazard curve). The sampled value of the MAPE for a particular event is used to determine the target peak ground velocity and the median peak ground acceleration.

3.4.3 Target Peak Ground Velocity

Once the mean annual frequency of exceedance is computed for a seismic event, the target peak ground velocity in the horizontal direction is obtained by interpolating between the peak ground velocities that bound the MAPE of the event given by Seismic_MAPE_PGV_PGAm_PGA_{sd}_CF_{min}_CF_{max}[1/yr,m/s,m/s²,_,_,_] as specified in *tpa.inp*.

3.4.4 Median Peak Ground Acceleration

When the target peak ground velocity of an event is known, the median peak ground acceleration in the vertical direction is obtained by linearly interpolating the parameter values of “MAPE” and “PGAm” in the seismic hazard curve Seismic_MAPE_PGV_PGAm_PGA_{sd}_CF_{min}_CF_{max}[1/yr,m/s,m/s²,_,_,_]. The standard deviation of the natural logarithm of the peak ground acceleration is obtained by interpolating “MAPE” and “PGA_{sd}.” Using the interpolated median and standard deviation of the natural logarithm of the peak ground acceleration, the peak ground acceleration for an event is sampled from a lognormal distribution.

3.4.5 Compaction of Rubble After Seismic Events

In TPA Version 5.1, rubble accumulated around the drip shield is assumed to be initially loosely compacted (Chapter 6). This material, however, is expected to compact over time from shaking due to seismic events. Compaction will decrease the rubble bulking factor resulting in an increase in the vertical static pressure. The lower and upper boundaries for compaction factors for discrete mean annual frequencies of exceedance are listed in the seismic hazard curve Seismic_MAPE_PGV_PGAm_PGA_{sd}_CF_{min}_CF_{max}[1/yr,m/s,m/s²,_,_,_] as “CF_{min}” and “CF_{max},” respectively. For a given MAPE, the values of CF_{min} and CF_{max} are interpolated. The compaction factor is then sampled using a uniform distribution between the interpolating CF_{min} and CF_{max} of that event.

3.5 Key Output

The key output information produced during a simulation is directed to the screen. Section 3.1 describes how this information can be captured in *tpa.out*. Many other output files with useful information are also generated as summarized in Chapter 19. A portion of screen output captured in *tpa.out* is shown in Figure 3-4. Only the beginning of the file is shown.

Notice that global parameters are echoed so the user can verify which flags have been set. For specific output relating to each of the modules, refer to the respective consequence module chapters and Chapter 19.

```
=====
      exec: Welcome to TPA Version 5.1
      Job started: Mon Jul 02 16:00:19 2007
=====
REPOSITORY DESIGN INFORMATION
Subarea  Area      Waste    Number of WP
#         [m^2]      [MTU]
1      224091.0      3025.5          526
2      448476.0      6108.4         1062
3     1241313.5     16703.3         2904
4      775953.1     10313.0         1793
5      605892.0      8351.7         1452
6      152357.0      1972.9          343
7      318122.0      4003.3          696
8      439350.0      5355.0          931
9      305880.0      4158.6          723
10     747165.5     10048.4         1747

Total Area [acre]      = 1299.382289078371
Total Buried Waste [MTU] = 70040.000000000000
Repository AML [MTU/acre] = 53.90253552684494
Watts per MTU [W/MTU]   = 1327.684245650000
Watts per linear meter of drift [W/m] = 1450.448314791551

Specified Global Parameters:

      Compliance Period = 10000.0 (yr)
      Maximum Simulation Time = 10000.0 (yr)
      Number Of Realizations = 500
      Number Of Subareas = 10
      Volcanism scenario = 0 (yes=1, no=0)
      Faulting scenario = 0 (yes=1, no=0)
      Mechanical failure scenarios:
          Seismicity = 0 (yes=1, no=0)
          Drift Degradation = 1 (yes=1, no=0)
      Distance to Receptor Group = 18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified <<<**
**>>> in the invent module. <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**

The specified path for data = d:\ronj-\tpa51\
The specified path for codes = d:\ronj-\tpa51\
```

Figure 3-4. Sample TPA Version 5.1 *tpa.out*

3.6 References

Bechtel SAIC Company, LLC. "Development of Earthquake Ground Motion Input for Preclosure Seismic and Postclosure Performance Assessment of a Geologic Repository at YM Nevada." MDL-MGR-GS-000003. Rev. 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2004.

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4 TPA VERSION 5.1 ARCHITECTURE (MODULES, SUBROUTINES, AND INFORMATION FLOW DIAGRAMS)

TPA Version 5.1 was specifically developed to independently develop risk insights that can help to risk-inform and focus regulatory activities and to help develop staff capability to review the U.S. Department of Energy (DOE) performance assessments. The architecture of the computer code comprises an executive module, several consequence modules, an extensive set of utility modules, libraries, and a combination of static and dynamic data files. As a result of using this approach, the source code includes a group of process simulation programs, numerous calculational subroutines, data storage and retrieval modules, and a set of lookup table libraries. This modular approach results in a large number of code components that permit detailed component testing and easier coding revisions. TPA Version 5.1 source code, which has in excess of 100,000 lines of FORTRAN, was written for execution on a personal computer using the Microsoft® Windows XP® operating system.

The main objective of this chapter is to describe the overall structure of TPA Version 5.1, explain the function of selected utility modules, delineate the types of module implementations, and outline the consequence modules in Chapters 5 through 17. This information ensures that a new user develops an understanding of the essential features of TPA Version 5.1. More detailed descriptions of the consequence modules are given in subsequent chapters.

4.1 Overall Control and Execution Flow

TPA Version 5.1 is composed of an executive driver program (EXEC)¹ with a set of consequence modules and a library of utility modules. The executive driver controls the sampling of stochastic input parameters, the calculational sequence, data transfers between modules, and the production of the main output files. Various intermediate output files are generated for later use in parameter sensitivity analyses or postprocessing for graphical presentations. Utility modules ensure that consistent data sets and computational algorithms are used by all consequence modules and facilitate the discretization of the potential repository system and surrounding geologic media.

EXEC calls a set of consequence modules for (i) the engineered system, which consists of the Drip Shield Corrosion Failure module (DSFAIL)² (Chapter 8), the Waste Package Corrosion Failure module (EBSFAIL)³ (Chapter 8), the Drip Shield and Waste Package Mechanical Failure module (MECHFAIL)⁴ (Chapter 9), and the Engineered Barrier System Radionuclide Release

¹An executive driver program is referenced frequently throughout this chapter. The abbreviation EXEC will be used.

²The Drip Shield Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation DSFAIL will be used.

³The Waste Package Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

⁴The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAIL will be used.

module (EBSREL)⁵ (Chapter 10); (ii) the natural system, which consists of the Climate and Infiltration module (UZFLOW)⁶ (Chapter 5), the Drift Degradation module (DRIFTFAIL)⁷ (Chapter 6), the Near-Field Environment module (NFENV)⁸ (Chapter 7), the Unsaturated Zone Flow and Transport module (UZFT)⁹ (Chapter 11), and the Saturated Zone Flow and Transport module (SZFT)¹⁰ (Chapter 12); (iii) faulting, which is modeled in the Direct Faulting Disruptive Event module (FAULTO)¹¹ (Chapter 13); (iv) direct releases from igneous activity, which includes the Igneous Disruptive Event Involving Magma module (VOLCANO)¹² (Chapter 14), the Igneous Activity Ash Remobilization module (ASHREMOB)¹³ (Chapter 15), the Igneous Activity Airborne Transport module (ASHPLUMO)¹⁴ (Chapter 16), and the Igneous Activity Deposition and Evolution of Ash module (ASHRMOVO)¹⁵ (Chapter 16); and (v) receptor doses that are calculated by the Dose Conversion Analysis for Groundwater module (DCAGW)¹⁶

⁵The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

⁶The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

⁷The Drift Degradation module is referenced frequently throughout this chapter. The abbreviation DRIFTFAIL will be used.

⁸The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

⁹The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

¹⁰The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

¹¹The Direct Faulting Disruptive Event module is referenced frequently throughout this chapter. The abbreviation FAULTO will be used.

¹²The Igneous Disruptive Event Involving Magma module is referenced frequently throughout this chapter. The abbreviation VOLCANO will be used.

¹³The Igneous Activity Ash Remobilization module is referenced frequently throughout this chapter. The abbreviation ASHREMOB will be used.

¹⁴The Igneous Activity Airborne Transport module is referenced frequently throughout this chapter. The abbreviation ASHPLUMO will be used.

¹⁵The Igneous Activity Deposition and Evolution of Ash module is referenced frequently throughout this chapter. The abbreviation ASHRMOVO will be used.

¹⁶The Dose Conversion Analysis for Groundwater module is referenced frequently throughout this chapter. The abbreviation DCAGW will be used.

(Chapter 17), ASHREMOB, and the Dose Conversion Analysis for Ground Surface module (DCAGS) (Chapter 17).¹⁷

Each execution of TPA Version 5.1 at the operating system command prompt is considered a single simulation. The consequence modules are shown in Figures 4–1A, 4–1B, and 4–1C. Note that the figures do not show every individual component; only the main components that are essential for understanding the information flow are shown. EXEC controls the sequences of consequence and utility module executions in a simulation. For example, EXEC begins the computational process sequence by calling the utility module READER (Section 4.3.1), which in turn reads *tpa.inp* and checks the file for errors such as zero time intervals, unqualified flag specifications, and improper range specifications for distribution functions. If errors are detected, READER writes diagnostic output, identifies the location of the error(s) in *tpa.inp*, and sends a flag to EXEC to terminate the run. If no errors are detected by READER, EXEC checks the scenario to be simulated and determines the ordered sequence of module executions required for that particular scenario. At this point, EXEC initiates a set of probabilistic calculations for the specified simulation period.

Before initiating a simulation, EXEC calls the statistical sampling utility module SAMPLER to generate sample values for the input parameters with assigned probability distributions (e.g., uniform, normal, lognormal, and others). SAMPLER produces the requisite number of random realizations; each realization is a collection of the random or optionally correlated variables drawn from their specified distributions. TPA Version 5.1 permits the user to select either Latin Hypercube Sampling or standard Monte Carlo Sampling (Chapter 3). Generally, Latin Hypercube Sampling is favored over Monte Carlo Sampling because it requires fewer realizations for the same level of statistical convergence. The required number of samples is user-selectable, depending on the degree of precision required, but correlated parameters cannot be properly generated unless the number of samples is greater than the number of sampled variables.

Prior to the realization loop, EXEC calculates the initial radionuclide inventories and thermal loading for the spent fuel and glass waste form characteristics defined in *nuclides.dat* and *burnup.dat*. This calculation is performed by the utility module INVENT that, based on the specified age of the waste, computes the inventory at the time of the potential repository closure for 43 radionuclides, as specified in the nuclides and chains input block in *tpa.inp* (Section 4.13). Although only a limited, user-specified set of these 43 radionuclides is considered in the groundwater pathway calculations to reduce computation time, the full set is considered in the igneous activity disruptive scenario.

Another preparatory step to initiating the realization loop involves setting up the spatial discretization of the potential repository region and the unsaturated zone (UZ)¹⁸ and saturated zone (SZ)¹⁹ flow fields. The potential repository is divided into a number of subareas using the coordinates specified in *tpa_include.inp* (Section 4.3.4). The SZ is discretized prior to the

¹⁷The Dose Conversion Analysis for Ground Surface module is referenced frequently throughout this chapter. The abbreviation DCAGS will be used.

¹⁸The unsaturated zone is referenced frequently throughout this chapter. The abbreviation UZ will be used.

¹⁹The saturated zone is referenced frequently throughout this chapter. The abbreviation SZ will be used.

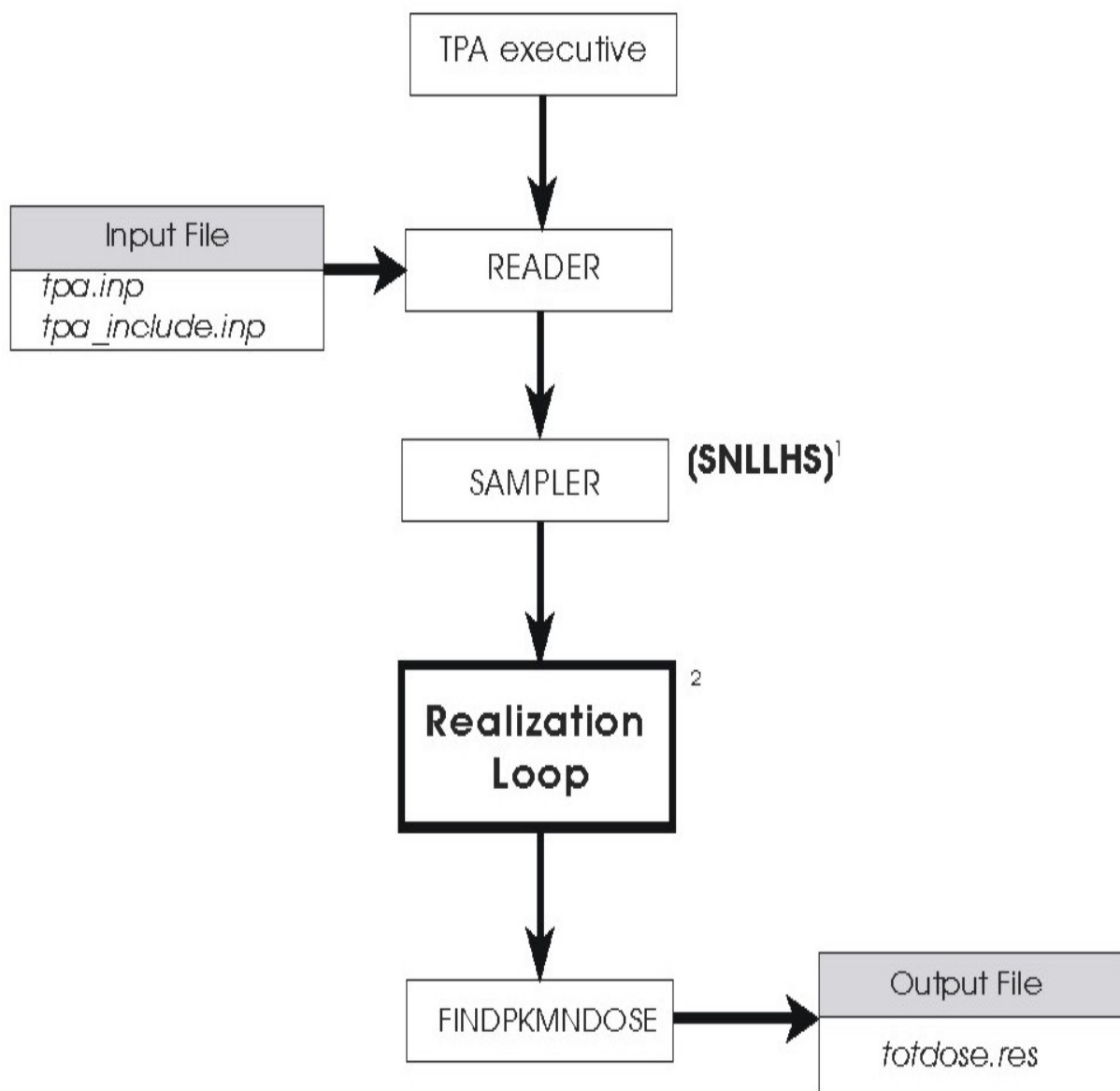


Figure 4–1A. TPA Version 5.1 Flow Diagram

¹Standalone code executed by SAMPLER.

²See details in Figure 4–1B.

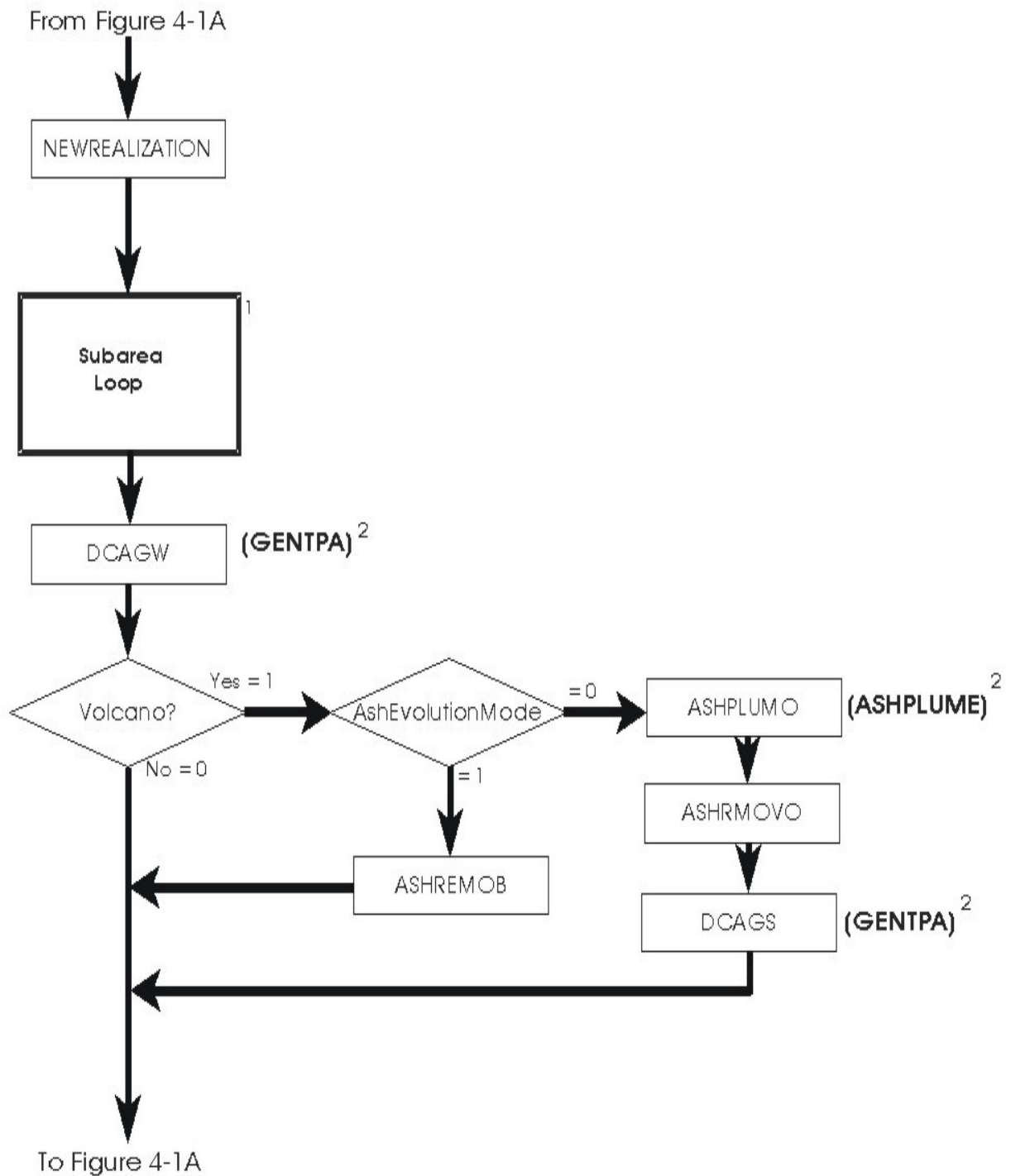


Figure 4-1B. TPA Version 5.1 Realization Loop Flow Diagram

¹See Figure 4-1C for details.

²Standalone codes executed by the associated consequence module.

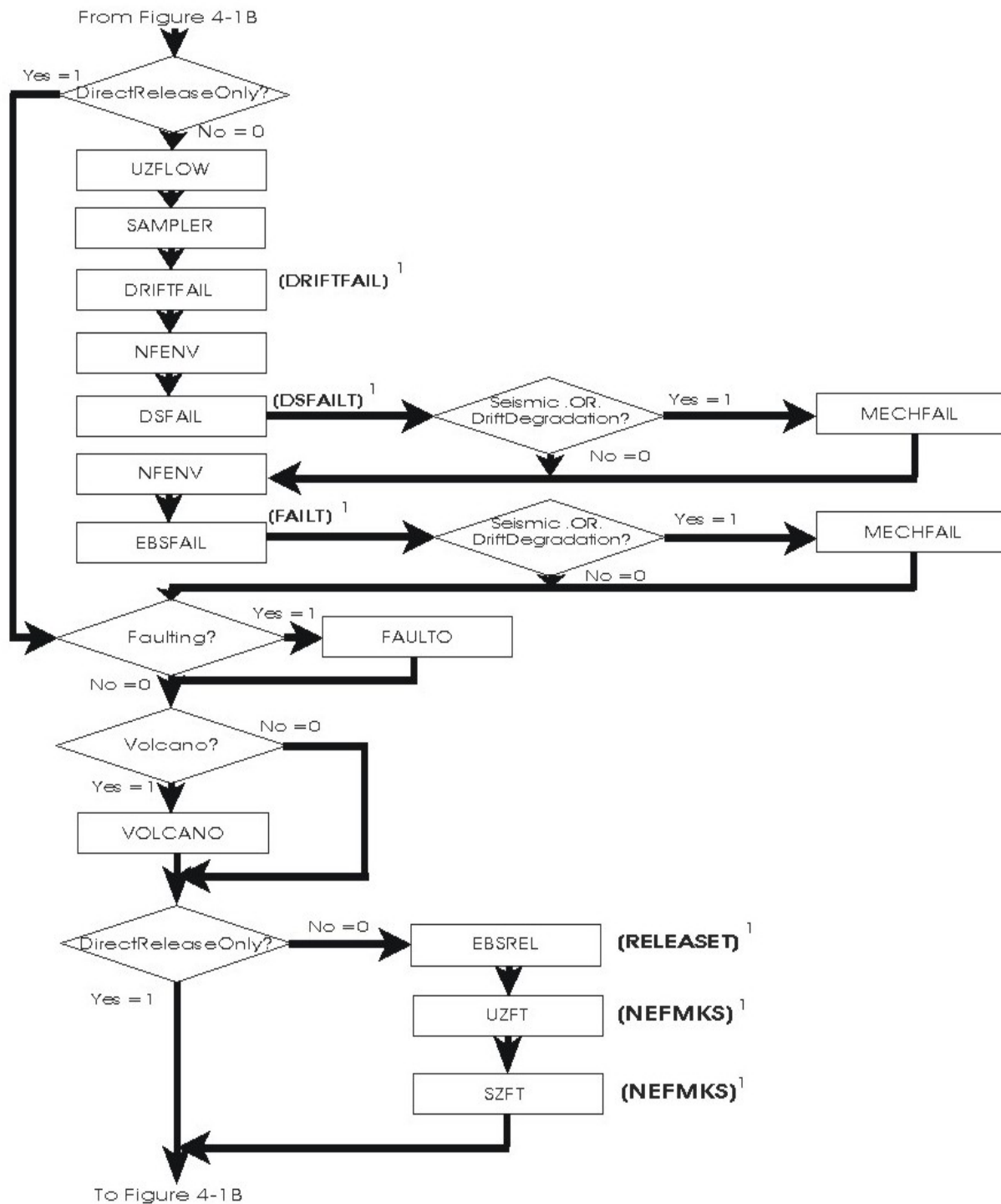


Figure 4-1C. TPA Version 5.1 Subarea Loop Flow Diagram

¹Standalone codes executed by the associated consequence module.

simulation into flow tube sections (Chapter 12), with the user specifying the geometry of the sections in *strmtube.dat*.

The user also discretizes the simulation period (e.g., 10,000 or 1 million years) into a two-level discretization scheme. At the highest level, the user specifies the duration of the first portion of the simulation period by setting the *tpa.inp* parameter DurationOfCompliancePeriod[yr]. When this value is less than the total simulation time, the duration of the second portion of the simulation is assigned to the remaining time by setting the *tpa.inp* parameter MaximumTime[yr]. At the second level of discretization, each of the two time periods is divided into timesteps. The step size for each period is specified in *tpa.inp* by the parameters NumberOfTimeStepsInCompliancePeriod, RatioOfLastToFirstTimeStepInCompliancePeriod, NumberOfTimeStepsAfterCompliancePeriod, and RatioOfLastToFirstTimeStepAfterCompliancePeriod for the two time periods, respectively. The simulation results TPA Version 5.1 provides in the output files correspond to these timesteps (Section 3.2.1.2).

After the full set of parameters and data files are assembled, EXEC executes the consequence modules (i.e., modules that simulate physical and chemical processes). Table 4-1 presents the order in which the TPA Version 5.1 modules are called during a simulation and their corresponding chapters in this user guide.

The consequence modules are implemented in the FORTRAN source code in one or more of the following ways: (i) table lookup; (ii) module/subroutine execution; and (iii) standalone codes.

Table 4-1. Module Descriptions in Sequential Order			
Module Name	Module Used for Reference Case	Calculated Parameters	Chapter
UZFLOW	Yes	percolation flux through the UZ	5
DRIFTFAIL	Yes	drift degradation	6
DSFAIL	Yes	drip shield corrosion	8
MECHFAIL	Yes	drip shield mechanical failure	9
NFENV	Yes	near-field thermohydrology and hydrochemistry	7
EBSFAIL	Yes	waste package corrosion failure	8
MECHFAIL	Yes	waste package mechanical behavior	9
FAULTO	No	faulting events and number of waste packages affected	13
VOLCANO	No	intrusive and extrusive magmatic events and amount of waste released	14
EBSREL	Yes	radionuclide release rate from the engineered barrier system	10

Table 4-1. Module Descriptions in Sequential Order (continued)			
Module Name	Module Used for Reference Case	Calculated Parameters	Chapter
UZFT	Yes	flow and transport through the UZ	11
SZFT	Yes	flow and transport through the SZ	12
DCAGW	Yes	groundwater concentrations and doses; biosphere dose conversion factors	17
ASHREMOB	No	airborne transport, redistribution, and inhalation dose (excludes ASHPLUMO, ASHRMOVO, and DCAGS)	15
ASHPLUMO	No	airborne transport and contaminated ash particle deposition; to be used for inhalation, external, and ingestion pathways (excludes ASHREMOB)	16
ASHRMOVO	No	radionuclide concentrations in soil (excludes ASHREMOB)	16
DCAGS	No	soil concentrations, dose, and biosphere dose conversion factors (excludes ASHREMOB)	17

Table lookup is an implementation in which the consequence module reads from one or more static data files. This method is illustrated in Figure 4-2(a). A table lookup code has been used for those consequence modules where a simulation of features, events, and processes was not computationally feasible (i.e., the module requires large execution times for individual realizations). The appropriate external process models are executed prior to executing TPA Version 5.1 for selected cases, and the results are abstracted and stored in a static data file. ASHREMOB is an example of a consequence module that uses a table lookup. ASHREMOB accesses data files that provide the mass of ash for various source regions that were generated separately using the external process model TEPHRA.

Another coding implementation approach embedded directly into the consequence modules is illustrated in Figure 4-2(b). In this case, calculations are performed without reliance on static data files or standalone programs. A consequence module using this type of coding is ASHRMOVO, which uses numerical algorithms to solve mathematical representations of abstracted process models. Because of the simplicity of these particular models and the fast calculational algorithms, ASHRMOVO was implemented as a set of subroutines rather than as a table lookup module.

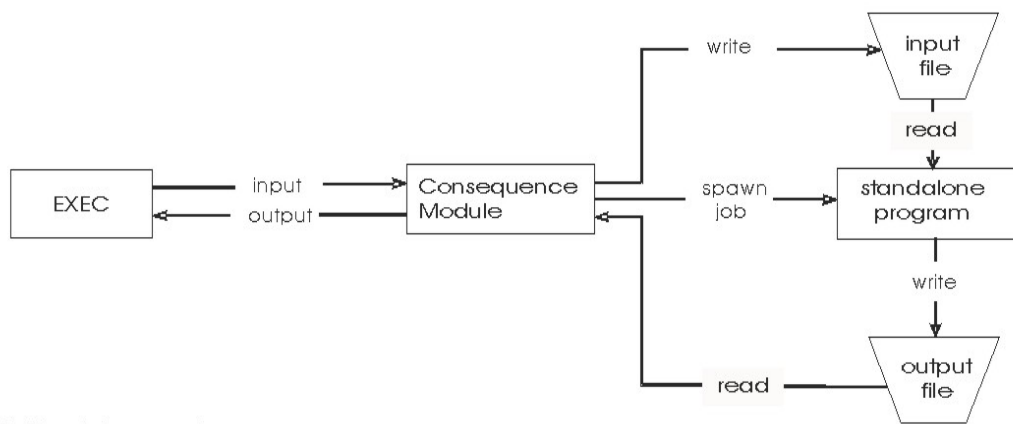
The third code implementation is execution of a standalone computer program illustrated in Figure 4-2(c). Standalone codes can be executed outside the TPA Version 5.1 environment. However, when they are executed under the control of the executive, intermediate data files are created by appropriate modules and associated with the standalone program for proper execution. This particular aspect of the design requires a nonstandard FORTRAN call within



(A) Table lookup



(B) Direct execution of consequence module



(C) Standalone code

Figure 4-2. Three Consequence Module Design Approaches Used in TPA Version 5.1

TPA Version 5.1 that spawns an external process that runs the standalone program. Although this feature is not part of FORTRAN 77, it is an option provided by all compilers. This method of executing a standalone code is currently used in DRIFTFAIL, DSFAIL, MECHFAIL, EBSFAIL, EBSREL, UZFT, SZFT, DCAGW, DCAGS, and ASHPLUMO. These modules are shown in Figure 4–1C with their respective standalone codes in parentheses.

4.2 Executive

This section briefly describes the sequence of operations in EXEC, including the individual calls to the consequence modules. At the start of execution, EXEC copies files from the *data* and *codes* subdirectories into the working directory. The *data* files are then read, and the standalone codes are invoked as needed. The input files contained in the *\data* subdirectory are listed and described in Chapter 18.

The first subroutine EXEC calls is the utility module READER. READER reads data from *tpa.inp* and stores the information in variables and arrays. After calling READER, EXEC opens and writes a five-line header to the output files. The headers contain the two-line title specified in *tpa.inp*, a two-line description of the output file contents, and a single line with the simulation starting time and date that uniquely identify one execution of TPA Version 5.1. The contents of each output file are discussed in Chapter 19. Before calculations are performed, EXEC prints to the screen selected input data specified in *tpa.inp*. This information allows the user to verify that certain critical values have been properly set in *tpa.inp* (e.g., subareas and their waste-loading characteristics, simulation time, and disruptive scenario flags). These screen prints (i) provide a quick synopsis of global parameter setup, (ii) identify the path for the primary input file, and (iii) present program execution progress and status.

4.2.1 The Realization Loop

The number of realizations is specified in *tpa.inp* with the NumberOfRealizations parameter. The realization loop is executed one time for each realization. In the realization loop, EXEC writes the results for all subareas processed to the screen or the screen capture file.

At the beginning of each realization, EXEC calls the utility module SAMPLER to obtain values of all sampled parameters defined in *tpa.inp* and stores the values in an array. These arrays are updated at the start of each cycle of the realization loop. These values may be used by EXEC or any of the consequence modules.

EXEC calls SAMPLER whenever one or more sampled parameters are specified in *tpa.inp*. SAMPLER spawns the Sandia National Laboratory Latin Hypercube Sampling standalone code (SNLLHS).²⁰ The SNLLHS program (Chapter 3) is executed only once at the beginning of a simulation and creates all of the sample values for all realizations. SNLLHS samples all specified parameters irrespective of whether the parameters are used by the consequence modules.

²⁰The Sandia National Laboratory Latin Hypercube Sampling standalone code is referenced frequently throughout this chapter. The abbreviation SNLLHS will be used.

When the *tpa.inp* parameter LatinHypercubeSampling(yes=1,no=0) parameter in *tpa.inp* is set to 1, the stratified sampling scheme is used by SNLLHS. When the parameter is set to 0, SNLLHS uses Monte Carlo sampling to generate the samples.

4.2.2 Subarea Loop

Contained within the realization loop, the subarea loop processes one subarea at a time. Using sampled parameter values, constants specified in *tpa.inp*, and static data, EXEC proceeds to call the consequence modules and pass the required intermediate results to subsequent modules. The subarea loop begins with a call to UZFLOW. The results from UZFLOW consist of the time-varying flow rate of water into the subarea. Using the total number of waste packages in the subarea and the UZFLOW output, EXEC generates the time-dependent flow rate per waste package, which is the primary input to DRIFTFAIL, NFENV, and DSFAIL. DRIFTFAIL provides equivalent diameter values to NFENV, vertical pressure values to MECHFAIL, and the fraction of waste packages in a subarea that have failed to EBSREL. NFENV provides water chemistry values to DSFAIL, and values of waste package temperature, relative humidity, water chemistry, and the time-varying flow rate of water contacting the waste package to EBSREL. DSFAIL provides drip shield thickness values to MECHFAIL, and seismic drip shield failure information to EBSFAIL.

EXEC then calls the consequence module EBSFAIL. The principal input to EBSFAIL is the NFENV output: waste package temperature, relative humidity, and water chemistry. EBSFAIL computes the failure time for corrosion failures for all waste packages in the subarea, which is written to the screen, and provides waste package thickness information to MECHFAIL. MECHFAIL then provides the fraction of waste packages in a subarea that have failed mechanically to EBSREL.

When either or both of the *tpa.inp* parameters FaultingDisruptiveScenarioFlag(yes=1,no=0) and VolcanismDisruptiveScenarioFlag(yes=1,no=0) flags are set to 1, FAULTO and/or VOLCANO are executed, respectively. FAULTO does not use any values calculated in other consequence modules. The output from FAULTO is an array with the fraction of waste packages failed by faulting events for each subarea. Similarly, VOLCANO does not use any values calculated in other consequence modules. VOLCANO output is an array containing the fraction of waste packages failed by the dike associated with the volcanic event for each subarea and the mass (in metric tons of uranium) of waste ejected from the volcanic conduit. The disruptive scenario modules perform calculations for all subareas during their first call in a realization and are executed in the first pass through the subarea loop. Disruptive scenario modules are not executed when their module-specific flag is set to 0.

When the *tpa.inp* parameter SeismicDisruptiveScenarioFlag(yes=1,no=0) is set to 1, EXEC calls SAMPLER, which uses the hazard curve defined in *tpa.inp* to determine the number and type of seismic events occurring during the simulation time for MECHFAIL.

After executing EBSFAIL and the selected disruptive consequence modules, the number of waste packages failed by initial defects, corrosion, faulting, igneous activity, and drift degradation are determined for the entire subarea. The times of failure are determined, and the number of failed waste packages is computed for each failure type.

The next consequence module called by EXEC, EBSREL, uses the number of initially defective waste packages and the time and number of waste packages failed by corrosion, faulting,

igneous activity, and mechanical failures, to write *ebsrel.inp*, which is an input file for the standalone code RELEASET (Figure 4–1C). The argument list for EBSREL also includes the flow rate of water potentially hitting the waste package before diversion, which is written to *ebsflo.dat*. Also written to *ebsflo.dat* is the time history of the two factors (F_{ow} and F_{mult}) from *wpflow.dat*. These two factors are used to determine the flow rate of water into the waste package. EBSREL then passes the engineered barrier system release rates to EXEC.

EXEC then calls UZFT to compute the release rates from the UZ. Inputs in the UZFT argument list include the flow rate of water into the subarea from UZFLOW and the engineered barrier system release rates from EBSREL. UZFT spawns the Network Flow and Transport in Time-Dependent Velocity Fields standalone code (NEFMKS),²¹ adapted from the code NEFTRAN II (Olague, et al., 1991), and maps the release rates calculated in NEFMKS to the timesteps. These release rates are passed back to EXEC in the UZFT argument list.

The final consequence module called by EXEC in the subarea loop is SZFT. SZFT uses release rates from UZFT as input to determine the SZ release rates at the receptor location. The receptor characteristics are specified in *tpa.inp*. The primary input and output items in the SZFT argument list are the UZ release rates from UZFT and SZ release rates, respectively. As with UZFT, SZFT spawns NEFMKS, which calculates release rates and maps these release rates to the timesteps.

Within the subarea loop, arrays store intermediate results that may be subsequently written to output files or summed for calculations performed later in the program execution outside of the subarea loop. In the subarea loop, UZFLOW, DRIFTFAIL, NFENV, DSFAIL, MECHFAIL, EBSFAIL, EBSREL, UZFT, and SZFT are executed for each subarea, while the disruptive modules selected in *tpa.inp* are called only on the first pass through the subarea loop.

4.2.3 Release to Biosphere Consequence Module

After completing the subarea loop, EXEC calls DCAGW. The principal input to DCAGW in the argument list consists of the release rates from SZFT summed for all subareas. DCAGW spawns the execution of the GENTPA standalone code, which computes biosphere dose conversion factors using exposure pathway input parameters specified in *tpa.inp*. DCAGW uses these biosphere dose conversion factors to calculate the dose from the groundwater pathway for the current realization. The calculated dose from groundwater is passed back to EXEC in the DCAGW argument list.

The effects of contaminated ash on the biosphere are calculated by either calling ASHREMOB for the reference case or the direct deposition suite of modules (ASHPLUMO, ASHRMOVO, and DCAGS) for nonreference cases. ASHREMOB is selected in the volcanic disruptive scenario reference case and considers the inhalation pathway. Input and output variables in the ASHREMOB argument list include the mass of spent fuel ejected and the resulting dose for the ground surface pathway.

²¹The Network Flow and Transport in Time-Dependent Velocity Fields code is referenced frequently throughout this chapter. The abbreviation NEFMKS will be used.

When the VOLCANO consequence module is executed for a nonreference case in the subarea loop, EXEC calls ASHPLUMO, ASHRMOVO, and DCAGS to evaluate the dose from the ground surface. Otherwise, following the call to DCAGW, EXEC has finished calculations for the current realization. EXEC then returns to the beginning of the realization loop and repeats the subarea loop for the next realization.

ASHPLUMO invokes the ASHPLUME standalone code to compute the areal density of spent fuel and ash deposited on the ground surface at the receptor location. Input variables in the ASHPLUMO argument list include the mass of spent fuel ejected, and the output variables include areal densities of spent fuel and ash. ASHRMOVO is then called and uses the output from ASHPLUMO to determine the spent fuel deposition on the ground surface at the receptor location. DCAGS is then called to calculate the dose for the ground surface pathway. DCAGS calls the GENTPA standalone code in a manner similar to the method used in DCAGW.

The DCAGS argument list contains the ASHRMOVO output for the ground surface spent fuel deposition. Using these values and dose conversion factors from GENTPA, DCAGS calculates the dose from the ground surface, which is passed back to EXEC in the DCAGS argument list.

Completion of DCAGS execution constitutes the end of the realization loop, and the simulation proceeds with the next realization. The number of realizations EXEC performs is specified in *tpa.inp*. When all realizations are complete, no further calls to consequence modules are performed. Throughout the program execution, EXEC writes headers and results to the output files. Primary and secondary output files have names with *res*, *abb*, *hdr*, *rlt*, *ech*, and *cum* extensions. A detailed description of the output files and their contents is provided in Chapter 19.

4.3 Utility Modules

TPA Version 5.1 has 13 utility modules: SAMPLER, INVENT, READER, MODULE VARIABLE, SUBAREA, ARRAY, FILEUNIT, FILEUTIL, NRUTIL, CUMFAIL2, NUMRECIP, PEAKFIND, and RAN. Each of these utility modules is composed of a variety of subroutines and function routines that provide centralized support to the algorithms in the consequence modules. EXEC and several of the utility modules produce output files. These files and their associated module are listed in Table 4-2. A description of the utility modules is provided next.

Table 4-2. Description of Output Files From Utility Modules		
File	Generated By Module	Description
<i>drifts.dat</i>	READER	Drift endpoint coordinates and number of waste packages in each drift in the repository.
<i>lhs.inp</i>	SAMPLER	Input data for SNLLHS. Contains all sampled parameters for all realizations.
<i>lhs.out</i>	SAMPLER	Contains all of the sampled parameters for all realizations. The block format of the file enables the efficient reading of the data in the SAMPLER utility module. All of the parameters for a given realization are grouped into a single block of data values.
<i>lhse.out</i>	SAMPLER	Captures the screen output of the SNLLHS standalone code.

Table 4-2. Description of Output Files From Utility Modules (continued)		
File	Generated By Module	Description
<i>tpamax.out</i>	READER	File produced by TPA Version 5.1 that is a version of <i>tpa.inp</i> with all parameters set to constant values that reflect the maximum value of the sample distribution.
<i>tpameans.out</i>	READER	File produced by TPA Version 5.1 that is a version of <i>tpa.inp</i> with all parameters set to constant values that reflect the mean value of the sample distribution (approximated for parameter distributions that do not have a closed-form analytical expression for mean value).
<i>tpamin.out</i>	READER	File produced by TPA Version 5.1 that is a version of <i>tpa.inp</i> with all parameters set to constant values that reflect the minimum value of the sample distribution.
<i>tpasys.tmp</i>	EXEC	Contains system path for folder containing TPA Version 5.1 used for the simulation.
<i>cp.tpa</i>	SAMPLER	List of all constant parameters and their values from <i>tpa.inp</i> .
<i>mv.tpa</i>	EXEC	Module variables are stored for each realization. This file captures the parameter names of the module variables generated by various modules of the TPA Version 5.1 code, as well as the values used for each realization. Calculated physical quantities are passed among modules using this mechanism.
<i>sp.tpa</i>	SAMPLER	Number of sampled parameters and sampled parameter values
<i>spquery.tpa</i>	SAMPLER	List of each parameter indicating the number of times the parameter is accessed per realization.

4.3.1 SAMPLER

The utility module SAMPLER performs two tasks. SAMPLER evaluates the seismic hazard curve to determine when seismic events occur, the mean annual frequency of exceedance of the seismic event, the target peak ground velocity, the median peak ground acceleration, the standard deviation of the natural logarithm of the peak ground acceleration, the lower boundary for the compaction factor, and the upper boundary for the compaction factor as described in Section 3.4. MECHFAIL uses these parameters to determine the timing and intensities of seismic events. Additional information on MECHFAIL is provided in Chapter 9. SAMPLER also prepares the input data for SNLLHS and executes SNLLHS. SNLLHS is executed once at the beginning of a simulation and creates all of the sample values for all parameters for all realizations, with the exception of those associated with the seismic hazard curve described above, irrespective of whether the parameters are used by the consequence modules.

4.3.2 INVENT

INVENT is a utility module that centralizes the computation and storage of radionuclide-specific information and inventory data for use throughout TPA Version 5.1. INVENT is called as needed throughout a realization by modules needing time-specific inventory (in Ci/MTU) of 43 radionuclides, accounting for chain decay and ingrowth of

daughters. INVENT also provides the time history of the thermal output of the average commercial spent nuclear fuel (in W/MTU). The user is cautioned to carefully consider the inventory to reasonably assess the inventory used for different simulation durations. This data is centralized to ensure data consistency between modules and to allow for variability of the initial nuclide inventories because of prolonged aging of the waste from the reactor to the potential repository and the composition of the waste.

The governing ordinary differential equation for predicting radionuclide inventories as a function of time is

$$\frac{dN_i(t)}{dt} = \lambda_{i-1}^P N_{i-1}(t) - \lambda_i^T N_i(t) \quad (4-1)$$

where

- $N_i(t)$ — atoms of i^{th} radionuclide as a function of time [mol]
- λ_{i-1}^P — radioactive decay constant for the parent radionuclide [1/yr]
- $N_{i-1}(t)$ — atoms of parent radionuclide as a function of time [mol]
- λ_i^T — i^{th} radionuclide total removal constant, which is a combination of radioactive decay and any other removal processes whose rate of removal is proportional to the number of atoms of the nuclide

The analytic solution to the above differential equation is (Jarzemba and Manteufel, 1997)

$$N_i(t) = \sum_{j=1}^i \left[\frac{\sum_{n=1}^j \left[\prod_{m=1}^{i-1} (TERM_m) \right] (N_{n,0})}{\prod_{\substack{k=j \\ k \neq i}}^i (\lambda_k^T - \lambda_j^T)} \right] \exp(-\lambda_j^T t) - \frac{\sum_{u=1}^i \left[\prod_{s=1}^{i-1} (TERM_s) \right]}{\prod_{q=1}^i \lambda_q^T} \quad (4-2)$$

$$TERM_m = \begin{cases} \lambda_{n-m}^T - \lambda_j^T & m < n \\ \lambda_m^P & m \geq n \end{cases}$$

$$TERM_s = \begin{cases} \lambda_s^T - \lambda_j^T & s < u \\ \lambda_s^P & s \geq u \end{cases}$$

where

- $N_i(t)$ — atoms of i^{th} radionuclide in decay chain as a function of time [mol]
- t — time
- λ_i^T — total removal constant for i^{th} radionuclide
- λ_i^P — decay constant for i^{th} radionuclide
- i — position in decay chain

j	—	member position in decay chain
k	—	member position in decay chain
$N_{n,0}$	—	initial number of atoms of n^{th} radionuclide in decay chain (atoms)
m	—	member position in decay chain
n	—	member position in decay chain
s	—	member position in decay chain
u	—	member position in decay chain

In the INVENT utility module in TPA Version 5.1, the total removal constant (λ_t^T) is equal to the decay constant of the parent (λ_t^P). Equation (4-2) was originally derived for calculating radionuclide leaching from contaminated volcanic ash blankets.

INVENT reads the initial inventories from the auxiliary input data file *nuclides.dat*. The 43 radionuclides in TPA Version 5.1 were selected from hundreds of radionuclides present in commercial spent nuclear fuel using radionuclide screening processes (Weldy and Peckenpaugh, 2003). Screening criteria included half-lives, solubilities, and radiotoxicities of the radionuclides. Although colloids have no initial inventory, they are included in this file to provide other radionuclide characteristics.

Waste inventories for commercial spent nuclear fuel and high-level waste glass were compiled (CRWMS M&O, 1999a,b; Bechtel SAIC Company, LLC, 2004a,b, 2003). The characteristics of the pressurized water reactor and boiling water reactor assemblies used in these calculations are

- Average pressurized water reactor assembly: 4.0 percent initial enrichment
48 Gwd/metric-ton-uranium burnup
25-year cooling time
- Average boiling water reactor assembly: 3.5 percent initial enrichment
40 GWd/metric-ton-uranium burnup
25-year cooling time

INVENT reads the time histories of thermal outputs from the data file *burnup.dat* and passes them to NFENV. In *burnup.dat*, the thermal outputs are included for 21 pressurized water reactor and 44 boiling water reactor waste packages. This auxiliary input data file contains auxiliary input data of 1-million-year time history thermal power profiles for a pressurized water reactor and a boiling water reactor commercial spent nuclear fuel. To generate the profiles, two average fuel assemblies, one for a pressurized water reactor and one for a boiling water reactor, were modeled with the external code SCALE version 5, ORIGEN-ARP sequence (Oak Ridge National Laboratory, 2000). The thermal output time history profiles were scaled down proportionally for *burnup.dat* so that the average initial emplacement lineal thermal power is 1.45 kW/m as required by the potential repository thermal design strategy (CRWMS M&O, 2000).

INVENT uses this information to determine the activity of each of the 43 radionuclides of interest in the high-level waste projected to the time of interest. The direct release calculation uses the first 43 nuclides, whereas a smaller set of nuclides is used for groundwater releases, though TPA Version 5.1 can use any number of nuclides from the list of 43.

The 43 radionuclides considered in INVENT for direct releases contain 4 major actinide element decay chains, as shown in Figures 4-3, 4-4, and 4-5. The specific nuclides being tracked are depicted in boxes in the decay chains. Additional radionuclides are tracked in the INVENT module that are not chain decay members; they are handled through simple decay equations. These radionuclides are typically fission or activation products and include U-232, Sm-151, Cs-137, Cs-135, I-129, Sn-126, Sn-121m, Ag-108m, Pd-107, Tc-99, Mo-93, Nb-94, Zr-93, Sr-90, Se-79, Ni-63, Ni-59, Cl-36, and C-14. INVENT treats the irreversible colloids of certain radionuclides as separate species with the corresponding half-lives of the associated radionuclide (Table 4-3). The colloidal species are presented with dashed boxes in Figures 4-3, 4-4, and 4-5.

The radionuclide inventory calculations INVENT performs have been verified by comparing the results with other published results and plotting the inventories for times from 1 to 1 million years (Figures 4-6 and 4-7). The trends in the inventories were compared with those published elsewhere (e.g., Roxburgh, 1987). As expected, most radionuclide inventories decrease with increasing time, some remain relatively constant over long periods of time (those with long half-lives), and others increase with time (daughters in a decay chain). For example, Pu-238 has a half life of 87.7 years, and its inventory can be observed to continuously decrease with time. Another example is U-234, which has a half-life of 244,500 years and remains relatively constant up to about 100,000 years. An example of daughter ingrowth can be seen with Th-230, Ra-226, and Pb-210, which are in the Cm-246 decay series of radionuclides (Figure 4-6). Hence, the inventories of these daughters increase with time. Due to removal during reprocessing that produces the glass waste, the Pu inventory per glass waste package and the total Pu glass inventory are much smaller than the corresponding spent fuel inventories. However, Pu inventories specified in units of Ci/MTU are comparable among the two waste forms because the inventory of U is also greatly reduced. In TPA Version 5.1, the DOE spent nuclear fuel inventory is disregarded because it is small compared to the spent nuclear fuel inventory.

4.3.3 READER

READER is a utility module that processes the data from *tpa.inp* and is the only subroutine that reads *tpa.inp*. The *tpa.inp* file contains data specific for TPA Version 5.1 execution as well as all probability density function definitions for sampled parameters that are provided to the consequence modules. The probability density function definitions are stored in an internal data base and prepared for use by SAMPLER. After SAMPLER has obtained the complete simulation sample set, it is presented in three output files, *samplpar.abb*, *samplpar.hdr*, and *samplpar.res*. *Samplpar.abb* contains both the parameter abbreviation and the full parameter name as specified in *tpa.inp*. The *samplpar.res* file contains the sampled values for all

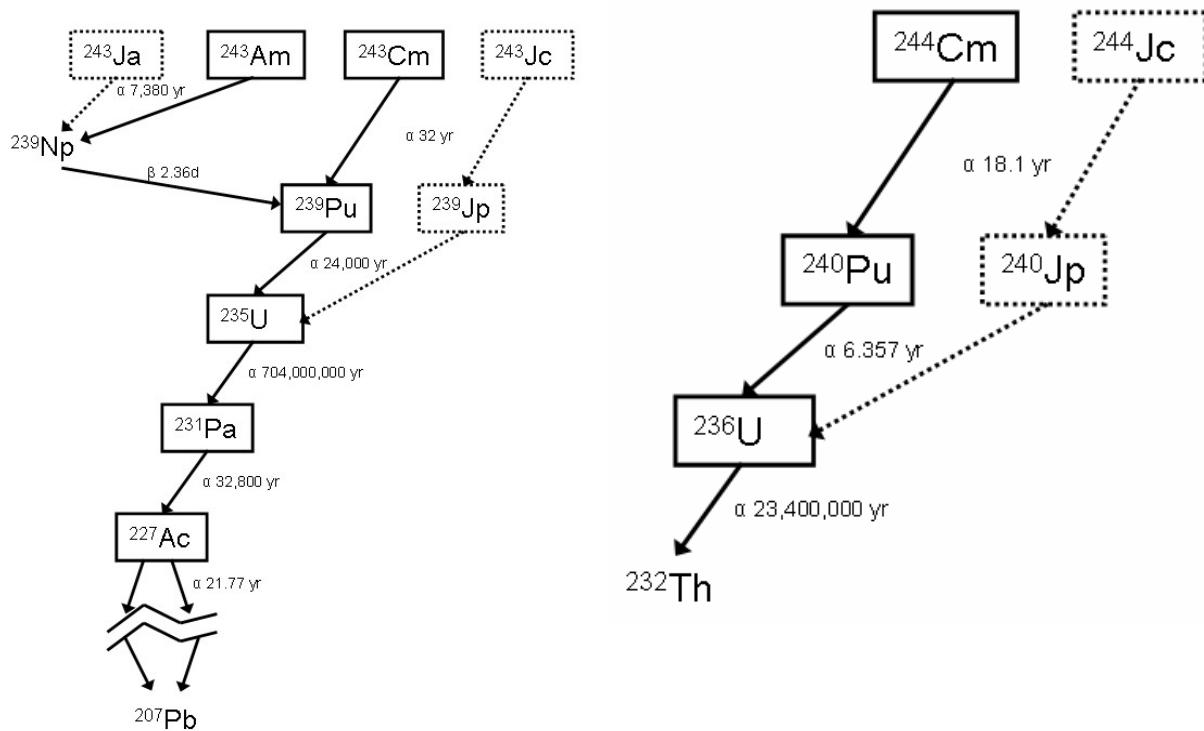


**Figure 4-3. Cm-243 and Cm-244 Decay Chains
(Dotted Components Indicate Irreversible Colloid Species)**

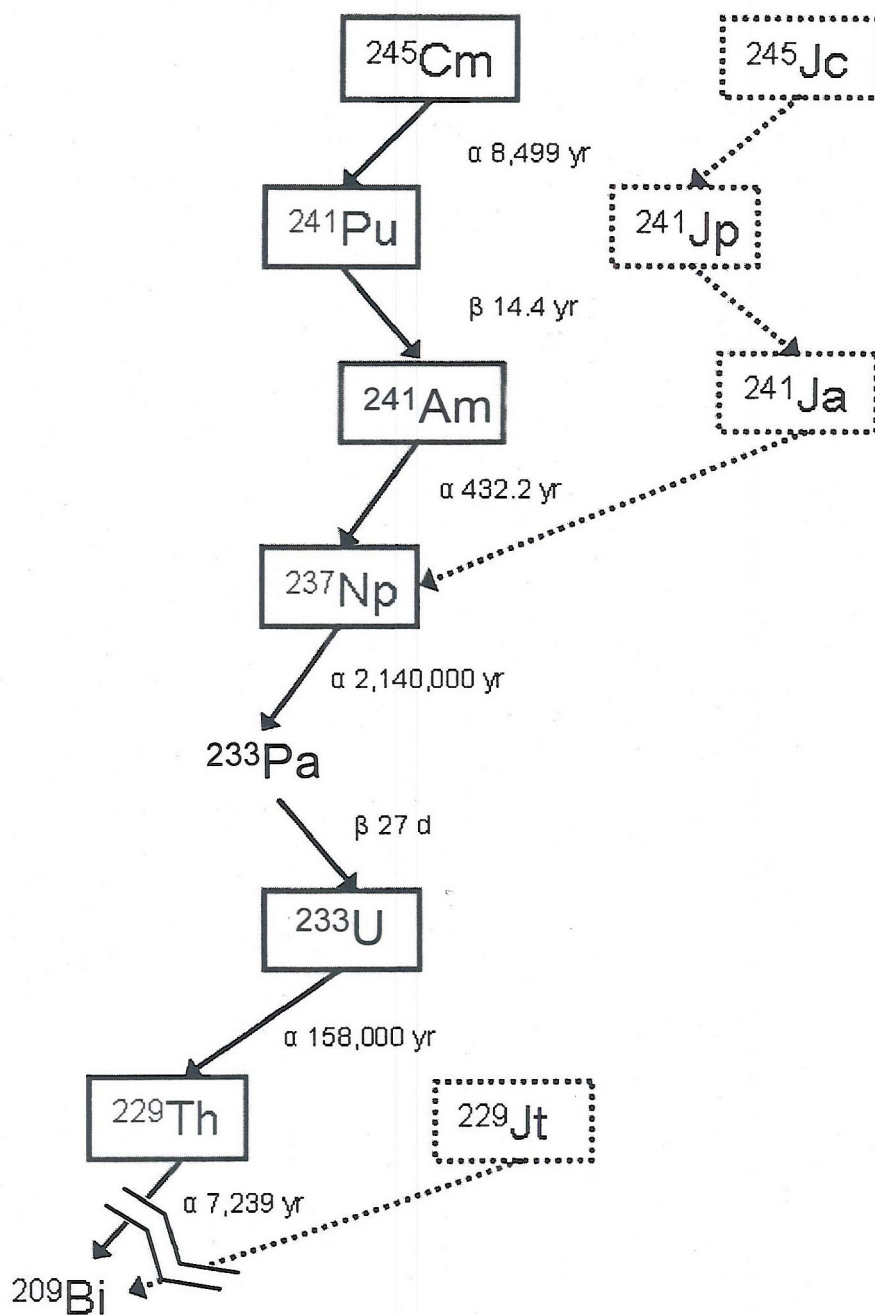


Figure 4-4. Cm-245 Decay Chain
(Dotted Components Indicate Irreversible Colloid Species)

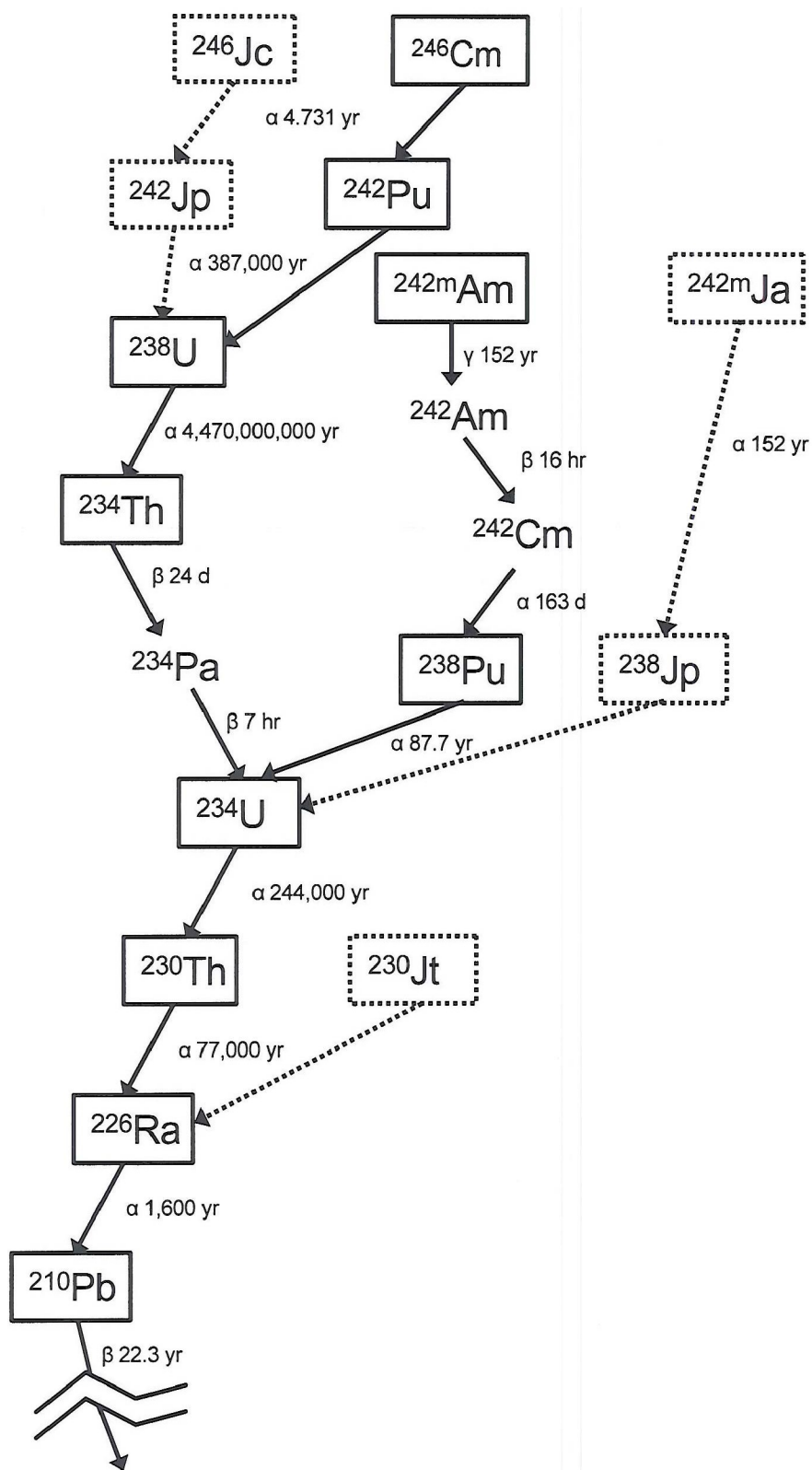


Figure 4-5. Cm-246 Decay Chain
(Dotted Components Indicate Irreversible Colloid Species)

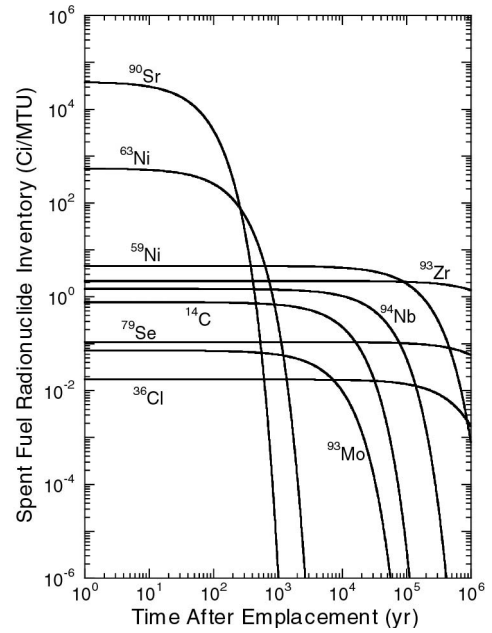
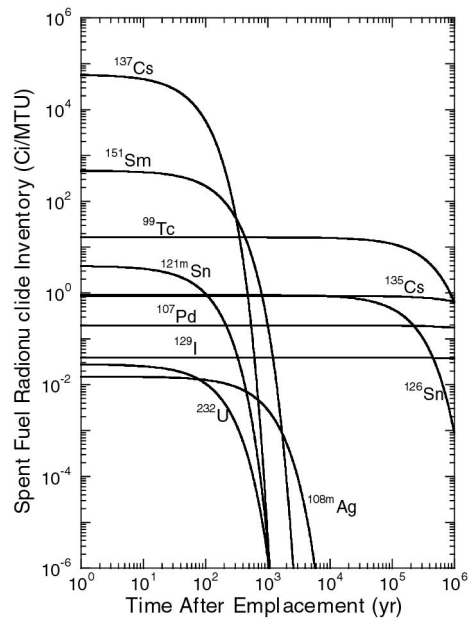
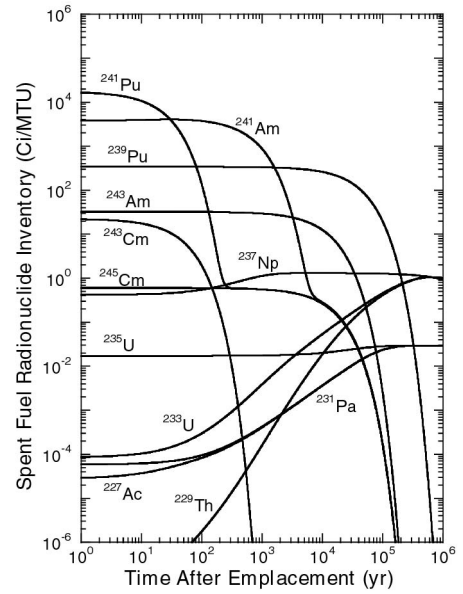
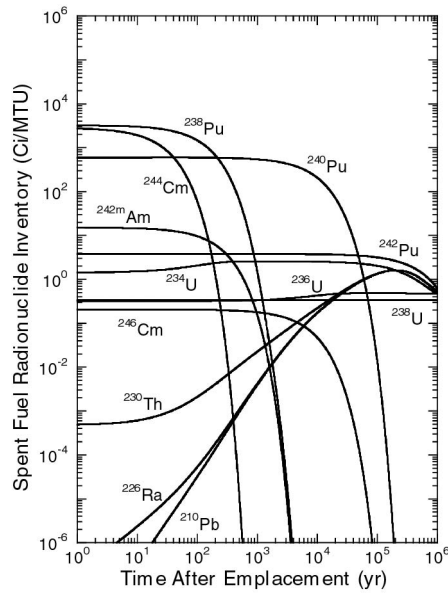


Figure 4-6. Commercial Spent Nuclear Fuel Radionuclide Inventories as a Function of Time as Calculated by INVENT

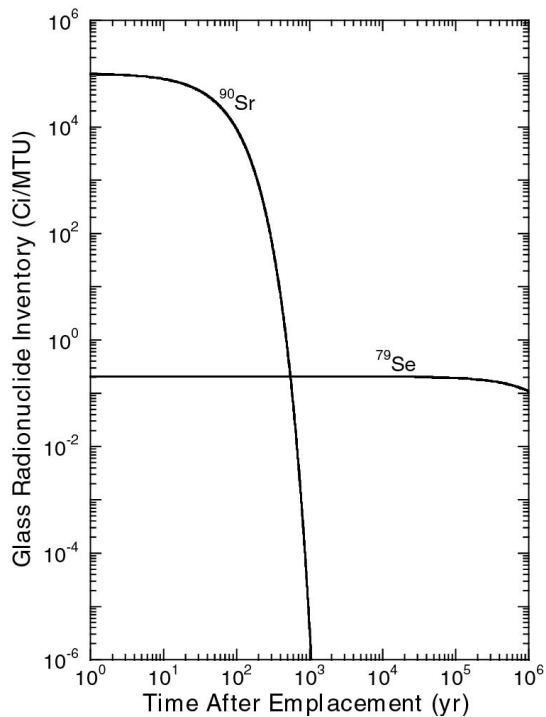
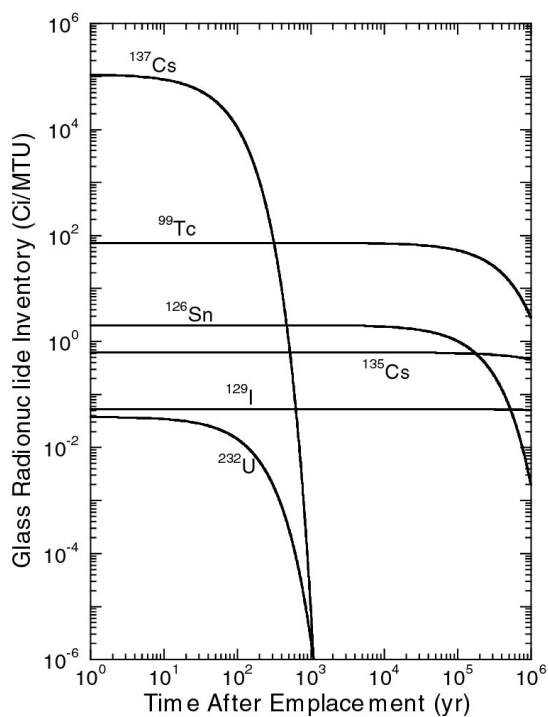
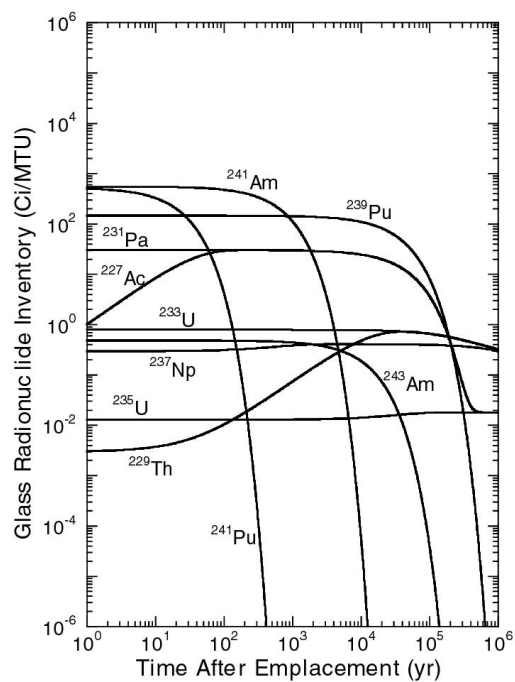
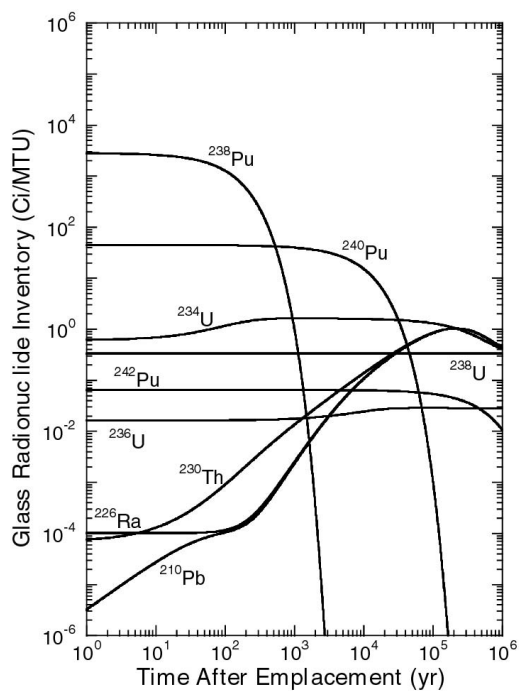


Figure 4-7. High-Level Waste Glass Form Radionuclide Inventories as a Function of Time as Calculated by INVENT

Table 4-3. List of 43 Nuclides and 14 Irreversible Colloid Species in the Invent Database			
Nuclide Number	Nuclide Name	Nuclide Number	Nuclide Name
1	²³⁸ U	30	¹²⁶ Sn
2	²⁴⁶ Cm	31	^{121m} Sn
3	²⁴² Pu	32	^{108m} Ag
4	^{242m} Am	33	¹⁰⁷ Pd
5	²³⁸ Pu	34	⁹⁹ Tc
6	²³⁴ U	35	⁹³ Mo
7	²³⁰ Th	36	⁹⁴ Nb
8	²²⁶ Ra	37	⁹³ Zr
9	²¹⁰ Pb	38	⁹⁰ Sr
10	²⁴³ Cm	39	⁷⁹ Se
11	²⁴³ Am	40	⁶³ Ni
12	²³⁹ Pu	41	⁵⁹ Ni
13	²³⁵ U	42	³⁶ Cl
14	²³¹ Pa	43	¹⁴ C
15	²²⁷ Ac	-----	-----
16	²⁴⁵ Cm	44	²⁴⁶ Jc
17	²⁴¹ Pu	45	²⁴² Jp
18	²⁴¹ Am	46	^{242m} Ja
19	²³⁷ Np	47	²³⁸ Jp
20	²³³ U	48	²³⁰ Jt
21	²²⁹ Th	49	²⁴³ Jc
22	²⁴⁴ Cm	50	²³⁹ Jp
23	²⁴⁰ Pu	51	²⁴³ Ja
24	²³⁶ U	52	²⁴⁵ Jc
25	²³² U	53	²⁴¹ Jp
26	¹⁵¹ Sm	54	²⁴¹ Ja
27	³⁷ Cs	55	²⁴⁴ Jc
28	¹³⁵ Cs	56	²⁴⁰ Jp
29	¹²⁹ I	57	²²⁹ Jt

parameters for each realization processed. They are presented in the standard SNLLHS output format of five per line. Each data block is preceded by the realization number and the number of sampled parameters.

One feature of READER is that it has a large number of error checks that detect problems with the input data and provide specific error messages directing the user to the problem. READER also calls other modules that have additional embedded error checks. EXEC contains additional error checks to ensure consistent format and content of input data. Most error checks also identify the line number of *tpa.inp* where the error was detected. Suggestions that may help to avoid the common errors are listed in Table 4-4.

Table 4-4. Hints to Prevent Common Errors in <i>tpa.inp</i>
First noncomment line of <i>tpa.inp</i> is keyword "title"
First line of title is not empty
Second line of title is not empty
All keywords are lowercase
Keyword "endoffile" is last line of <i>tpa.inp</i>
Probability density function distributions are physically consistent (e.g., min < max)
No duplicate values in user-defined distributions
Radionuclides specified are correctly defined for aqueous releases
Subarea definitions have consistent coordinates
Probability density function-type keywords are correct
Random number seed is a constant between 2^{30} and 2^{31}
Waste package payload (in metric tons of uranium) is a constant
Potential repository area and areal mass loading are consistent
Number of realizations is constant
Number of timesteps is defined, integer constant, greater than 1
Ratio of last to first timestep is defined (when ratio is between 0 and 1, equal timesteps are assigned)
All defined variable names are present
All named variables are defined correctly

A few examples of READER-generated errors and associated error messages follow.

READER enters an error trap when the user has only one title line in *tpa.inp*. Here is an example of a title being defined ("title" is the keyword), with the second title line missing:

```

**
title
First line of title - Only one title line supplied
**

```

The asterisks (**) are comment lines that help the user visually block the input data into groups. The READER generated error is

```

***>>> Error in Reader <<<***
  Second line of title is blank or comment line
  title line is:
**
  Look on Line Number = 4

```

The error message prints the second line of the title (which is read as a comment line, **) and the line number in *tpa.inp* where the error was detected.

Another example of a READER error trap is when the user specifies that zero timesteps are to be used:

```
**
iconstant
NumberOfTimeStepsInCompliancePeriod
0
**
```

then READER provides the following error message [le = less than equal to]

```
***>>> Error in Reader <<<***
NumberOfTimeStepsInCompliancePeriod .le. 1
needs to be >= 2
```

The last example of a READER error check is when the user specifies a uniform distribution with the lower limit greater than the upper limit:

```
**
uniform
DriftDegradationGeometrySelectionValue
1.0, 0.0
**
```

READER generates the following error message:

```
***>>> Error in Reader <<<***
for uniform distribution
name = DriftDegradationGeometrySelectionValue
xmax .le. xmin
xmax =      1.000000000000000
xmin =      0.000000000000000
Look on Line Number =    826
```

An error identified in SAMPLER when called by READER occurs when a flag value is set to a value other than zero or one

```
**
iflag
SeismicDisruptiveScenarioFag(yes=1,no=0)
5
**
```

The resulting error message is [ne = not equal to]

```
***>>> Error in Reader <<<***  
  (iflag .ne. 0) .and. (iflag .ne. 1)  
  iflag =    5  
  Look on Line Number =   16
```

In addition to those previously described, READER uses two other input files. The input file *tpanames.dat* is an ASCII file of all TPA Version 5.1 input parameter names and their associated eight-character abbreviations. Finally, the legacy file *ia.dat* contains a hierarchical system of identifiers (subsystem, barrier, component, and parameter) for importance analysis, which is no longer supported.

4.3.3.1 Drift Calculator

Another feature of READER is that it contains a drift calculator. The calculator creates an output file called *drifts.dat* that contains the endpoint coordinates of each drift in the potential repository. The drift calculator reads the repository design auxiliary input data file (*repdes.dat*) that contains the coordinates defining the repository outline being modeled. The coordinate pairs represent Universal Transverse Mercator easting and northing in meters. This discretization is illustrated in Figure 4-8, which reflects the input parameters for the reference case. If other input parameters are used, the boundaries shown in Figure 4-8 would be different. Information provided in *tpa_include.inp* to define the subarea coordinates must coincide with the potential repository outline coordinates presented in this file. This file also provides the angle (in radians) of inclination of the drift with respect to the east-west direction. The potential repository is divided into four large blocks, referred to as emplacement blocks, as denoted by blue, orange, red, and green lines in Figure 4-8. Each emplacement block is defined by coordinate pairs in *repdes.dat* and by two corner points, referred to as starting and stopping points. The drift emplacement algorithm starts in the first emplacement block indicated in *repdes.dat*. If the amount of emplaced waste has not exceeded the maximum specified for the potential repository (as defined in *tpa.inp* parameters *EmplacementDriftSpacing[m]*, *WastePackageSpacingAlongEmplacementDrifts[m]*, and *TotalWasteEmplacedInRepository[MTU]*), then drift emplacement continues with the second block. The direction in which drifts are advanced during drift emplacement depends on the coordinates of the stopping point relative to the starting point.

If the *tpa.inp* parameters are adjusted to create additional drifts, the subarea boundaries should be adjusted in *tpa_include.inp* to include the additional drifts. Consulting the drift calculator output in *drifts.dat* will aid in determining proper coordinate values.

If the *tpa.inp* parameters are adjusted to create fewer drifts, the subarea boundaries should be adjusted to maintain a consecutive numbering scheme starting at 1. Subarea boundaries are usually placed between drifts to avoid roundoff errors in assigning the waste package emplacement locations.

The READER module calculates the start and stop points for the drifts and the number of waste packages in each. The number of waste packages is needed to check the total emplaced waste based on the payload of spent fuel and glass waste forms, and the percentage of inventory corresponding to each waste form. The number of waste packages is also used to calculate the

thermal line load for temperature calculations and the areal mass load of the repository being modeled.

The drift calculator determines the endpoints of each drift based on the emplacement angle; the TPA Version 5.1 potential repository outline, which is an equal area transformation of the DOE potential repository outline that reduces the number of boundary edges; and the simplified internal boundary segments of the DOE panels. DOE panel boundaries were simplified by removing edge irregularities while maintaining a constant area and combining adjacent panels where convenient. The panels are defined in a potential repository design file (*repdes.dat*). To assign drifts to these panels, TPA Version 5.1 uses a construct referred to as “emplacement blocks,” which are quadrilaterals defined by two diagonal reference points that surround each panel. Drift creation proceeds from east to west and with the north or south drift advance direction as determined by the implied direction of the two diagonal reference points within these emplacement blocks. The drift endpoints and the number of waste packages in each drift are stored in *drifts.dat*. The number of waste packages assigned to each subarea is calculated in TPA Version 5.1 by comparing each drift location to the boundaries defined for each subarea.

Waste packages are assigned to subareas for drifts and portions of drifts that fall within the subarea boundaries. When adjusting the subarea boundaries, waste package payload, or other parameters that affect the distribution of waste in the potential repository, the user should check the last drift in *drifts.dat* and note where the emplacement stops. If the user changes the amount of wastes, the waste package payloads, or the spacing of the waste from those values in the reference case, resulting in a substantial portion of the last subarea being unused, the user should consider changing the coordinates for that subarea to reduce the size so that calculated values of areal mass loading remain meaningful.

4.3.4 SUBAREA

SUBAREA is a utility module that stores and retrieves potential repository subarea information. The data are read in the READER utility module and stored in SUBAREA for use by all modules. The consequence modules can acquire information about the subarea discretization from SUBAREA, but are not allowed to change (i.e., inadvertently corrupt) the information.

The subareas are defined in *tpa_include.inp* by providing Universal Transverse Mercator location coordinates for the vertices of quadrilateral elements. The SUBAREA utility module has subroutines that determine

- Footprint area of subarea
- Metric tons of uranium in subarea
- Number of waste packages in subarea
- Subarea coordinates
- Total number of subareas
- Coordinates of a subarea midpoint (centroid)
- Whether a point is located within a specified subarea
- Whether a circle is located within a specified subarea
- Whether a line is located within a specified subarea

TPA 5.1 Subareas

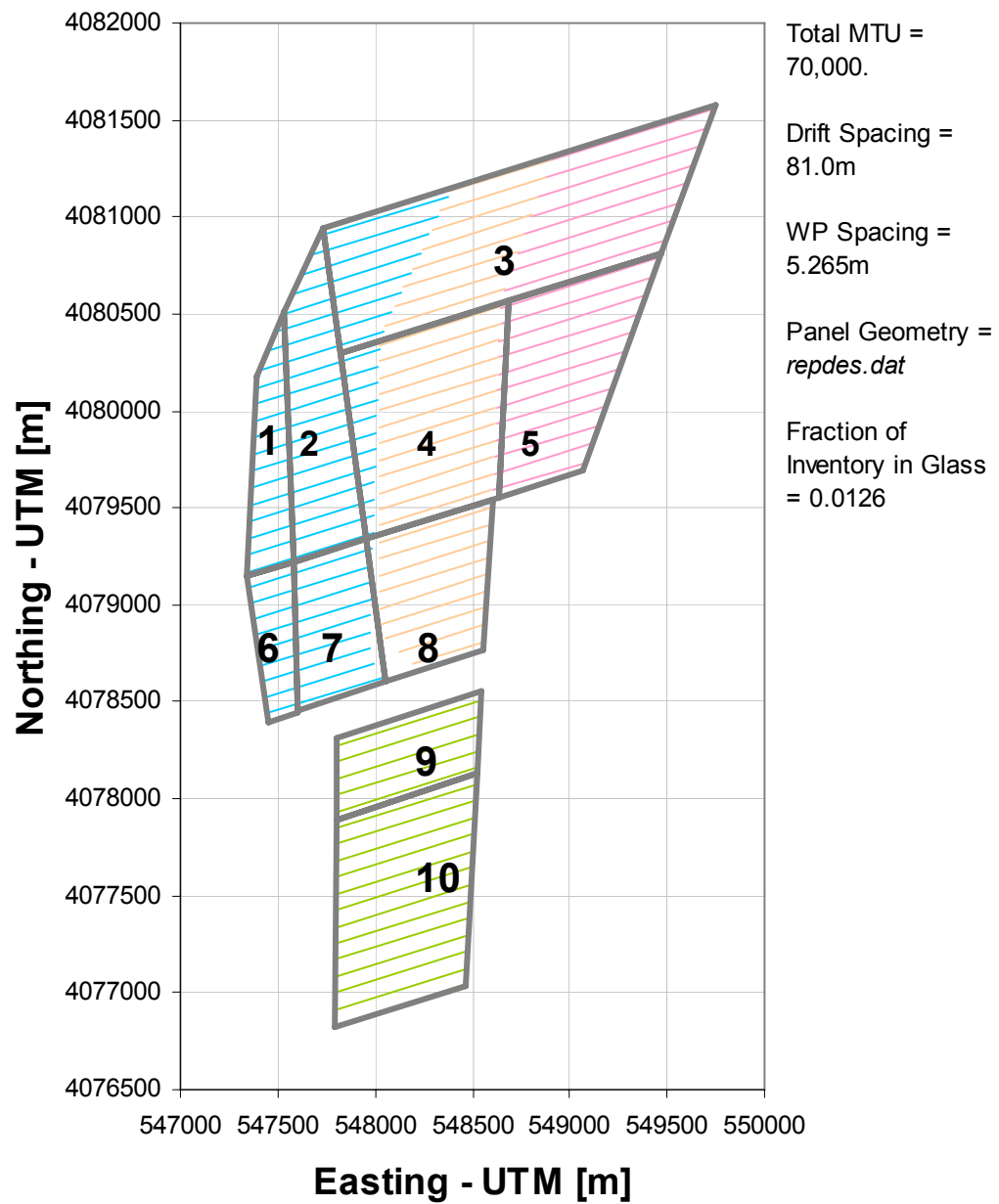


Figure 4-8. Subarea Geometry Used for the Reference Case in TPA Version 5.1

For example, Figure 4-9 shows four line segments that represent faults or volcanic dikes that intersect a given subarea. Subroutines in SUBAREA are called from FAULTO, SZFT, READER, and VOLCANO for these calculations. SUBAREA takes, as input, the coordinates of the endpoints of a given line segment and the subarea number. The routine then uses each segment of the boundary of the emplacement area, checks whether there is a real intersection, and calculates the intersection point. SUBAREA then determines whether both ends of the line fall within the given region. When both ends of the line are within the given region, the intersection length is the length of the line. When one end or both ends fall outside the given region, SUBAREA determines the intersection point(s) of the line with the sides of the quadrilateral region. There may be one or two real intersection points, depending on whether one or two endpoints fall outside the region. The intersection length for the first case is the distance between the real intersection point and the endpoint of the line that falls within the region. The intersection length for the second case is the distance between the two intersection points. In Figure 4-9, for example, the intersection length of Line 1 is the full length, Line 2 intersection length is AB (need to find B only), and for Lines 3 and 4, the intersection length is AB (need to find both A and B). SUBAREA calculates the intersection lengths of the lines in this example.

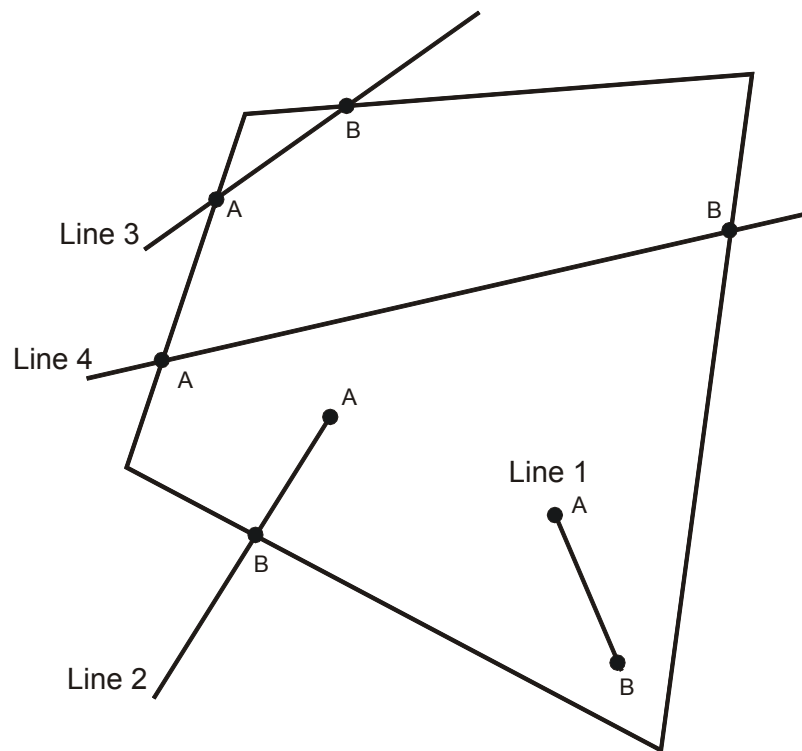


Figure 4-9. Four Cases of a Line Segment Intersecting a Quadrilateral

4.3.5 MODULE VARIABLE

The MODULE VARIABLE utility module stores values computed by consequence modules. MODULE VARIABLE provides a database for storing consequence module results (i.e., subsystem and system performance measures) and provides a special index to identify each parameter value. This procedure provides data security, such that only the subroutine that introduced the data knows the index for a given parameter and may change its value within the database. Other modules within TPA Version 5.1 are allowed to query the value; however, they cannot change the value in the database.

MODULE VARIABLE gives the TPA Version 5.1 user a tool for storing parameter values for later correlation with the output. For example, the user may decide to save the time for each faulting event to assess the sensitivity of the resulting dose to the event time. Examples of the types of variable information generally saved to the MODULE VARIABLE utility module include

- Waste package failure time (yr)
- Fractional release rate (1/yr)
- Time of peak annual dose (yr)
- Magnitude of peak annual dose (rem/yr)
- Cumulative normalized release

4.3.6 ARRAY

ARRAY, which is a utility module, manipulates various data types (i.e., floating point, integer, and character). These subroutines can be called by other modules to perform routine functions. The functionality of these subroutines includes utility operations such as initialization, vector operations, variance calculations, index mapping, and sorting. The subroutines called by ARRAY are identified and described in Table 4-5.

Table 4-5. Standard Subroutines Located in the ARRAY Utility Module	
Subroutine	Operational Description
zero	zeros out a real vector
zeroi	zeros out an integer vector
clearchar	clears character string
initr	sets all elements of a double precision array to a given value
initi	sets all elements of an integer array to a given value
initchar	sets all characters of a string to a given character
transpose	transposes the contents of a matrix
scale	scales a vector
scopy	scales and copies a vector
acopy	copies vector and adds a constant to each entry
ascopy	adds, scales, and copies a vector
addto	adds one vector to another
isoneofset	determines whether an integer is part of an integer set

Table 4-5. Standard Subroutines Located in the ARRAY Utility Module (continued)	
Subroutine	Operational Description
ainterl	linearly interpolates in list of {time, value} data to find value at time of interest
avar	calculates variance of an array of values
amean	calculates mean of an array of values
checkinorder	determines whether array of values is in order, either ascending or descending
sortqr	sorts based on pointers to array of values—sorts from smallest to largest value
maplist	maps data in first list into second list given the first set of {x,y} and the second set of {x}, and finds the second set of {y}
maptimeofevent	fills each element of an array with one of two input values depending on the time of the event
checkforduplicates	determines whether a double precision array of sorted values has any duplicates
icheckforduplicates	determines whether an integer array of sorted values has any duplicates

4.3.7 Secondary Utility Modules

Secondary utility modules include FILEUNIT, FINDELEV, NUMRECIP, PEAKFINDER, RAN, NRUTIL, and CUMFAIL2. These modules primarily support the utility modules previously described in this chapter, but may also be called by other TPA Version 5.1 modules. Table 4-6 lists the function of each of these secondary modules.

Table 4-6. Description of Secondary Utility Modules	
Module	Function
FILEUNIT	assigns unit numbers to all modules and ensures different modules have unique unit numbers
FINDELEV	finds elevation of ground surface for a given set of Universal Transverse Mercator coordinates
NUMRECIP	contains multiple subroutines for solving equations as modified from Press, et al. (1986)
PEAKFINDER	finds and reports time and magnitude of peak doses for each nuclide and summed dose for all nuclides
RAN	generates random values for the seismic hazard curve
NRUTIL	contains several routines to calculate drip shield and waste package temperature
CUMFAIL2	provides the number of failed waste packages for each failure type to EBSREL, based on the fraction of waste packages in a subarea failed received from the consequence models, and the associated P_{contact} and $P_{\text{allowance}}$ parameters from <i>tpa.inp</i>

4.4 Consequence Modules and Standalone Codes

4.4.1 Consequence Modules

This section outlines the information provided in Chapters 5 through 17 for each of the consequence modules associated with TPA Version 5.1.

The information in Chapters 5 through 17 is intended to allow the TPA Version 5.1 user to either develop or modify the input files based on an understanding of the relationship of the input parameters to the calculational approach in TPA Version 5.1 and to know the types of results available for analyzing performance.

TPA Version 5.1 execution requires a variety of input. The primary input file, *tpa.inp*, controls the attributes of the simulation (e.g., inclusion of disruptive events, number of realizations in the probabilistic analyses, and length of simulation) and specification of parameters. It is anticipated that TPA Version 5.1 will be used in a probabilistic mode (i.e., performing a large number of realizations based on Monte Carlo Sampling or Latin Hypercube Sampling of the input parameters) due to uncertainty and variability in parameters describing the potential repository system (e.g., porosity, retardation, and solubility limits). The input parameters included in *tpa.inp* and *tpa_include.inp* are the only input that can be sampled. Other inputs, not considered appropriate for sampling, specify constants of the analysis (e.g., elevation of the subarea and radionuclide half-life) or abstractions of detailed models (e.g., definition of streamtube characteristics based on a two-dimensional analysis). A variety of auxiliary input data files, generally designated by the extension *.dat*, supply the deterministic information. For completeness, Chapters 5 through 17 identify input relevant to a particular module; however, the user should only modify the values in *tpa.inp*. Chapter 3 contains additional information on the input structure for TPA Version 5.1.

Two general types of consequence modules are incorporated in TPA Version 5.1: (i) nominal scenario modules primarily associated with the groundwater pathway—UZFLOW, DRIFTFAIL, DSFAIL, NFENV, EBSFAIL, MECHFAIL, EBSREL, UZFT, SZFT, and DCAGW and (ii) disruptive scenario modules associated with damage to the waste package and release of radionuclides from faulting and igneous activity—FAULTO, VOLCANO, ASHREMOB, ASHPLUMO, ASHRMOVO, and DCAGS. Overall, the consequence modules described in Chapters 5 through 17 estimate

- Water infiltration from the land surface to the subsurface and, subsequently, into the emplacement drifts onto waste packages
- Environment around the waste packages (temperature, humidity, and water chemistry) that affects waste package degradation or radionuclide release
- Drip shield failure times due to corrosion and mechanical processes and seismicity-induced rock fall
- Waste package failure times due to corrosion and mechanical processes, seismicity-induced rock fall, faulting, igneous activity, and waste packages that are initially defective

- Release of radionuclides from failed waste packages through the invert to the groundwater transport pathway
- Release of radionuclides from the extrusive component of igneous activity to the air pathway
- Transport of radionuclides in groundwater through the UZ and the SZ
- Transport of radionuclides in volcanic ash
- Doses to the receptor through the radiological contamination in groundwater
- Doses to the receptor through the radiological contamination of the ground surface (released from the potential repository by an extrusive volcanic event)

4.4.2 Standalone Codes

The standalone codes are independent from EXEC and its subroutines and modules. This independence is maintained to such a degree that to execute the standalone codes, a special operation system call is required to transfer control to them. Transferring control to an independent code is frequently referred to as “spawning a task” from the point of view of the operating system. The standalone codes are kept in the *codes* subdirectory in the TPA Version 5.1 directory structure. They differ from the TPA Version 5.1 subroutines in that, with properly prepared input files, they can be executed independently of the TPA Version 5.1 environment using their program executable name.

The standalone codes differ from external codes in that they are routinely “spawned” in the normal operation of TPA Version 5.1, and TPA Version 5.1 modules automatically prepare their input files. EXEC copies the standalone codes to the *run* directory before they are used by TPA Version 5.1. Table 4-7 lists the TPA Version 5.1 standalone codes.

Table 4-7. TPA Version 5.1 Standalone Codes		
Standalone Code	Description	Associated With Module
ASHPLUME	Generates ash plume data for ASHRMOVO and DCAGS	ASHPLUMO
DRIFTFAIL	Generates drift degradation data	DRIFTFAIL
DSFAILT	Calculates drip shield corrosion failure time	DSFAIL
EBSFILT	Calculates invert transport data (legacy code)	EBSREL
FAILT	Calculates waste package corrosion failure time	EBSFAIL

Table 4-7. TPA Version 5.1 Standalone Codes (continued)		
Standalone Code	Description	Associated With Module
GENTPA	Calculates receptor intakes and exposure time-weighted ground surface concentrations	DCAGW DCAGS
MECHFALL	Calculates mechanical failure time of drip shield and waste package	MECHFALL
NEFMKS	Calculates flow and transport for UZ and SZ	UZFT SZFT
RELEASET	Calculates the waste package release data	EBSREL
SNLLHS	Latin Hypercube Sampling code	SAMPLER

4.5 Input Parameters in *tpa.inp*

The *tpa.inp* parameters EXEC uses are contained in Table 4-8.

Table 4-8. Summary of Global Input Parameters <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Disruptive Scenario Flag	DriftDegradationScenario Flag(yes=1,no=0)	Activates the thermally driven drift degradation scenario calculations	iflag 1	The reference case for the nominal scenario includes the drift degradation disruptive process.
Disruptive Scenario Flag	SeismicDisruptive ScenarioFlag(yes=1, no=0)	Activates the seismic disruptive scenario	iflag 0	This flag must be set to 1 for the seismic disruptive scenario to be simulated; the nominal scenario does not include this disruptive scenario.
Disruptive Scenario Flag	FaultingDisruptive ScenarioFlag(yes=1, no=0)	Activates the faulting disruptive scenario calculations	iflag 0	This flag must be changed to 1 for a faulting event to be simulated. The nominal scenario does not include faulting events, so the flag is set to zero.
Disruptive Scenario Flag	VolcanismDisruptive ScenarioFlag (1=yes, 0=no)	Activates the igneous activity disruptive scenario calculations	iflag 0	This flag must be set to 1 for the igneous disruptive scenario to occur; the nominal scenario does not include this disruptive scenario.
Disruptive Scenario Flag	DirectReleaseOnlyFlag (yes=1,no=0)	This flag can disable the processing of all groundwater calculations	iflag 0	This flag streamlines calculations and reduces execution times for TPA Version 5.1 simulations of extrusive igneous activity events. Because ASHREMOB is designed specifically for modeling extrusive igneous activity events, it is recommended that this flag be set to a value of 1 for ASHREMOB if groundwater doses from igneous intrusion are not needed.
Disruptive Scenario Flag	AshEvolutionMode [0=no_ashremob, 1=ashremob]	User-selected flag for calculating evolution of ash at receptor location	iconstant 1	0 implies wind direction fixed toward the receptor without ash remobilization (i.e., ASHPLUMO/ASHRMOVO/DCAGS); 1 implies the wind direction is sampled and ash remobilization effects are included (i.e., ASHREMOB).
Simulation Times	DurationOfCompliance Period[yr]	Duration of first simulation period [yr]	constant 1.0e4	May be set as high as 1 million years.

Table 4-8. Summary of Global Input Parameters (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Simulation Times	MaximumTime[yr]	Simulation time period [yr]	constant 1.0e4	Maximum time may be set as high as 1 million years.
Simulation Times	NumberOfTimeStepsIn CompliancePeriod	Number of timesteps in the first simulation period [unitless]	iconstant 201	User option. Program control switch: specifies the number of timesteps within the first simulation period specified by DurationOfCompliancePeriod[yr].
Simulation Times	RatioOfLastToFirstTime StepInCompliancePeriod	Ratio of last to first timestep in the first simulation period. [unitless]	constant 100.0	User option. This parameter, together with DurationOf CompliancePeriod[yr] and NumberOfTimeStepsInCompliancePeriod determines the times used in calculations, from time = 0 to the end of the first simulation period {i.e., DurationOfCompliancePeriod[yr]}. As values increase for this parameter, the times (timesteps) closer to time = 0 become finer, while the times (timesteps) closer to the end of the first simulation period are coarser. As values approach 1 for this parameter, the times throughout the compliance period become closer to uniform (equal) timesteps. Because the thermal pulse occurs in the first thousand years, it is desirable to have more information at these earlier times. Thus, the reference value equals 100.0. 1. For values less than or equal to 1e-5, there is an ERROR message, and execution stops. 2. For values greater than 1e-5 and less than or equal to 1.0001, value is reset to 1.0 (i.e., uniform timesteps). 3. For values greater than 1.0001, timesteps increase geometrically, such that the ratio of the last timestep to the first timestep equals the value for this parameter.
Simulation Times	NumberOfTimeStepsAfter CompliancePeriod	Number of timesteps in the interval after the first simulation period specified by DurationOf CompliancePeriod [yr] [unitless]	iconstant 100	User option. Specifies the number of timesteps after the first simulation period; maximum number is 4,800; sum must not exceed 5,001 for the entire simulation time. This parameter is ignored when MaximumTime[yr] = DurationOfCompliancePeriod[yr].

Table 4-8. Summary of Global Input Parameters (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Simulation Times	RatioOfLastToFirstTime StepAfterCompliance Period	Ratio of the last to the first timestep in the second simulation period. [unitless]	constant 1.0	This parameter, together with MaximumTime[yr] and NumberOfTimeStepsAfterCompliancePeriod determines the times used in calculations, from time = DurationOfCompliancePeriod[yr] to the end of the simulation {i.e., MaximumTime[yr]}. This parameter is not used when MaximumTime[yr] equals DurationOfCompliancePeriod[yr], which is the reference case. If the user modifies the <i>tpa.inp</i> parameter MaximumTime[yr] to a time greater than DurationOfCompliancePeriod[yr], the following description is applicable. As values increase for this parameter, the times (timesteps) closer to time = first simulation period become finer, while the times (timesteps) closer to the maximum time are coarser. As values approach 1 for this parameter, the times throughout this time interval become closer to uniform (equal) timesteps. Because the thermal pulse occurs in the first thousand years, it is desirable to have more information at these earlier times, while at later times uniform timesteps are reasonable. 1. For values less than or equal to 1e-5, there is an ERROR message, and execution stops. 2. For values greater than 1e-5 and less than or equal to 1.0001, value is reset to 1.0 (i.e., uniform timesteps). 3. For values greater than 1.0001, timesteps increase geometrically, such that the ratio of the last timestep to the first timestep equals the value for this parameter.
Parameter Sampling	LatinHypercubeSampling (yes=1,no=0)	Latin Hypercube Sampling flag [unitless]	iflag 1	User option. When set to 0, TPA Version 5.1 uses the Monte Carlo method. When set to 1, Latin Hypercube Sampling is used.
Parameter Sampling	SeedForRandomNumber	Seed for random number generator [unitless]	constant 1456789101.0	Seed must be an odd number between 2^{30} and 2^{31} (Wyss and Jorgensen, 1998). Good seeds tend to be large and odd (Iman and Shortencarier, 1984).
Parameter Sampling	NumberOfRealizations	Number of realizations [unitless]	iconstant 500	User option. Specifies the number of realizations (simulations, vectors) to run.
Parameter Sampling	StartAtRealization	Realization at which to start processing data [unitless]	iconstant 1	User option. Program control parameter for first user-defined realization.

Table 4-8. Summary of Global Input Parameters (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Parameter Sampling	StopAtRealization	Realization at which to stop processing data [unitless]	iconstant 1	User option. Program control parameter for last user-defined realization. When zero, perform all remaining realizations after StartAtRealization. Set to 1 in the reference case to prevent a large run being started inadvertently.
Parameter Sampling	StartAtSubarea	Selects subarea at which to start simulation [unitless]	iconstant 1	User option. Program control parameter for first user-defined subarea. User can select 1–10. The reference case defines 10 subareas, which approximate the potential repository.
Parameter Sampling	StopAtSubarea	Selects subarea at which to stop simulation; user can select 0–10 [unitless]	iconstant 0	User option. Program control parameter for last user-defined subarea. When zero, perform simulation on all subareas after StartAtSubarea.
Parameter Sampling	AverageCalendarYear AssumedFor Emplacement[A.D.]	Calendar year in which the spent fuel is emplaced in the potential repository [A.D.]	constant 2033.0	Based on data from CRWMS (1999a,b).
Nuclides and Chains	CheckNuclidesAndChains (yes=1,no=0)	Compares completeness and order of decay chains currently used to an ordered listing of all known decay chains [unitless]	iflag 0	User option. The reference case does not include all nuclides and chains—only those that are specified in <i>tpa.inp</i> . In TPA Version 5.1, this parameter should always be set to 0.

Table 4-8. Summary of Global Input Parameters (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Nuclides and Chains		List of aqueous phase groundwater pathway radionuclides to analyze; fixed format data listing nuclide names	aqueousnuclides 21 12 2 Cm246 U238 5 Cm245 Am241 Np237 U233 Th229 2 Am243 Pu239 1 Pu240 4 U234 Th230 Ra226 Pb210 1 Cs135 1 I129 1 Tc99 1 Ni59 1 Se79 1 Nb94 1 Cl36	The first number defines the total number of aqueous radionuclides. The second number defines the total number of decay chains. The remainder of list defines the length and members of individual decay chains. There is no parameter name in <i>tpa.inp</i> , only the distribution type and parameter values.

Table 4-8. Summary of Global Input Parameters (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Nuclides and Chains		List of irreversible colloidal phase groundwater pathway radionuclides to analyze; fixed format data listing nuclide names	colloidalnuclides 11 5 2 Jc246 U238 3 Jc245 Ja241 Np237 2 Ja243 Jp239 1 Jp240 3 Jl230 Ra226 Pb210	The first number defines the total number of colloidal radionuclides. The second number defines the total number of colloidal decay chains. The remainder of the list defines the length and members of individual colloidal decay chains. There is no parameter name in <i>tpa.inp</i> , only the distribution type and parameter values. An irreversible colloid is distinguished from simple radionuclides with an initial letter of "J" and a second letter that corresponds to the first letter of its associated radionuclide. Elements americium, curium, plutonium, and thorium have irreversible colloid species symbols of Ja, Jc, Jp, and Jt, respectively.
Output Print Options	OutputMode(0=None, 1=All, 2=User Defined)	Flag for appending intermediate output to files [unitless]	iconstant 0	User option. 0 = no realizations are processed for append option, 1 = all realizations are processed, and 2 = append processing for only user-defined realizations. Note: set to 1 to get <i>spquery.tpa</i> (file contains number of times a parameter is accessed per realization).
Output Print Options	UserDefinedLower RealizationAppended	For output mode = 2, append files are written beginning with this realization [unitless]	iconstant 1	User option.
Output Print Options	UserDefinedUpper RealizationAppended	For output mode = 2, append files are written ending with this realization	iconstant 1	User option.

Table 4-8. Summary of Global Input Parameters (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Output Print Options	SelectAppendFiles	User-specified files to append	iconstant 0	User option. Program control parameter; user can append inputs and intermediate outputs either to all .rit, .ech, and .cum files or can select such information to be appended for a particular module. 0 = append all files; 1 = uzflow.ech and uzflow.rit only; 2 = nflow.ech and nflow.rit only; 3 = ebsrel.ech and ebsrel.rit only; 4 = drifftail.ech, drifftail.rit, mechtail.ech, and mechtail.rit only; 5 = faulto.ech and faulto.rit only; 6 = volcano.ech and volcano.rit only; 7 = ebsrel.ech, ebsrel.rit, and ebsrel.cum only; 8 = uzft.ech and uzft.rit only; 9 = szft.ech and szft.rit only; 10 = dcagw.ech and dcagw.rit only; 11 = ashplumo.ech and ashplumo.rit only; 12 = ashrmovo.ech and ashrmovo.rit only; 13 = dcags.ech and dcags.rit only; 14 = ashplume.cum only; 15 = failt.cum only; 16 = refliuz.cum and refisz.cum only; 17 = releaset.cum only; 18 = ggenii.cum only; 19 = genv.cum only; 20 = dcfw.cum and dcfws.cum only; 21 = dsfail.ech and dsfail.rit only; 22 = files needed by the graphical postprocessor; and 23 = infilper.cum only
tpa_include. inp	ImportanceAnalysisFlag (yes=1,no=0)	Flag to activate importance analysis [unitless]	iflag 0	Legacy user option. Only enabled for specialized runs configured for nonreference cases. Not supported for TPA Version 5.1.
tpa_include. inp	GenerateRestartFiles(yes=1,no=0)	Flag to save data values per realization during execution [unitless]	iflag 0	User option. Program control switch: if code execution is interrupted, execution can be resumed from the last completed realization. Data is saved check.pnt, which can become quite large. Only use if executing TPA Version 5.1 on an unstable machine, where the process may be interrupted or halted by external circumstances. Not supported for runs with simulation times greater than 10,000 years.
Groundwater Protection	GroundwaterProtection Calc(yes=1,no=0)	Enables groundwater protection calculations	iflag 1	Enables the generation of files that contain groundwater protection dose in a manner that is convenient for comparison with applicable standards.
Groundwater Protection	WellPumpingRate Groundwater Protection[gal/day]	Well pumping rate groundwater protection	constant 2676394.0	Value is based on the representative volume specified in 10 CFR 63.332.

Table 4-8. Summary of Global Input Parameters (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Groundwater Protection	FractionPlumeCapture GroundwaterProtection	Consideration of portion of water containing radionuclides entering test well	constant 1.0	Fraction adds flexibility to TPA Version 5.1 by allowing flexibility to consider scenarios in which the contamination plume is wider than the capture zone of the well.

4.6 References

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5 CLIMATE AND INFILTRATION (UZFLOW)

The Climate and Infiltration (UZFLOW)¹ module calculates the deep percolation flux above the repository horizon in the absence of thermal effects, thus providing the upper flow boundary conditions for the unsaturated zone. UZFLOW accomplishes the following main functions: (i) providing subarea-average deep percolation fluxes to the Near Field Environment (NFENV)² module (Chapter 7), which estimates thermally altered water fluxes entering the drifts; (ii) providing subarea-average deep percolation fluxes to the Unsaturated Zone Flow and Transport (UZFT)³ module (Chapter 11), which estimates radionuclide transport in the unsaturated zone; (iii) providing relative change in mean annual precipitation (MAP)⁴ and mean annual temperature (MAT)⁵ from present day to full glacial maximum to the Saturated Zone Flow and Transport module (SZFT)⁶ (Chapter 12); and (iv) MAP and MAT to the Dose Conversion Analysis for Groundwater (DCAGW)⁷ mode (Chapter 17), which converts groundwater combinations at the receptor location to annual pathway and radionuclide-specific doses. These linkages are shown in Figure 5-1. UZFLOW is executed for each repository subarea in every realization of a reference-case simulation.

5.1 Conceptual Model

Deep percolation is derived from a portion of precipitation infiltrating at the ground surface. The term “deep percolation” is used to refer to the downward-moving water immediately above the repository horizon. A portion of the infiltrated water may escape the effects of evapotranspiration in the rooting zone to become net infiltration, which is described herein using the term mean annual infiltration (MAI),⁸ when averaged over several years (e.g., more than a decade). When sufficient infiltrated water escapes evapotranspiration, gravity is expected to drive the water downward through the upper unsaturated zone within the bedrock matrix and fractures to the repository horizon. Downward moving waters can be diverted laterally by capillary and permeability barriers, whereas secondary heterogeneities such as small faults

¹The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

²The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

³The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

⁴Mean annual precipitation is referenced frequently throughout this chapter. The abbreviation MAP will be used.

⁵Mean annual temperature is referenced frequently throughout this chapter. The abbreviation MAT will be used.

⁶The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

⁷The Dose Conversion Analysis for Groundwater module is referenced frequently throughout this chapter. The abbreviation DCAGW will be used.

⁸Mean annual infiltration is referenced frequently throughout this chapter. The abbreviation MAI will be used.

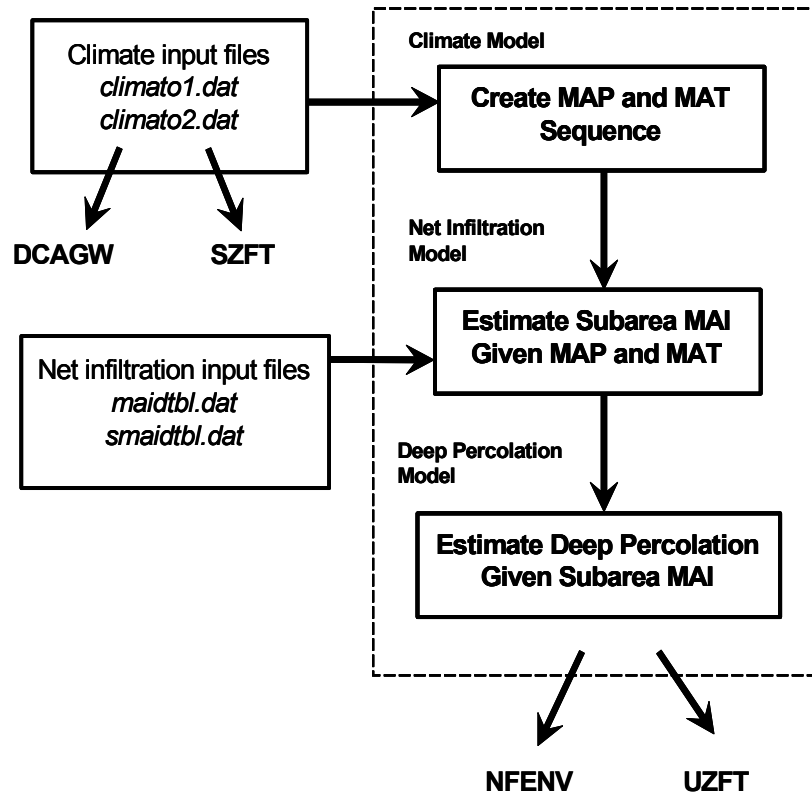


Figure 5-1. Information Flow Diagram for UZFLOW

tend to restrict lateral movement. Deep percolation affects the repository near-field environment, radionuclide release, and transport in the unsaturated zone below the repository.

The UZFLOW conceptual model considers the impact of changes in MAP and MAT at the ground surface for changes in MAI over glacial cycles. UZFLOW consists of three components: (i) a climate model specifying the time history of climatic change, (ii) a net infiltration model calculating MAI under different climates, and (iii) a deep percolation model calculating subarea-averaged percolation flux at the repository horizon. The concepts included in UZFLOW are discussed next.

5.1.1 Climate Model

The climate model represents partially deterministic and partially stochastic time evolution of the two climatic variables, MAP and MAT, that have the dominant effect on infiltration in numerical simulations (Stothoff, 1999). Both MAP and MAT are conceptually linked to the volume and extent of the North American continental ice sheets, which in turn are related to orbital dynamics. MAP is linked to the ice sheets because the jet stream and associated storm tracks are deflected by large ice sheets. MAT is linked to the ice sheets because (i) the ice sheets wax and wane with changes in global temperature and (ii) the temperature gradient between equator and pole is affected by ice sheet extent. The links between ice sheet volume and climate are implemented indirectly by correlating past climate to orbital dynamics.

5.1.2 Net Infiltration Model

The net infiltration model calculates the fraction of MAP that becomes MAI. In the net infiltration conceptual model, some precipitation is lost to direct evaporation before infiltrating into the soil, and some moves laterally due to overland flow before infiltrating. Once in the soil, some of the water is removed by evapotranspiration and some is rendered essentially immobile by capillary and surface tension forces. Any remaining water moves downward, driven by gravity, to enter the fracture system and bedrock matrix underlying the unconsolidated soil system. Once below the evapotranspiration zone, the water is called net infiltration. Thus, net infiltration is affected by the interplay of precipitation events, precipitation seasonality, overland flow, and evapotranspiration as mediated by topography, soil depth and texture, fractured bedrock, vegetation, and climate.

5.1.3 Deep Percolation Model

Percolating water is expected to move vertically in the unsaturated zone unless capillary or permeability barriers force lateral redistribution. Most of the unsaturated zone between the ground surface and the repository horizon is fractured welded tuff with small matrix permeability relative to MAI and plentiful subvertical fractures. These hydraulic properties are expected to promote predominantly vertical flow. A nonwelded tuff unit intermediate between ground surface and repository horizon, the Paintbrush Tuff (PTn),⁹ has large matrix permeability relative to MAI, numerous small faults and fault-related deformation features, and dips to the east. The hydraulic properties of the nonwelded tuff are expected to dampen wetting pulses, and the numerous fault-related heterogeneities are expected to channel flow vertically to counteract the tendency for lateral diversion due to the contrast in hydraulic properties between welded and nonwelded units.

5.2 Model Support and Assumptions

Model support and assumptions are discussed separately for the climate, net infiltration, and deep percolation models in the following sections.

5.2.1 Climate Model

The UZFLOW climate model is a stylized representation of potential future climate sequences. The UZFLOW climate model assumes that (i) MAP and MAT are the dominant climatic parameters needed to estimate MAI, (ii) changes in future regional lapse rates for MAP and MAT are small relative to changes in MAP and MAT, (iii) future climate sequences will be driven by the same naturally occurring processes that drove climate sequences over the past 800,000 years, (iv) the processes driving climate at Yucca Mountain can be paced by peak summer insolation at 65° N latitude, and (v) climate change under peak glacial conditions is the dominant uncertainty in representing the magnitude of future climate change. These assumptions have the logical consequences that (i) the timing of climate change is considered relatively well known, because insolation is dependent on orbital parameters that are readily calculated for millions of years into the future and (ii) climate at a future point in time can be calculated as a weighted sum of present-day and full-glacial-maximum climatic conditions.

⁹Nonwelded Paintbrush Tuffis frequently referenced throughout this chapter. The abbreviation Ptn will be used.

The assumption that MAP and MAT are the dominant climatic parameters needed to estimate MAI is based on the analysis by Stothoff (1999), which found that the numerical model used to estimate MAI is most sensitive to MAP, is less sensitive to MAT, and is relatively insensitive to other annual-average climatic parameters. Various lines of field evidence are consistent with the numerical results (Stothoff and Walter, 2007; Stothoff and Musgrove, 2006), as is the observation that MAP and MAT are the climatic parameters that are typically identified using paleoclimate proxy records.

The assumption that changes in regional lapse rates for MAP and MAT are small relative to changes in MAP and MAT is fundamentally based on unchanging topography and distance to the ocean. This assumption allows specified values of MAP and MAT at a Yucca Mountain reference elevation to be interpolated to other elevations using present-day lapse rates. This assumption further implies that relative changes in MAP and MAT at Yucca Mountain were similar to other locations in the region under past climates.

The assumption that future climate sequences will be driven by the same naturally occurring processes that drove climate sequences over the past 800,000 years is a fundamental assumption. This assumption implies that future climate is based on observations from past glacial cycles.

The assumption that processes driving climate at Yucca Mountain can be paced by peak summer insolation at 65° N latitude is based on (i) the correlation between global ice sheet volume and peak summer insolation at this latitude (the Milankovitch cycle) and (ii) the inferred influence of Northern Hemisphere ice sheets on storm tracks and temperature distributions. Sharpe (2002) provides a basis for this assumption.

The assumption that climate change under peak glacial conditions is the dominant uncertainty in representing the magnitude of future climate change comes about because (i) peak glacial conditions represent the largest change from present-day conditions in the past million years and (ii) paleoclimate proxy records tend to be easier to interpret as relative changes in climate than as absolute changes in climate.

Estimates of full-glacial-maximum MAP and MAT in the Yucca Mountain region are based on several lines of evidence for the last glacial maximum, adjusted to the previous glacial maximum (which represents the full glacial maximum in the UZFLOW model) using inferences from moraines in the Sierra Nevada range (Stothoff and Walter, 2007).

5.2.2 Net Infiltration Model

The net infiltration model consists of two submodels: (i) an external process model that estimates net infiltration statistics on a grid at the ground surface and (ii) the UZFLOW net infiltration model in TPA Version 5.1. Model support and assumptions are discussed separately for these submodels in the following sections.

5.2.2.1 Infiltration Tabulator for Yucca Mountain

The net infiltration model implemented in UZFLOW assumes that any given climatic state (characterized by MAP and MAT at a reference elevation) has a unique spatial distribution of MAI that can be estimated by interpolation between MAI estimates at reference climatic states.

UZFLOW uses input files to provide MAI estimates for several reference climatic states. These input files are typically generated using the preprocessor module Infiltration Tabulator for Yucca Mountain (ITYM).¹⁰ ITYM performs Monte Carlo analyses of net infiltration using abstractions for distributed net infiltration and overland flow based on numerical simulations. Additional details on ITYM are found in Appendix A.

The infiltration abstraction embodied in the ITYM external process model is based on a number of assumptions. In general, ITYM assumes that MAI is dominated by distributed infiltration rather than channel infiltration (although channel infiltration is considered), net infiltration is only influenced mildly by lateral overland and subsurface redistribution, and plant transpiration reduces the net infiltration that would occur under unvegetated conditions by a multiplicative fraction that is not affected by climate. The conceptual model further assumes that vegetative cover reduces net infiltration by a fixed ratio (dependent on soil depth) for any combination of MAP and MAT. The ITYM user documentation (Appendix A) discusses the model assumptions in detail.

The ITYM external process model evaluates MAI for a list of MAP values and a list of MAT values. All combinations of the MAP and MAT values are considered. Figure 5-2 shows areal-average mean infiltration predicted using the base ITYM input file compared with other estimates from Yucca Mountain and nearby areas. Infiltration is averaged over a rectangular box bounding the subareas. Recharge relationships derived for east-central Nevada hydrobasins (Stothoff and Musgrove, 2006) are shown for comparison. The horizontal pink band in Figure 5-2 represents one standard deviation above and below the median areal-average infiltration under present-day conditions. The vertical blue band in Figure 5-2 represents the range of precipitation over all elevations within the same rectangular box. Observations from locations at Yucca Mountain and around Nevada are shown (Stothoff and Walter, 2007), as well as elevation-dependent recharge relationships for east-central Nevada hydrobasins (Stothoff and Musgrove, 2006).

The relationship labeled “ITYM footprint box” in Figure 5-2 describes the hypothetical effect of physically changing the elevation of the Yucca Mountain region (i.e., changing both MAP and MAT according to regional lapse rates) to better compare with the regional estimates. The ITYM relationship is consistent with Yucca Mountain estimates using temperature profiles and saturated zone chloride mass balance calculations, but is approximately an order of magnitude greater than unsaturated zone chloride mass balance calculations. Yucca Mountain estimates are dominated by observations made at lower elevations, which are thought to have less recharge than upland areas. The ITYM relationship tracks the preferred hydrobasin-derived recharge relationship over the precipitation range of 100 to approximately 500 mm/yr [3.9 to 20 in/yr], covering all but the most extreme glacial conditions.

The comparisons suggest that the MAI estimates provided by ITYM with the default input parameters match available present-day data reasonably well and track changes in MAI that may be expected under climate change reasonably well.

¹⁰The Infiltration Tabulator for Yucca Mountain module is referenced frequently throughout this chapter. The abbreviation ITYM will be used.

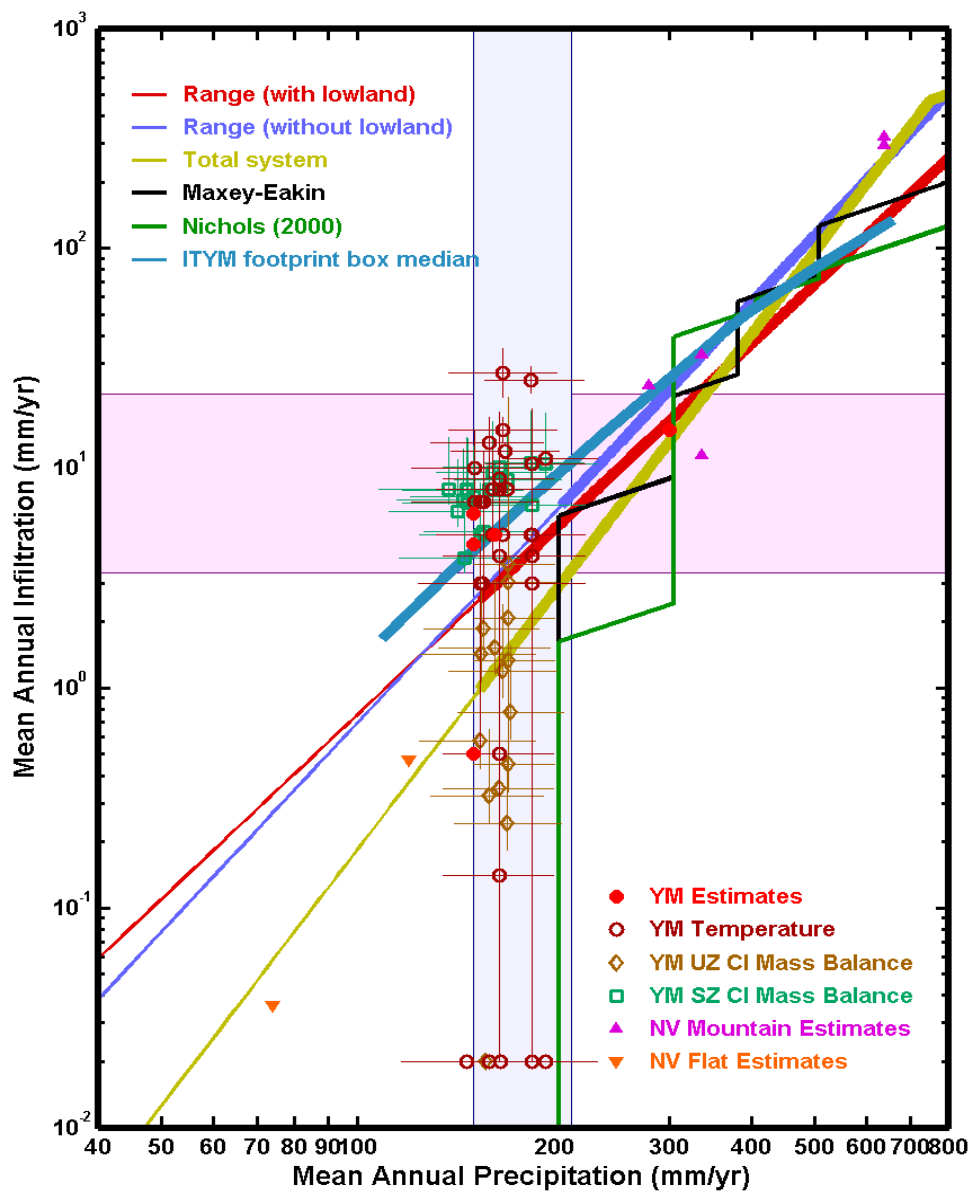


Figure 5-2. Change in Areal-Average Mean Annual Infiltration Predicted by ITYM as a Result of Changing MAP and MAT According to Regional Elevation-Dependent Gradients

ITYM uses the same set of input properties for each MAP and MAT pair, essentially assuming that uncertainty in the input properties is dominant relative to systematic differences in input properties for different climates. Climatic properties, such as cloud cover, relative humidity, and wind speed, are expected to change somewhat over glacial cycles, but MAP and MAT have the dominant influence on calculated MAI (Stothoff, 1997) so systematic variation in other climatic properties is neglected. The bedrock matrix properties are assumed to be unlikely to change over glacial cycles. Little information is available regarding fracture-fill material; thus it is assumed that the fracture-fill material properties represent average properties over a glacial cycle.

The ITYM input parameters describing soil depth and hydraulic properties are expected to vary over glacial cycles, although changes to the soil may not occur synchronously with climate change. Hillslope soil reservoirs in the arid American southwest are thought to be dynamic over glacial time scales, with soils developing over tens of thousands of years during wetter or cooler periods and rapidly being stripped from hillslopes as plant cover drops below a threshold value during interglacial periods (Bull, 1991). The soil thickness distribution and soil hydraulic properties used by ITYM are representative of present-day conditions. A numerical experiment performed by Stothoff, et al. (1999) suggests that neglecting changes in soil properties is expected to cause an average discrepancy of less than a factor of 2. The good agreement shown in Figure 5-2 between ITYM results and regional climate changes due to elevation changes further supports the assumption that changes in the soil characteristics over glacial cycles are dominated by other factors.

5.2.2.2 Subarea Infiltration Table Lookup

The UZFLOW model estimates subarea-average net infiltration using a lookup table. It is assumed that the uncertainty in subarea-average net infiltration is lognormally distributed, and it is further assumed that the mean and standard deviation of subarea-average net infiltration are well described using the average values for all of the fine-scale pixels within the subarea.

The lookup table approach provides a reasonable approximation, as may be seen from the cumulative probability distribution functions in Figure 5-3. The three curves represent (i) the cumulative frequency for 2,000 realizations of areal-average MAI using ITYM; (ii) the cumulative probability distribution function for a lognormal distribution with the mean and standard deviation of the 2,000 realizations (i.e., the statistics of the mean); and (iii) the cumulative probability distribution function for a lognormal distribution with the average mean and average standard deviation of MAI in each of the 59,700 pixels used to estimate MAI (i.e., the mean of the statistics). The two lognormal distributions match closely. The 2,000 realizations are well approximated by a lognormal distribution, but the lognormal distributions have greater probability in the tails than the empirical cumulative distribution function.

5.2.2.3 Deep Percolation Model

The deep percolation model has two primary assumptions: (i) the change in water storage within the unsaturated zone above the repository horizon is small relative to total subarea-integrated net infiltration over a timestep, and (ii) net lateral flow into or out of each subarea is small relative to the total subarea-integrated net infiltration over a timestep. These assumptions result in the subarea-averaged deep percolation averaged over a timestep, being approximately equal to subarea-average MAI, averaged over the same timestep.

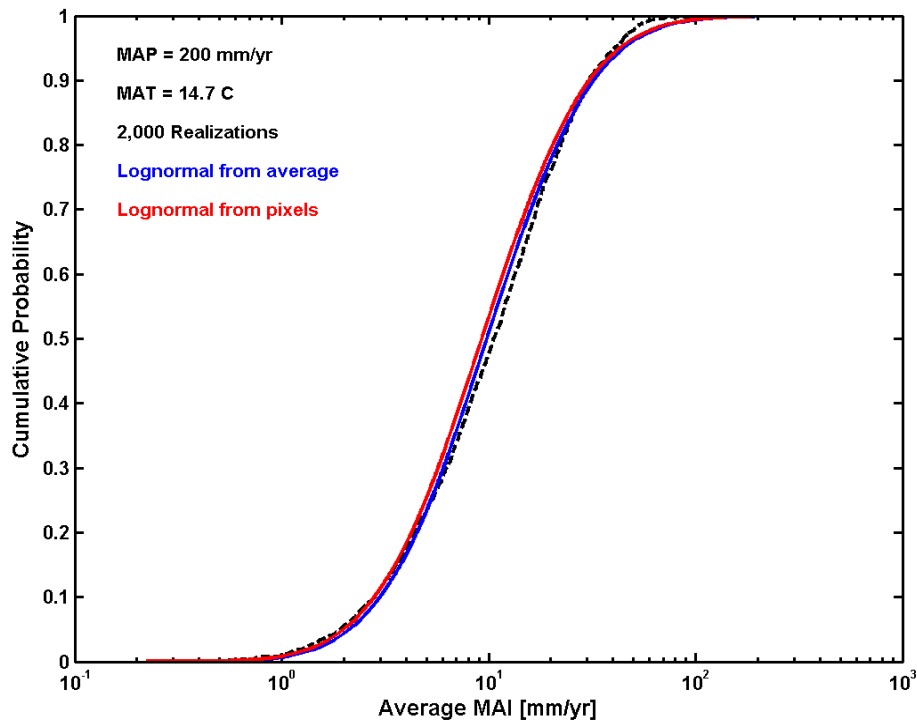


Figure 5-3. Cumulative Probability Distribution Function for Areal-Average MAI

The assumption that there is small change in stored water volume in the unsaturated zone is based on several considerations. The welded tuff matrix above the repository typically remains close to saturation because of the hydraulic properties of the tuff and the fracture system has little volume available for storage; thus neither can appreciably change storage. The PTn does have storage available, but typically responds to wetting pulses quickly relative to a UZFLOWS timestep. Manepally, et al. (2007) suggest that wetting pulses are transmitted through the PTn thickness on the order of one to four decades (wetting pulses propagate more rapidly than the average water velocity through a porous medium, because water entering the top of the medium displaces water at the bottom of the medium). In comparison, a TPA timestep is typically several centuries in duration.

The assumption that net lateral flow into or out of each subarea is small relative to the total subarea-integrated net infiltration is based on observations by Manepally, et al. (2007) that secondary heterogeneities in the form of numerous small faults and fault-related deformation features may limit lateral displacement through the PTn to a scale of tens of meters. All subareas are at least 140 m [460 ft] across in the dip direction, much larger than the lateral diversion through the PTn, and to a certain extent, lateral outflow in the dip direction is balanced by lateral inflow in the dip direction.

5.3 Implementation of Conceptual Model in TPA Version 5.1

The UZFLOW model estimates a time sequence of subarea-average MAI by first using an abstraction for climate to provide a time sequence of MAP and MAT and then table lookup with MAP and MAT to derive subarea-average MAI.

It is computationally intensive to calculate detailed process-level estimates of net infiltration, particularly at the scale necessary to resolve the details of the many washes above the potential repository footprint. Because of this computational burden, UZFLOW does not explicitly incorporate a process-level net infiltration model. Instead, at the onset of a simulation, UZFLOW merges tabular results of external calculations on a fine grid to create a lookup table that relates climate to areal-average MAI for each repository subarea. During runtime, UZFLOW relies on table lookup and interpolation within the merged results. The external calculations are performed with the ITYM preprocessor code for the reference case prior to execution of TPA Version 5.1.

The first time UZFLOW is called during a TPA simulation, *climato1.dat* and *climato2.dat* are read and subarea-average tables of MAI as a function of MAP and MAT are prepared from detailed infiltration results captured in *maidtbl.dat* and *smaidtbl.dat*. The auxiliary data files are independent of the subarea coordinates, which are defined in *tpa_include.inp*; thus there is no need to prepare new *maidtbl.dat* and *smaidtbl.dat* if subareas are revised, unless a new subarea lies outside the area covered by *maidtbl.dat* and *smaidtbl.dat*. The *maidtbl.dat* and *smaidtbl.dat* files encompass contingency areas for the repository as well as previously potential repository designs. Each subarea-average table is calculated by averaging all cell values within the subarea.

UZFLOW is called once for each subarea during each realization. Output from UZFLOW consists of time- and space-averaged deep percolation flux for each timestep in each subarea, and it is used as input by NFENV and UZFT (Figure 5-1).

The first time UZFLOW is called during a realization, all UZFLOW-specific *tpa.inp* parameters describing the realization are used to generate a climate sequence in increments of the internal UZFLOW timestep. This climate sequence is used for all subareas in the realization. Section 5.3.1 describes how the climate sequence is generated.

The climate sequence is used to interpolate within the table of subarea-average MAI to provide a constant value of median MAI for each UZFLOW timestep. In the MAI-sampled mode, the interpolated MAI value is adjusted to honor the sampled footprint-average MAI as described in Section 5.3.2.1. In the property-sampled mode (Section 5.3.2.2), the subarea-average standard deviation of MAI is also determined by interpolation, and a sampled zero-mean, unit-variance normal deviate representing uncertainty in footprint-average net infiltration is used with the median and standard deviation to calculate the realization of subarea-average MAI. It is assumed that uncertainty in subarea-average MAI can be described by a lognormal distribution. Cumulative MAI is obtained at the end of each TPA timestep, with the average MAI for each timestep calculated as the difference between cumulative MAI over the timestep divided by the timestep duration.

5.3.1 Climate Model

The climate abstraction relies on the following three components: (i) user-defined auxiliary input file *climato2.dat*, describing a mean sequence of climates, specified relative to initial and full glacial climates; (ii) user-defined auxiliary input file *climato1.dat*, describing perturbations to the mean sequence of climates; and (iii) user-defined parameters describing the actual climatic conditions under initial and full glacial climates and the uncertainty in these climatic states.

Three climate modes are used to describe climate change: (i) the time-varying mode, which uses an input sequence of MAP and MAT over the period of interest in conjunction with table lookup to estimate MAI in each subarea; (ii) the maximal-infiltration mode, in which MAI is assumed to equal MAP using the same MAP sequence; and (iii) the long-term-average mode, in which a long-term-average value for MAI is used. The time-varying and maximal-infiltration modes apply at the beginning of a simulation. The long-term-average mode (if used) applies from a fixed onset time to the end of a simulation. Once the long-term-average mode begins, calculations from the time-varying and maximal-infiltration modes are ignored.

5.3.1.1 Time-Varying Mode

The time-varying mode of the climate model is signaled by setting the *tpa.inp* parameter *uzflow_SampleMode* to 1 or 2 [representing the MAI-sampled and property-sampled modes of the net infiltration model (see Section 5.3.2)]. The time-varying mode accounts for the different sources of climate change using the vector equation

$$\mathbf{V}^k = \begin{bmatrix} V_{op} \\ V_{ot} \end{bmatrix} + \mathbf{F}^k \begin{bmatrix} V_{gp} - V_{op} \\ V_{gt} - V_{ot} \end{bmatrix} + \boldsymbol{\chi}^k \quad (5-1)$$

where

$\mathbf{V}^k$	—	climate vector at UZFLOW climate step k
V_{op}	—	MAP value at the start of the realization as specified by the <i>tpa.inp</i> parameter <i>uzflow_ReferenceMAPAtStart</i> [mm/yr]
V_{ot}	—	MAT value at the start of the realization as specified by the <i>tpa.inp</i> parameter <i>uzflow_ReferenceMATAtStart</i> [degC]
V_{gp}	—	MAP value at the reference full glacial maximum for the realization
V_{gt}	—	MAT value at the reference full glacial maximum for the realization
$\mathbf{F}^k$	—	vector of relative climate change from the initial to full glacial maximum at UZFLOW climate step k
$\boldsymbol{\chi}^k$	—	vector of perturbations

The $\mathbf{F}^k$ and $\boldsymbol{\chi}^k$ parameters are specified in *climato2.dat* and *climato1.dat*, respectively, as described in Section 5.5.

Full glacial maximum is described relative to the conditions at the start of the simulation, with MAP described as a multiple of initial conditions and MAT described as an offset from initial conditions

$$V_{gp} = F_{gp} V_{op} \quad (5-2)$$

$$V_{gt} = V_{ot} + \Delta_{gt} \quad (5-3)$$

where

- F_{gp} — ratio of full-glacial to present-day MAP as specified by the *tpa.inp* parameter `uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum`
- Δ_{gt} — increase in temperature from present-day to full-glacial MAT (usually Δ_{gt} is negative) as specified by the *tpa.inp* parameter `uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]`

UZFLOW assumes that perturbations to MAP and MAT obey a bivariate normal distribution within a UZFLOW climate step, and these perturbations are not correlated with perturbations from previous UZFLOW climate steps. Correlated perturbations to MAP and MAT are sampled from a bivariate normal distribution using

$$\chi^k = \begin{bmatrix} \sigma_p & 0 \\ \sigma_t \rho & \sigma_t (1 - \rho^2)^{1/2} \end{bmatrix} \epsilon^k \quad (5-4)$$

where

- σ_p — standard deviation of the precipitation perturbation as specified by the *tpa.inp* parameter `uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]`
- σ_t — standard deviation of the temperature perturbation as specified by the *tpa.inp* parameter `uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]`
- ρ — correlation between precipitation and temperature perturbations as specified by the *tpa.inp* parameter `uzflow_CorrelationBetweenMAPAndMATPerturbations`
- ϵ^k — vector of normally distributed perturbations with zero mean and unit variance

Parameters σ_p , σ_t , and ρ are defined in *tpa.inp*. A large number of ϵ^k values are specified in *climato1.dat*, which can be used to generate several sets of climatic-perturbation sets.

All UZFLOW calculations are done with an internal constant timestep, *tpa.inp* parameter `uzflow_TimeStep[yr]`, that is independent of the overall TPA Version 5.1 timestep. Climate, net infiltration fluxes, and deep percolation fluxes are all assumed to be constant throughout a UZFLOW timestep. TPA Version 5.1 provides UZFLOW with the start and end of each TPA timestep. Average deep percolation flux over TPA Version 5.1 timestep is the cumulative UZFLOW-calculated deep percolation flux from the start to end of TPA Version 5.1 timestep, divided by the step size.

5.3.1.2 Maximal-Infiltration Mode

The maximal-infiltration mode of operation assumes that all precipitation becomes deep percolation (i.e., no loss of water from the subarea due to evapotranspiration and runoff). The maximal-infiltration mode is signaled by setting *tpa.inp* parameter `uzflow_SampleMode` to 3.

5.3.1.3 Long-Term-Average Mode

A simplified mode of operation considers long-term-average MAI. The long-term-average period begins at an onset time specified by the *tpa.inp* parameter called *uzflow_LongTermAverageOnsetTime[yr]*, which may be before the start of simulation or after the end of the performance period. UZFLOW selects random values for long-term repository-average deep percolation using *tpa.inp* parameter *uzflow-LongTermAverageFootprintAverageMeanAnnualInfiltration[mm/yr]*. The deep percolation flux within an individual subarea may vary from the repository average, but the area-weighted average is preserved using the representation

$$Q_i = f_i Q_a \quad (5-5)$$

$$\sum_{i=1}^N w_i f_i = 1 \quad (5-6)$$

$$\sum_{i=1}^N w_i = 1 \quad (5-7)$$

where

- Q_i — deep percolation flux [mm/yr] for repository subarea i
- Q_a — deep percolation flux [mm/yr] averaged over the repository footprint as specified by the *tpa.inp* parameter *uzflow_LongTermAverageFootprintAverageMeanAnnualInfiltration[mm/yr]*
- w_i — fraction of the repository area in subarea i
- f_i — fraction of the deep percolation flux in subarea i

The w_i values lie between 0 and 1. The f_i values are calculated using tabulated fluxes for a climate representative of intermediate glacial conditions and are usually close to 1.

5.3.2 Net Infiltration Model

Four modes for estimating subarea-average MAI are available. The MAI-sampled and property-sampled infiltration modes both use the time-varying climate sequence from Section 5.3.1.1 to interpolate in the subarea-average MAI tables described in Section 5.2.2.2 that relate MAI to climate, but the tables are interpreted differently in the two modes. The maximal-infiltration climate mode described in Section 5.3.1.2 assumes that the generated MAP sequence is converted directly into net infiltration. The long-term-average mode directly specifies the magnitude of the footprint-average MAI, but ensures that the spatial patterns of MAI in the subarea-average MAI tables are preserved. The maximal-infiltration and long-term-average climate modes are described in Sections 5.3.1.2 and 5.3.1.3, respectively. The MAI-sampled and property-sampled infiltration modes are described in Sections 5.3.2.1 and 5.3.2.2, respectively, as are strategies for considering modifications in MAI due to climatic variability and change in precipitation seasonality (Section 5.3.2.3).

5.3.2.1 MAI-Sampled Mode

The MAI-sampled mode is specified by setting *tpa.inp* parameter *uzflow_SampleMode* to 1. The MAI-sampled mode uses a normalized version of the MAI input specified in *maidtbl.dat* to define MAI in each subarea as a function of climate. The user directly specifies footprint-average MAI at the start of the simulation using a sampled parameter. In this mode, the tables of subarea-average MAI as a function of MAP and MAT are replaced with scaled tables at the start of each realization.

The scaling factor is simply the ratio of sampled footprint-average MAI to the calculated footprint-average MAI using *maidtbl.dat*. All MAI values in the table are multiplied by the scaling factor using the formula

$$I^* = \left[\frac{I_o}{I(P_o, T_o)} \right] I \quad (5-8)$$

where

- I^* — scaled table entry [mm/yr]
- I — subarea-average MAI [mm/yr] derived from *maidtbl.dat* [mm/yr]
- I_o — sampled initial footprint-average MAI [mm/yr] as specified by the *tpa.inp* parameter [mm/yr]
uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
- $I(P_o, T_o)$ — footprint-average MAI under initial climatic conditions [mm/yr]

5.3.2.2 Property-Sampled Mode

The property-sampled mode is used when both spatially distributed MAI and its variability are well estimated by the input files. The property-sampled mode is specified by setting *uzflow_SampleMode* to 2 in *tpa.inp*.

The property-sampled mode has similar assumptions regarding *maidtbl.dat* as the MAI-sampled mode, but in the property-sampled mode, uncertainty is accounted for with *smaidtbl.dat*. The MAI values can be scaled using a parameter in *tpa.inp*, accounting for climatic variability at time scales smaller than individual UZFLOW timesteps.

In the property-sampled mode, tables are created for subarea-average MAI and the standard deviation of MAI. In this mode, the tables of subarea-average MAI as a function of MAP and MAT are replaced with scaled tables at the start of each realization. Each subarea MAI in the table is modified using the formula

$$I^* = F_i I + \sigma_h N_h \quad (5-9)$$

where

- I^* — scaled table entry [mm/yr]
- I — subarea-average MAI [mm/yr] derived from *maidtbl.dat*
- F_i — sampled MAI scaling factor as specified by the *tpa.inp* parameter
uzflow_SampledMAIScalingFactor

σ_h	—	subarea-average standard deviation of MAI [mm/yr] from <i>smaidtbl.dat</i>
N_h	—	sampled zero-mean, unit-variance normal deviate as specified by the <i>tpa.inp</i> parameter <code>uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]</code>

5.3.2.3 Climate-Variability-Induced MAI Scaling

Climatic variability exists over a wide range of time scales. Long-term variability is considered using *climato2.dat*. The abstractions embedded in the ITYM external process model account for the variability at hourly to annual time scales; thus variability at less than the decadal scale is implicitly considered in *maidtbl.dat*.

Two general approaches are implemented to scale MAI due to intermediate-scale climatic variability. One method relies on explicitly calculated perturbations in climate (i.e., the χ^k values discussed in Section 5.1.1). The second method explicitly increases the tabulated MAI values to represent expected MAI augmentation due to climatic variability. The second method provides a smoother sequence of deep percolation, which is more computationally efficient.

The second method is implemented differently depending on the net infiltration mode. In the MAI-sampled and long-term-average modes, the MAI values used in *tpa.inp* represent augmented MAI. In the property-sampled mode, all subarea-averaged MAI values are assumed to incorporate intermediate-scale variability

5.4 Input Parameters in *tpa.inp*

All input parameters to UZFLOW are located in the UZFLOW section of *tpa.inp* and are listed in Table 5-1.

5.5 Auxiliary Input Data and External Process Modules

5.5.1 Auxiliary Input Data

Auxiliary input data files used by UZFLOW provide detailed information on future climatic conditions and tables that specify the statistics of estimated MAI distributed across the ground surface as a function of MAP and MAT. Table 5-2 lists and describes the auxiliary input data files for UZFLOW.

Table 5-1. Reference Data for Parameters of <i>tpa.inp</i> Used by UZFLOW (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFLOW	uzflow_SampleMode	Flag specifying the method for estimating net infiltration using data from <i>maidtbl.dat</i> and <i>smaidtbl.dat</i> prior to the long-term-average period. Sample mode 1 is the reference-case climate mode with sampled mean annual infiltration (<i>maidtbl.dat</i> used), 2 is the reference-case climate mode with sampled hydraulic properties (<i>maidtbl.dat</i> and <i>smaidtbl.dat</i> used), and 3 is the maximal-infiltration mode (infiltration equals precipitation).	iconstant 1	User option. Program control switch: for value = 1, the mean values of net infiltration from <i>maidtbl.dat</i> , when aggregated for each subarea, are scaled to the sampled value for uzflow_FootprintAverageMean AnnualInfiltrationAtStart[mm/yr]; for value = 2, the mean values for the subarea are aggregated, no scaling is used, and uncertainty is obtained from <i>smaidtbl.dat</i> ; and for value = 3, infiltration is assumed to be equal to mean annual precipitation at the reference elevation (maximal-infiltration mode). The <i>maidtbl.dat</i> and <i>smaidtbl.dat</i> files are created by ITYM prior to a TPA simulation.
UZFLOW	uzflow_ReferenceMAPAtStart[mm/yr]	V_{op} MAP at the reference elevation of 1,400 m at the start of the simulation [mm/yr]	constant 185	Reference value of MAP at a reference elevation for present-day conditions; used in conjunction with the precipitation multiplier for glacial conditions. Stothoff and Walter (2007) discuss elevation-dependent variation of MAP in the Yucca Mountain region.
UZFLOW	uzflow_ReferenceMATAtStart[degC]	V_{ot} MAT at the reference elevation of 1,400 m at the start of the simulation [°C]	constant 15.7	Reference value of MAT at a reference elevation for present-day conditions; used in conjunction with the temperature increase for glacial conditions. Stothoff and Walter (2007) discuss elevation-dependent variation of MAT in the Yucca Mountain region.

Table 5-1. Reference Data for Parameters of <i>tpa.inp</i> Used by UZFLOW (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFLOW	uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]	I_o MAI [mm/yr] for the initial (modern) climate averaged over the repository footprint	lognormal 0.465, 156	Estimate from Stothoff and Walter (2007), with median = 8.5 mm/yr and coefficient of variation = 1.19.
UZFLOW	uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum	F_{MAP}^{gp} multiplier at glacial maximum	uniform 1.8, 2.3	Estimate from Stothoff and Walter (2007).
UZFLOW	uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]	Δ_{MAT}^{gp} increase at glacial maximum [°C]	uniform -9.7, -6.9	Estimate from Stothoff and Walter (2007).
UZFLOW	uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]	N_h Used to determine deviation of net infiltration extracted from <i>smaiddtbl.dat</i> (table of standard deviations) to use with the annual average net infiltration from <i>maiddtbl.dat</i>	normal -3.0902, 3.0902	Values are based on 0.1- and 99.9-percent quantiles of the standard normal distribution (e.g., Abramowitz and Stegun, 1972).
UZFLOW	uzflow_LongTermAverageOnsetTime[yr]	Time after start when the long-term-average sample mode begins	constant 10,000	Time after start when the long-term-average sample mode begins. The climate mode set by UZFLOW_SampleMode is ignored during the long-term-average mode.
UZFLOW	uzflow_LongTermAverageFootprintAverageMeanAnnualInfiltration [mm/yr]	Q_a MAI [mm/yr] after onset of the long-term-average period, averaged over the repository footprint	lognormal 3.577, 285.3	Values define the relationship found by Stothoff and Walter (2007) with median = 31 mm/yr and coefficient of variation = 0.81.

Table 5-1. Reference Data for Parameters of tpa.inp Used by UZFLOW (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFLOW	uzflow_TimeStep[yr]	Internal timestep used for UZFLOW calculations	constant 500	Value is based on staff expert judgment for representing smooth and step variations in <i>climato2.dat</i> for creating input for estimating net infiltration. The value of 500-year step size also factors in efficiency of TPA Version 5.1 simulations.
UZFLOW	uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod [mm/yr]	σ_p Standard deviation of MAP about mean in one time period [mm/yr]	constant 0.0	Needed to incorporate intermediate scale variation in climate using <i>climato1.dat</i> . Including intermediate scale climate variation is not in the reference case because deviation about the mean is not considered to have a significant effect (per current staff expert judgment) and allows efficient execution for TPA Version 5.1. This parameter is not used when set to zero.
UZFLOW	uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod [degC]	σ_t Standard deviation of MAT about mean in one time period [°C]	constant 0.0	Needed to incorporate intermediate scale variation in climate using <i>climato1.dat</i> . Including intermediate scale climate variation is not in the reference case because deviation about the mean is not considered to have a significant effect (per current staff expert judgment) and allows efficient execution for TPA Version 5.1. This parameter is not used when set to zero.
UZFLOW	uzflow_CorrelationBetweenMAPAndMAT Perturbations	ρ Correlation coefficient between MAP and MAT perturbations	constant -0.8	The value is a best estimate of staff drawing from climate expert elicitation described by DeWispelare, et al. (1993). Parameter is used when uzflow_SampleMode is 1 and both uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] and uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod [degC] are nonzero.

Table 5-1. Reference Data for Parameters of <i>tpa.inp</i> Used by UZFLOW (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFLOW	uzflow_ClimatePerturbationSet	Program control parameter used to specify which part of <i>climato1.dat</i> is to be used for climate perturbations to represent intermediate scale variations	iconstant 1	The number of sets of data in <i>climato1.dat</i> is determined by dividing the number of values in <i>climato1.dat</i> by two times the number of UZFLOW timesteps needed for a TPA simulation. There are 50,000 values in the <i>climato1.dat</i> for the reference case. Generally, a small value (1 to 12) should be selected for ClimatePerturbationSet for long TPA simulations with numerous timesteps.
Correlated Parameters	Independent Variable uzflow_FootprintAverage MeanAnnualInfiltrationAt Start[mm/yr] Dependent Variable uzflow_HydraulicProperty UncertaintyDeviation [N(0,1)]	Correlation between I_o and N_h	correlateinputs 0.9999	Ensures that correlation between infiltration and parameters from NFENV is unaffected by infiltration sample mode.
Correlated Parameters	Independent Variable uzflow_FootprintAverage MeanAnnualInfiltrationAt Start[mm/yr] Dependent Variable uzflow_LongTerm AverageFootprintAverage MAI[mm/yr]	Correlation between I_o and Q_a	correlateinputs 0.98	Correlation between I_o and Q_a is assumed to be dominated by site hydraulic properties.

Table 5-1. Reference Data for Parameters of tpa.inp Used by UZFLOW (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Correlated Parameters	Independent Variable uzflow_HydraulicProperty UncertaintyDeviation [N(0,1)]	Correlation between Q_a and N_h	correlateinputs 0.98	A necessary consequence of the perfect correlation between I_o and N_h .
	Dependent Variable uzflow_LongTerm AverageFootprintAverage MAI[mm/yr]			
Correlated Parameters	Independent Variable uzflow_FootprintAverage MeanAnnualInfiltrationAt Start[mm/yr]	Correlation between I_o and SubAreaWetFraction*	correlateinputs 0.7	Staff best estimate.
	Dependent Variable SubAreaWetFraction			
Correlated Parameters	Independent Variable uzflow_FootprintAverage MeanAnnualInfiltrationAt Start[mm/yr]	Correlation between I_o and WastePackageFlow MultiplicationFactor*	correlateinputs -0.7	Must be the opposite of the correlation between I_o and SubAreaWetFraction.
	Dependent Variable WastePackageFlow MultiplicationFactor			
Correlated Parameters	Independent Variable uzflow_FootprintAverage MeanAnnualInfiltrationAt Start[mm/yr]	Correlation between I_o and XOFmultCoefficient*	correlateinputs 0.6	Consistent with other correlations.
	Dependent Variable XOFmultCoefficient			

Table 5-1. Reference Data for Parameters of tpa.inp Used by UZFLOW (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Correlated Parameters	Independent Variable uzflow_HydraulicProperty UncertaintyDeviation [N(0, 1)]	Correlation between N_h and SubAreaWetFraction*	correlateinputs 0.7	Must be identical to the correlation between I_o and SubAreaWetFraction.
	Dependent Variable SubAreaWetFraction			
Correlated Parameters	Independent Variable uzflow_HydraulicProperty UncertaintyDeviation [N(0, 1)]	Correlation between N_h and WastePackageFlow MultiplicationFactor*	correlateinputs -0.7	Must be the opposite of the correlation between N_h and SubAreaWetFraction.
	Dependent Variable WastePackageFlow MultiplicationFactor			
Correlated Parameters	Independent Variable uzflow_HydraulicProperty UncertaintyDeviation [N(0, 1)]	Correlation between N_h and X0FmultCoefficient*	correlateinputs 0.6	Must be identical to the correlation between I_o and XDFmultCoefficient.
	Dependent Variable X0FmultCoefficient			
Correlated Parameters	Independent Variable uzflow_LongTerm AverageFootprintAverage MAI[mm/yr]	Correlation between Q_a and SubAreaWetFraction*	correlateinputs 0.7	Consistent with other correlations.
	Dependent Variable SubAreaWetFraction			

Table 5-1. Reference Data for Parameters of tpa.inp Used by UZFLOW (continued)				
(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Correlated Parameters	Independent Variable uzflow_LongTerm AverageFootprintAverage MAI[mm/yr]	Correlation between Q_a and WastePackageFlow MultiplicationFactor*	correlateinputs -0.7	Must be the opposite of the correlation between Q_a and SubAreaWetFraction.
	Dependent Variable WastePackageFlow MultiplicationFactor			
Correlated Parameters	Independent Variable uzflow_LongTerm AverageFootprintAverage MAI[mm/yr]	Correlation between Q_a and X0FmultCoefficient*	correlateinputs 0.6	Consistent with other correlations.
	Dependent Variable X0FmultCoefficient			
*See Chapter 10 for descriptions of SubAreaWetFraction, WastePackageFlowMultiplicationFactor, and X0FmultCoefficient.				

Table 5-2. Auxiliary Input Data Files Used by UZFLOW	
Input File	Contents
<i>climato1.dat</i>	Data file <i>climato1.dat</i> provides normally distributed random numbers used in computing time-varying MAP and MAT [the ϵ_k values used in Eq. (5-4)]. Each of the N UZFLOW timesteps requires two random numbers, for a total of $2N$ random numbers per sequence. The numbers provided are reorganized into perturbation sets of length $2N$ at run time. There are 50,000 numbers in <i>climato1.dat</i> provided with TPA Version 5.1, yielding 12 perturbation sets for a 1-million-year simulation using 500-year timesteps. The perturbation set used for each realization is selected with <i>tpa.inp</i> parameter <i>uzflow_ClimatePerturbationSet</i> . The header of the reference-case <i>climato1.dat</i> for TPA Version 5.1 describes the format for the file.
<i>climato2.dat</i>	Data file <i>climato2.dat</i> provides a time history of climate expressed as a relative change in MAP and MAT from initial state (present day) to full glacial maximum, as described in Section 5.1.1. From 10,000 years to 1,000,000 years in the future, <i>climato2.dat</i> for the reference case is based on the sequence developed by Sharpe (2002), and the first 10,000 years represent a gradual transition from present day conditions to year 10,000. The header of the reference-case <i>climato2.dat</i> for TPA Version 5.1 describes the format for the file.
<i>maidtbl.dat</i>	This file contains several sets of the mean of MAI for each grid block of the digital elevation model. Each set represents a distinct MAP and MAT value at a reference elevation. This file is generated with an external process model, the ITYM preprocessor code. ITYM is included with TPA Version 5.1. The reference case uses a 120-m [394-ft] grid to describe the spatial distribution of MAI. UZFLOW averages the values in the grid blocks within each subarea to derive a table of subarea-average MAI, as described in Section 5.3.
<i>smaidtbl.dat</i>	This file contains several sets of the standard deviation of MAI for each grid block of the digital elevation model. The file format must match <i>maidtbl.dat</i> .

5.5.2 External Process Model—ITYM

ITYM is an external process model that creates *maidtbl.dat* and *smaidtbl.dat*. The shallow infiltration model in ITYM calculates the mean annual net-infiltration flux below the root zone moving vertically downward into the deeper subsurface. The net-infiltration flux is directly linked to the MAP and MAT climatic parameters used in TPA Version 5.1. Appendix A further details the use of ITYM.

5.5.2.1 ITYM Process Representation

ITYM directly considers water balances on a fine grid. Each grid block, or pixel, in TPA Version 5.1 is a square with 30-m [98-ft] sides. ITYM embodies abstractions developed from numerous one-dimensional simulations that consider a mass and energy balance in the absence of plant transpiration (i.e., bare soil) with various combinations of soil, bedrock, and climatic properties that span the range of potential values expected over the performance period. The simulations were driven by a decade of hourly meteorological observations from Desert Rock, Nevada, approximately 45 km [28 mi] east-southeast of Yucca Mountain. These simulations and the abstraction process are described by Stothoff (1999, 1997).

The one-dimensional abstractions represent local-scale net infiltration without lateral subsurface redistribution, which would tend to move water from shallow soils with high net infiltration rates to deeper soils with lower net infiltration rates. ITYM estimates are anticipated to be slight overestimates of net infiltration on upper hillslopes and slight underestimates at the foot of hillslopes. Lateral subsurface redistribution will tend to slightly reduce areal-average net infiltration by disproportionately reducing infiltration in high-infiltration zones.

The one-dimensional abstraction values are adjusted within ITYM to account for runoff and vegetation. As discussed in Appendix A, ITYM considers runoff by increasing the precipitation levels for each pixel based on contributing upslope area and soil volume.

ITYM uses a heuristic model to account for plant transpiration. The one-dimensional simulations only considered evaporation, which is ineffective at removing water from deep in the soil column. The presence of vegetation tends to reduce net infiltration by removal of water that would otherwise escape evaporation. Essentially all soil water is scavenged from deep soil in arid climates, but there is less time for plant uptake to occur in shallow soils above fractured bedrock before water enters the bedrock fracture system and becomes inaccessible to uptake. The heuristic transpiration model assumes that the scavenging fraction is smallest with zero soil thickness and increases exponentially to a limiting value as soil depth increases.

5.5.2.2 ITYM Inputs

ITYM is a distributed model for net infiltration. Each pixel requires information on elevation, soil type, bedrock type, soil depth, mean annual windspeed, contributing upslope area, and contributing upslope soil volume, all provided as digital elevation model files. ITYM also uses an input file relating mean annual insolation to ground slope and aspect. These files are described in Appendix A.

ITYM explicitly considers uncertainty in each input parameter. For example, the probability distribution for each parameter in each soil type is provided in the master ITYM input file, including correlations between parameters. The explicit representation of uncertainty within the ITYM calculations allows a statistical description to be estimated for MAI.

5.6 Intermediate Outputs and Information Passed to Other Modules

The intermediate outputs from UZFLOW are available in *infilper.res*. For all realizations, *infilper.res* contains the deep percolation rate averaged over all subareas for every 10 timesteps used in a simulation. The *infilper.res* file is described in Chapter 19.

In addition to the intermediate output file described above, the user can specify that calculated information passed to and from UZFLOW be saved as intermediate output for specific realizations. Table 5-3 lists and describes these optional intermediate output files.

To specify optional intermediate output files, the user can set *tpa.inp* parameter OutputMode(0=None,1=All,2=UserDefined) to a value of 1 or 2. When set to 1, all optional intermediate output for UZFLOW will be saved for all realizations. When set to 2, optional intermediate output selected will be saved for realizations starting from *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by *tpa.inp* parameter UserDefinedUpperRealizationAppended. The user can select UZFLOW optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter SelectAppendFiles to 1 for just *uzflow.ech* and *uzflow.rlt*, or 23 for just *infilper.cum*.

UZFLOW passes the volumetric flow rate of water infiltrating toward the repository in each subarea for each timestep to NFENV to estimate groundwater reflux during the repository thermal phase and to UZFT to determine transport velocities. UZFLOW passes time-dependent climate state information to SZFT (Chapter 12). In addition, UZFLOW passes the MAP and MAT sequences to DCAGW (Chapter 17).

5.7 Techniques for Understanding Module Performance

While there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of processes modeled by UZFLOW. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques may be useful to understand their effects on system-level performance.

In addition, “pinch-point” techniques, wherein output or intermediate results produced from UZFLOW can be understood in combination with output or intermediate results from other modules [e.g., NFENV, Contaminant Release (EBSREL), and UZFT], may help to better evaluate subsystem processes. The *infilper.res* file is a key output file that lists the time history of deep percolation fluxes by subarea, as well as fluxes within the drift. The influence of deep

Table 5-3. Optional Intermediate Output Files Created During Execution of UZFLOW	
Output File	Contents
<i>uzflow.ech</i>	Contains the time intervals at which UZFLOW outputs are written
<i>uzflow.rlt</i>	Contains the volumetric deep percolation flow rates into each subarea for each timestep in each realization
<i>infilper.cum</i>	Identical to <i>infilper.res</i> except that every timestep is reported.

percolation on processes associated with the engineered barrier system can be understood by comparing release data stored in *ebsrel.rlt* (see Chapter 10) with fluxes in *infilper.res*.

Further, single parameter importance analyses can be performed by repetitively varying input parameters associated with particular subsystem processes modeled by UZFLOW and analyzing output and intermediate results from various consequence modules, as mentioned previously. Single parameter importance analyses could be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, a single parameter importance analysis could be performed by repetitively specifying smaller ranges within the parameter's original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges. The user should exercise care in interpreting results from simulations in which input are altered beyond their intended ranges. Key input parameters that can influence dose calculations include `uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]`, `uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum`, `uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]`, and `uzflow_LongTermAverageFootprintAverageMeanAnnualInfiltration[mm/yr]`.

The overall effect of surface and shallow subsurface processes on repository performance can be understood by setting the `uzflow_SampleMode` to 3 to allow all precipitation to become deep percolation.

5.8 References

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6 DRIFT DEGRADATION (DRIFTFAIL)

The Drift Degradation module (DRIFTFAIL)¹ calculates the magnitude and time of occurrence of static vertical pressure on a drip shield resulting from accumulated rubble in the drift and the equivalent diameter of the degraded drift. Vertical pressures calculated by DRIFTFAIL are passed to the Drip Shield and Waste Package Mechanical Failure module (MECHFALL)² (Chapter 9), which calculates mechanical drip shield and waste package failures. Equivalent drift diameters calculated by DRIFTFAIL are passed to the Near-Field Environment module (NFENV)³ (Chapter 7), which calculates surface temperatures for the waste package and drip shield. DRIFTFAIL performs calculations for thermally or seismically induced drift degradation depending on the status of two flags: DriftDegradationScenarioFlag(yes=1,no=0) and SeismicDisruptiveScenarioFlag(yes=1,no=0). DRIFTFAIL executes once for each subarea in every realization.

6.1 Conceptual Model

DRIFTFAIL calculates rubble accumulation in an emplacement drift. This accumulation is caused by drift degradation from the effects of rock stress changes due to excavation, thermal loading, and/or seismic ground motion. In DRIFTFAIL, drift degradation from the effects of excavation and thermal loading occurs at a steady rate, but degradation from seismic ground motions is controlled by earthquakes that are strong enough to cause rock failure around the drift openings. Rubble from drift degradation may occupy more volume than the rock that breaks up to form rubble. This rock bulking may result in a self-arresting mechanism for drift degradation. Detachment of blocks from the host rock above a drift may cause the drift opening to expand, but the resulting rubble fills the opening at a faster rate. Thus, the drift opening may be ultimately filled with rubble, thereby terminating the degradation process. The volume of rubble needed to fill a drift is calculated by invoking a mass balance between rock blocks above the drift opening and the rubble formed when the blocks break up and fall.

The volume of a rock block ($V_{initial}$) and the volume of rubble (V_{final}) formed after the rock block breaks up and falls into the drift are related through the equation

$$V_{final} = V_{initial}(BF) \quad (6-1)$$

where

BF — the bulking factor of the rock, which describes the volumetric expansion of the rock when it breaks up to form rubble [dimensionless]

¹The Drift Degradation module is referenced frequently throughout this chapter. The abbreviation DRIFTFAIL will be used.

²The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFALL will be used.

³The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

Assuming that the cross-sectional area of the degraded drift is constant along the drift axis, the volumes $V_{initial}$ and V_{final} can be replaced with cross-sectional areas $A_{initial}$ and A_{final} , respectively, which results in the equation

$$A_{final} = A_{initial}(BF) \quad (6-2)$$

The area $A_{initial}$ is associated with the cross-sectional area of rock above the initial drift opening, and A_{final} is associated with the sum of $A_{initial}$ and the cross-sectional area of the initial drift opening. Values of the two areas depend on the degraded-drift configuration (Figure 6-1). Implementing Eq. (6-2) in the module as described in Section 6.3 uses the initial cross-sectional diameter of a circular drift, height and width of the drip shield, height of the invert, and the bulking factor (Figure 6-1). The height of rubble that corresponds to a given area is calculated using an assumed degraded-drift shape [i.e., chimney or trapezoidal (Figure 6-1)]. The equivalent degraded-drift diameter is calculated using the model described in NFENV.

6.2 Model Support and Assumptions

DRIFTFAIL is supported by process-level analyses that have evaluated (i) the potential for degradation of emplacement drifts after closure, (ii) termination mechanisms for drift degradation, and (iii) the potential shapes of a degraded drift. Assumptions used in the model include a constant rate of rubble accumulation for drift degradation caused by the stress effects of excavation and thermal loading and a linear relationship between ground motion magnitude and rubble accumulations caused by the ground motion. For a given seismic event, the relationship is defined using the threshold ground motion needed to initiate degradation, the magnitude of ground motion needed to cause a drift to collapse and fill with rubble, the volume of rubble needed to fill a drift, and the volume of accumulated rubble prior to the seismic event.

6.2.1 Potential for Drift Degradation

The understanding that emplacement drifts can fill with rubble during the period of regulatory concern after closure of a potential Yucca Mountain repository is consistent with (i) DOE information that indicates drift degradation may result from low probability seismic events (Bechtel SAIC Company, LLC, 2004a) and (ii) independent analyses that indicate potential repository thermal loading alone can cause degradation of emplacement drifts and accumulations of rubble (Ofoegbu, et al., 2007, 2006).

6.2.2 Termination Mechanisms for Drift Degradation

DRIFTFAIL is based on drifts being filled with rubble before mechanical conditions at the drift wall can change enough to terminate degradation. This understanding is consistent with results of thermal-mechanical analyses that indicate overstress of drift-wall rock for several hundred years (Ofoegbu, et al., 2007, 2006). Persistent overstress of drift-wall rock in the thermal-mechanical models indicates a potential for progressive spallation of the drift wall until the drift fills with rubble (Ofoegbu, et al., 2006).

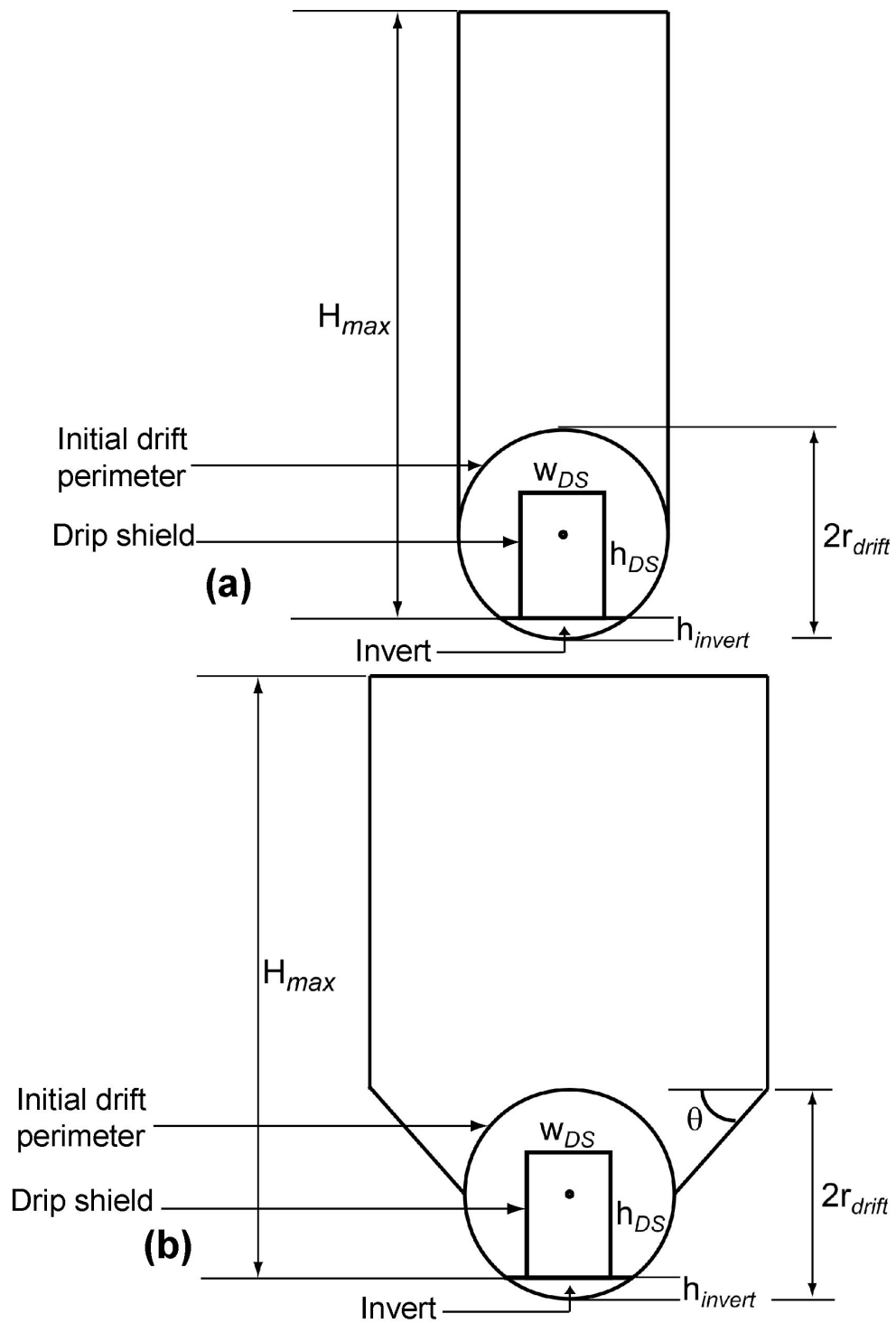


Figure 6-1. Degraded Drift Configurations: (a) Chimney Shape and (b) Trapezoidal Shape

6.2.3 Shape of Degraded Drift

The degraded-drift shapes in DRIFTFAIL were inferred from results of thermal-mechanical analyses (Ofoegbu, et al., 2006) that indicate progressive spallation of drift walls initiating in a zone around the drift perimeter and a few tens of centimeters deep. The analyses indicate spallation initiating at the drift sidewall in low-grade lithophysal rock or the drift roof in high-grade lithophysal rock. Ofoegbu, et al. (2006) estimated that progressive spallation of drift sidewalls can increase roof instability, resulting in a drift degrading laterally first and vertically thereafter, which is represented using a trapezoidal configuration. Progressive spallation of the drift roof, in contrast, is estimated to result in a drift degrading vertically, which is represented using the chimney configuration. The chimney and trapezoidal configurations are assumed to represent the range of potential degraded drift shapes.

6.3 Implementation of Conceptual Model in TPA Version 5.1

Rubble accumulation can result from thermally or seismically induced drift degradation. Two control flags trigger or suppress calculations for seismic or thermal degradation: (i) SeismicDisruptiveScenarioFlag(yes=1,no=0), which identifies whether rubble accumulation from seismically induced degradation occurs, and (ii) DriftDegradationScenarioFlag(yes=1,no=0), which identifies whether rubble accumulation from thermally induced degradation will occur. The calculation is performed for each of the two rock types: lithophysal rock (type one) and nonlithophysal rock (type two).

6.3.1 Rubble Accumulation

The volume of rubble that fills a drift and the height of the rubble above the drip shield are determined by the bulking factor and the degraded drift shape. The bulking factor is initially provided as *tpa.inp* input parameters BulkingFactorRockTypeOneSubarea_#[] and BulkingFactorRockTypeTwoSubarea_#[].⁴ The parameters are described in Table 6-1 (Section 6.4).

The degraded drift shape is either chimney, as shown in Figure 6-1(a), or trapezoidal, as shown in Figure 6-1(b). The selection of the degraded drift shape is controlled by two parameters in *tpa.inp*, FractionDriftDegradationOccursByChimney and DriftDegradationGeometrySelectionValue. The selection is performed by comparing FractionDriftDegradationOccursByChimney and DriftDegradationGeometrySelectionValue. Values of DriftDegradationGeometrySelectionValue smaller than or equal to FractionDriftDegradationOccursByChimney result in a chimney shape. Other values result in a trapezoidal shape. The probability of selection of the chimney shape is equal to the value of FractionDriftDegradationOccursByChimney.

⁴Where the term “_#” appears in a formal *tpa.inp* parameter name in this chapter, it refers to a particular potential repository subarea.

6.3.1.1 Chimney-Shaped Degradation Zone

Geometric analysis of a chimney-shaped degraded drift [Figure 6-1(a)] using Eq. (6-2) results in the following equation for the maximum height of rubble above the drift invert (i.e., when the drift is filled with rubble)⁵

$$H_{max} = \frac{\pi r_{drift}}{2(BF - 1)} - \frac{(w_{DS} h_{DS} + A_{invert})}{2(BF - 1)r_{drift}} - \left(1 - \frac{\pi}{4}\right)r_{drift} + 2r_{drift} - h_{invert} \quad (6-3)$$

where

- H_{max} — maximum height of rubble above the invert [m]
- r_{drift} — drift radius [m], which is half of the drift diameter as specified in *tpa.inp* as EmplacementDriftDiameter[m]
- w_{DS} — drip shield width [m], which is specified in *tpa.inp* as DripShieldEqvWidth[m]
- h_{DS} — drip shield height [m], which is specified in *tpa.inp* as DripShieldEqvHeight[m]
- BF — bulking factor, which is initially specified in *tpa.inp* as BulkingFactorRockTypeOneSubarea_#[] and BulkingFactorRockTypeTwoSubarea_#[]
- h_{invert} — height of the invert [m], which is specified in *tpa.inp* as InvertHeight[m]
- π — the transcendental number π , which is the mathematical constant that begins 3.1415926...
- A_{invert} — area filled by the invert [m²]

The area filled by the invert is determined using the following relationship

$$A_{invert} = r_{drift}^2 \arccos\left(\frac{r_{drift} - h_{invert}}{r_{drift}}\right) - (r_{drift} - h_{invert})\sqrt{(2r_{drift}h_{invert} - h_{invert}^2)} \quad (6-4)$$

where

- A_{invert} — area filled by the invert [m²]
- r_{drift} — drift radius [m], which is half of the drift diameter as specified in *tpa.inp* as EmplacementDriftDiameter[m]
- h_{invert} — height of the invert [m], which is specified in *tpa.inp* as InvertHeight[m]

6.3.1.2 Trapezoidal-Shaped Degradation Zone

Geometric analysis of a trapezoidal degraded drift [Figure 6-1(b)] using Eq. (6-2) results in the following equation for the maximum height of rubble above the drift invert (i.e., when the drift is filled with rubble)

⁵Implementation equations reported in Section 6.3 were derived from CNWRA Scientific Notebook 760E.

$$H_{max} = \frac{1}{2r_{drift}} \left[\frac{\left(\frac{\pi^2 r_{drift}^2 - w_{DS} h_{DS} - A_{invert}}{BF - 1} \right) - r_{drift}^2 \left(\cot(\theta) + 2 \left(1 - \frac{\pi}{4} \right) \right)}{1 + \cot(\theta)} \right] + 2r_{drift} - h_{invert} \quad (6-5)$$

where

- H_{max} — maximum height of rubble above the invert [m]
- r_{drift} — drift radius [m], which is half of the drift diameter as specified in *tpa.inp* as EmplacementDriftDiameter[m]
- w_{DS} — drip shield width [m], which is specified in *tpa.inp* as DripShieldEqvWidth[m]
- h_{DS} — drip shield height [m], which is specified in *tpa.inp* as DripShieldEqvHeight[m]
- BF — bulking factor, which is initially specified in *tpa.inp* as BulkingFactorRockTypeOneSubarea_#[] and BulkingFactorRockTypeTwoSubarea_#[]
- h_{invert} — height of the invert [m], which is specified in *tpa.inp* as InvertHeight[m]
- θ — base angle of the trapezoid [degrees] [see Figure 6-1(b)], which is specified in *tpa.inp* as TrapezoidBaseAngle
- π — the transcendental number π , which is the mathematical constant that begins 3.1415926...
- A_{invert} — area filled by invert [m²] [see Eq. (6-4)]

6.3.2 Rubble Accumulation From Thermally Induced Drift Degradation

Rubble accumulation resulting from thermally induced drift degradation is evaluated when the *tpa.inp* parameter DriftDegradationScenarioFlag(yes=1,no=0) is set to one. Rubble from thermally induced drift degradation accumulates at a constant rate starting at the time of potential repository closure and ending at a time established by the *tpa.inp* parameters DegradationTimeRockTypeOneSubarea_#[yr] and DegradationTimeRockTypeTwoSubarea_#[yr]. Thus for thermally induced drift degradation, the time of drift fill up (time at which the drift is filled with rubble) is the sum of the degradation time and the potential repository closure time.

The maximum height of rubble above the invert (H_{max}) is used to calculate the height of rubble above the drip shield, H_{rubble} , at a given time. First, the cross-sectional area of the potential maximum rubble accumulation, A_{max} , is determined using the maximum rubble height H_{max} .

Then the rate of change of rubble cross-sectional area (i.e., rate of rubble accumulation) is calculated thereafter using A_{max} and the drift degradation time {*tpa.inp* parameters DegradationTimeRockTypeOneSubarea_#[yr] and DegradationTimeRockTypeTwoSubarea_#[yr]} with the following equation

$$\frac{dA}{dt} = \frac{A_{max}}{t_d} \quad (6-6)$$

where

- dA/dt — rate of rubble accumulation [m^2/yr]
- t_d — degradation time of rock type in drift (after potential repository closure) [yr]
which is initially specified in *tpa.inp* as
DegradationTimeRockTypeOneSubarea_#[] and
DegradationTimeRockTypeTwoSubarea_#[]
- A_{max} — rubble cross-sectional area at drift fill up [m^2]

The rubble cross-sectional area at a given time is then calculated incrementally as

$$A_{rubble}(t_{j+1}) = A_{rubble}(t_j) + \frac{dA}{dt} \Delta t_j \quad (6-7)$$

where

- $A_{rubble}(t_j)$ — cross-sectional area of rubble accumulated with respect to time, with a limiting maximum value of less than or equal to A_{max} [m^2]
- Δt_j — length of time increment [yr]
- dA/dt — rate of rubble accumulation [m^2/yr]
- j — the index of the timestep

The height of rubble accumulation above the drip shield, H_{rubble} , is then evaluated using an area-filling geometric analysis of the degraded drift in conjunction with the accumulated rubble cross-sectional area [$A_{rubble}(t)$]. In a similar manner and in concurrence with these calculations, the time-dependent height of the drift ceiling is also evaluated.

6.3.3 Rubble Accumulation From Seismically Induced Drift Degradation

Rubble accumulation resulting from seismically induced drift degradation is evaluated when the *tpa.inp* parameter SeismicDisruptiveScenarioFlag(yes=1,no=0) is set to one. When the *tpa.inp* parameter DriftDegradationScenarioFlag(yes=1,no=0) also is set to one, then rubble accumulation from thermally induced drift degradation also is evaluated, with the two contributions to rubble accumulation being additive.

When the SeismicDisruptiveScenarioFlag(yes=1,no=0) is set to one, calculations are performed to evaluate (i) the change in bulking factor resulting from rubble compaction and (ii) the rubble accumulation resulting from seismically induced drift degradation. The compaction effect is calculated using a rubble compaction factor defined as the fractional reduction in the bulking factor as a result of seismic compaction. The effect of the compaction factor on bulking is defined as (Ibarra, et al., 2007)

$$BF_i = (BF_{i-1} - 1)(1 - CF_i) + 1 \quad (6-8)$$

where

- i — index of the seismic event
- BF_i — bulking factor at end of seismic event i [dimensionless]
- CF_i — compaction factor of the seismic event, which is specified in *tpa.inp* by Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax [dimensionless]

BF_0 is the initial bulking factor as specified in *tpa.inp* as BulkingFactorRockTypeOneSubarea_#[] and BulkingFactorRockTypeTwoSubarea_#[]. A change in the bulking factor results in a recalculation of H_{max} and H_{rubble} . A minimum value for the bulking factor is defined in *tpa.inp* as the SeismicMinimumBulkingFactor. After each seismic event, the new bulking factor (BF_i) is compared to the SeismicMinimumBulkingFactor to ensure that the bulking factor is greater than or equal to the SeismicMinimumBulkingFactor. When the initial bulking factor is less than the SeismicMinimumBulkingFactor, the bulking factor is unaffected by seismic compaction calculations.

For seismic events occurring before the emplacement drifts are filled with rubble, damage to the drift from a seismic event is proportional to the magnitude of the seismic event and the amount of previously accumulated rubble. Rubble accumulation from such a seismic event is given as (Gute, et al., 2003)

$$\Delta A_{seismic\_event} = \frac{(A_{max} - A_{rubble})}{(g_{max} - g_{init})} (PGA_{seismic\_event} - g_{init}) \quad (6-9)$$

where

- $\Delta A_{seismic\_event}$ — incremental increase in rubble cross-sectional area from the seismic event [m²]
- A_{max} — potential maximum rubble cross-sectional area [m²]
- A_{rubble} — cross-sectional area of accumulated rubble prior to seismic event [m²]
- g_{max} — seismic ground acceleration that would cause drift to completely degrade and fill with rubble, which is specified in *tpa.inp* as GroundAccelerationMaximumRockTypeOneSubarea_#[pga] and GroundAccelerationMaximumRockTypeTwoSubarea_#[pga]. The parameter is expressed in multiples of g (i.e., 9.81 m/s²).
- g_{init} — minimum seismic ground acceleration that would initiate seismically driven drift degradation, which is specified in *tpa.inp* as GroundAccelerationInitialRockTypeOneSubarea_#[pga] and GroundAccelerationInitialRockTypeTwoSubarea_#[pga]. The parameter is expressed in multiples of g (i.e., 9.81 m/s²).

$PGA_{seismic\_event}$ — seismic ground acceleration along the vertical direction of the seismic event (g), which is specified in *tpa.inp* by Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax.

The change in the rubble cross-sectional area from a seismic event is applied at the time of the seismic event to the existing rubble accumulation. For seismic events that occur after the drift has filled with rubble (based on the bulking factor of the rock prior to any seismic rubble compaction), the drift height, rubble height, and vertical pressures are immediately set to their new maximum values based on the new bulking factor.

6.3.4 Seismic Degradation With No Thermal Degradation

Drift degradation can be evaluated for seismic degradation without the occurrence of thermal drift degradation by setting the *tpa.inp* parameter DriftDegradationScenarioFlag(yes=1,no=0) to zero while setting the parameter SeismicDisruptiveScenarioFlag(yes=1,no=0) to one. Using these settings, rubble accumulation from thermal degradation of the drift is not calculated, so rubble accumulates only when seismic events occur. The amount of rubble that results from each seismic event is evaluated using Eq. (6-7), and the rubble cross-sectional area (A_{rubble}) is the cumulative sum of contributions from individual seismic events. The height of rubble is evaluated as described in Sections 6.3.2 and 6.3.3 at the time of seismic events in addition to TPA Version 5.1 time increments.

In the seismic degradation calculation, a minimum bulking factor, below which the bulking factor cannot be reduced, is evaluated. This value is defined in *tpa.inp* as the SeismicMinimumBulkingFactor. After each evaluation of a seismic event, the new bulking factor is compared to the SeismicMinimumBulkingFactor to ensure that the bulking factor is greater than or equal to the SeismicMinimumBulkingFactor.

6.3.5 Static Vertical Pressures on Drip Shield Crown

The static vertical pressure on the drip shield crown resulting from the accumulated rubble (P_{vert}) is determined using the following equation

$$P_{vert} = \frac{H_{rubble} g \rho_{rock}}{BF} \quad (6-10)$$

where

- H_{rubble} — the current height of accumulated rubble above the drip shield [m]
- ρ_{rock} — bulk density of the host rock, which is specified in *tpa.inp* as RockMassDensityForRockTypeOne[kg/m³] and RockMassDensityForRockTypeTwo[kg/m³]
- g — gravitational acceleration [9.81 m/s²]
- BF — bulking factor of the rock [unitless]; either the values initially specified in *tpa.inp* as BulkingFactorRockTypeOneSubarea_#[] and BulkingFactorRockTypeTwoSubarea_#[] or values which have been altered through seismic compaction [Eq. (6-3)]

The static vertical pressure (kPa) is reported by DRIFTFAIL for each timestep and at the moment of each seismic event. The pressure reported for a seismic event does not include any effects of the event (i.e., the pressure reported for event i does not include the rubble compaction effect or accelerated drift degradation effect of event i).

6.4 Input Parameters in *tpa.inp*

Table 6-1 lists the parameters specified in *tpa.inp* that are used by DRIFTFAIL.

6.5 Auxiliary Input Data and External Process Models

DRIFTFAIL requires no auxiliary input data or external process models.

6.6 Intermediate Outputs and Information Passed to Other Modules

Table 6-2 describes the intermediate output files that are created during the execution of DRIFTFAIL. Table 6-3 describes the optional output files that are created when selected by the user. This functionality can be implemented in the *tpa.inp* input block titled <<Output Print Options>> by setting the output mode parameter, `OutputMode(0=None,1=All,2=UserDefined)`, to a value of one or two. When set to one, the optional output files are saved for all realizations; when set to two, these files are saved for realizations starting with the one specified by `UserDefinedLowerRealizationAppend` and ending with the realization specified by `UserDefinedUpperRealizationAppend`.

To obtain intermediate outputs from DRIFTFAIL, the `SelectAppendFiles` parameter in the <<Output Print Options>> input block should be set to a value of four. When the `SelectAppendFiles` parameter is set to a value of zero, then setting the output mode parameter, `OutputMode(0=None,1=All,2=UserDefined)`, to a value of one or two causes intermediate output files to be written for numerous modules including DRIFTFAIL. Some files can be very large and can quickly fill up available storage if all intermediate outputs are specified for all realizations.

6.7 Techniques for Understanding Module Performance

Although there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of the drift degradation processes modeled by DRIFTFAIL. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques (e.g., Mohanty, et al., 2004) may be useful to understand their effects on system-level performance.

In addition, “pinch-point” techniques, where output or intermediate results produced by DRIFTFAIL can be understood in combination with output or intermediate results from other modules (e.g., MECHFAIL), may help evaluate subsystem processes. Key files useful for these comparisons include *driftfail.inp* and *driftfail.dat*, which contain the inputs and results for individual drift degradation calculations. An examination of these files allows the user to

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	DripShieldEqvHeight[m]	h_{DS} Height of an equivalent rectangle representing the drip shield [m]	constant 2.508	Derived from DOE drip shield design as described in CNWRA Scientific Notebook 410, page 73.
DRIFTFAIL	DripShieldEqvWidth[m]	w_{DS} Width of an equivalent rectangle representing the drip shield [m]	constant 2.082	Derived from DOE drip shield design as described in CNWRA Scientific Notebook 410, page 73.
DRIFTFAIL	InvertHeight[m]	h_{invert} The height of the invert [m]	constant 0.806	Engineering specification taken from DOE information (CRWMS M&O, 2000).
DRIFTFAIL	RockMassDensityForRockTypeOne[kg/m ³]	ρ_{rock} Parameter approximating the average rock mass density for the lower lithophysal rock unit [kg/m ³]	constant 2139	Represents moist density of lithophysal rock for average saturation, as described in CNWRA Scientific Notebook 612-8E.

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	RockMassDensityForRockTypeTwo[kg/m ³]	ρ_{rock} Parameter approximating the average rock mass density for the middle nonlithophysal rock unit [kg/m ³]	constant 2322	Represents moist density of nonlithophysal rock for average saturation, as described in CNWRA Scientific Notebook 612-8E.
DRIFTFAIL	FractionRockTypeOneInSubarea_1[] FractionRockTypeOneInSubarea_2[] FractionRockTypeOneInSubarea_3[] FractionRockTypeOneInSubarea_4[] FractionRockTypeOneInSubarea_5[] FractionRockTypeOneInSubarea_6[] FractionRockTypeOneInSubarea_7[] FractionRockTypeOneInSubarea_8[] FractionRockTypeOneInSubarea_9[] FractionRockTypeOneInSubarea_10[]	Fraction of lithophysal rock in the potential repository footprint [unitless]	constant 0.85	Based on DOE information (Bechtel SAIC Company, LLC, 2004b). Note that the fraction of lithophysal rock could vary between subareas, data do not currently exist that would establish which subareas contain lithophysal rock and which do not. Therefore, all subareas are modeled as being 85 percent lithophysal rock.

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	BulkingFactorRockType OneSubarea_1[] BulkingFactorRockType OneSubarea_2[] BulkingFactorRockType OneSubarea_3[] BulkingFactorRockType OneSubarea_4[] BulkingFactorRockType OneSubarea_5[] BulkingFactorRockType OneSubarea_6[] BulkingFactorRockType OneSubarea_7[] BulkingFactorRockType OneSubarea_8[] BulkingFactorRockType OneSubarea_9[] BulkingFactorRockType OneSubarea_10[]	<i>BF</i> Estimated bulking factor for lower lithophysical rock unit [unitless]	beta 1.01, 2.0, 23.17, 92.70	Based on information calculated by DOE (Bechtel SAIC Company, LLC, 2004a). The bulking factor distribution has a mean of 1.2 and a standard deviation of 0.037. This shifted beta distribution includes 83 percent of its probability density area between bulking factor values of 1.15 and 1.25. Probability density areas for different bulking factor intervals of interest are as follows (Ibarra, et al., 2007): P(BF < 1.1) – 0.08 percent P(BF < 1.15) – 8.0 percent P(BF < 1.25) – 90.6 percent P(1.15 < BF < 1.25) – 82.5 percent P(BF < 1.35) – 100.0 percent It is normally thought that the bulking factor distributions are in the range from 1 to 2 and that the boundary point would not be selected under normal sampling techniques. However, a value of 1 for the lower limit causes a numerical instability in TPA Version 5.1 when <i>tpamin.out</i> is used as an input file. To avoid this condition, a lower limit of 1.01 is specified because this is a small change and does not significantly change the distribution of parameter values.

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	BulkingFactorRockType TwoSubarea_1[] BulkingFactorRockType TwoSubarea_2[] BulkingFactorRockType TwoSubarea_3[] BulkingFactorRockType TwoSubarea_4[] BulkingFactorRockType TwoSubarea_5[] BulkingFactorRockType TwoSubarea_6[] BulkingFactorRockType TwoSubarea_7[] BulkingFactorRockType TwoSubarea_8[] BulkingFactorRockType TwoSubarea_9[] BulkingFactorRockType TwoSubarea_10[]	<i>BF</i> Estimated bulking factor for middle nonlithophysal rock unit [unitless].	beta 1.01, 2.0, 23.17, 92.70	Based on information calculated by DOE for lithophysal rock (Bechtel SAIC Company, LLC, 2004a). The use of lithophysal rock bulking data has been used for the nonlithophysal rock because there is currently insufficient data to differentiate the bulking properties of the two rock types. The bulking factor distribution has a mean of 1.2 and a standard deviation of 0.037. This shifted beta distribution includes 83 percent of its probability density area between bulking factor values of 1.15 and 1.25. Probability density areas for different bulking factor intervals of interest are as follows (Ibarra, et al., 2007): P(BF < 1.1) – 0.08 percent P(BF < 1.15) – 8.0 percent P(BF < 1.25) – 90.6 percent P(1.15 < BF < 1.25) – 82.5 percent P(BF < 1.35) – 100.0 percent It is normally thought that the bulking factor distributions are in the range from 1 to 2 and that the boundary point would not be selected under normal sampling techniques. However, a value of 1 for the lower limit causes a numerical instability in TPA Version 5.1 when <i>tpamin.out</i> is used as an input file. To avoid this condition, a lower limit of 1.01 is specified because this is a small change and does not significantly change the distribution of parameter values.

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	DegradationTimeRocktypeOneSubarea_1[yr]	Time for a complete drift degradation for lower lithophysical rock unit [yr]	lognormal 369.32, 1523.05	Based on analysis described in Ofoegbu, et al. (2007). The lognormal distribution has a median value of 750 years and a logarithmic standard deviation (i.e., standard deviation of the natural logarithm of the data) of 0.23, resulting in the following probability density areas for different values of drift degradation time (Ibarra, et al., 2007): P(t < 400 years) – 0.3 percent P(t < 500 years) – 3.9 percent P(t < 1,000 years) – 89.5 percent P(t < 1,280 years) – 99.0 percent
	DegradationTimeRocktypeOneSubarea_2[yr]			
	DegradationTimeRocktypeOneSubarea_3[yr]			
	DegradationTimeRocktypeOneSubarea_4[yr]			
	DegradationTimeRocktypeOneSubarea_5[yr]			
	DegradationTimeRocktypeOneSubarea_6[yr]			
	DegradationTimeRocktypeOneSubarea_7[yr]			
	DegradationTimeRocktypeOneSubarea_8[yr]			
	DegradationTimeRocktypeOneSubarea_9[yr]			
	DegradationTimeRocktypeOneSubarea_10[yr]			

Table 6-1. Reference Data for Parameters of tpa.inp Used by DRIFTFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	Degradation TimeRocktype Two Subarea_1[yr]	Time for a complete drift degradation for middle nonlithophysal rock unit [yr]	lognormal 369.32, 1523.05	Based on analysis described in Ofoegbu, et al. (2007). The use of lithophysal rock degradation time data has been used for the nonlithophysal rock because there is currently insufficient data to differentiate the properties of the two rock types. The lognormal distribution has a median value of 750 years and a logarithmic standard deviation (i.e., standard deviation of the natural logarithm of the data) of 0.23, resulting in the following probability density areas for different values of drift degradation time (Ibarra, et al., 2007): P(t < 400 years) – 0.3 percent P(t < 500 years) – 3.9 percent P(t < 1,000 years) – 89.5 percent P(t < 1,280 years) – 99.0 percent
	Degradation TimeRocktype Two Subarea_2[yr]			
	Degradation TimeRocktype Two Subarea_3[yr]			
	Degradation TimeRocktype Two Subarea_4[yr]			
	Degradation TimeRocktype Two Subarea_5[yr]			
	Degradation TimeRocktype Two Subarea_6[yr]			
	Degradation TimeRocktype Two Subarea_7[yr]			
	Degradation TimeRocktype Two Subarea_8[yr]			
	Degradation TimeRocktype Two Subarea_9[yr]			
	Degradation TimeRocktype Two Subarea_10[yr]			

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	GroundAccelerationInitialRock	g_{init} Smallest acceleration that will cause rockfall in a drift for lower lithophysical rock unit [g] ($1g = 9.81 \text{ m/s}^2$)	beta 0.5, 0.6, 2.21, 5.85	Based on empirical data cited in Gute, et al. (2003); see also CNWRA Scientific Notebook 410, p. 25. The beta distribution has a mean of 0.527 g and standard deviation of 0.015, resulting in the following probability density areas: $P(g_{init} < 0.502 \text{ g}) - 0.3 \text{ percent}$ $P(g_{init} < 0.506 \text{ g}) - 3.9 \text{ percent}$ $P(g_{init} < 0.548 \text{ g}) - 89.5 \text{ percent}$ $P(g_{init} < 0.567 \text{ g}) - 99.0 \text{ percent}$
	TypeOneSubarea_1[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_2[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_3[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_4[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_5[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_6[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_7[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_8[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_9[pga]			
	GroundAccelerationInitialRock			
	TypeOneSubarea_10[pga]			

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	GroundAccelerationInitialRock	g_{init} Smallest acceleration that will cause rockfall in a drift for middle nonlithophysal rock unit $[g \text{ (} 1g = 9.81 \text{ m/s}^2\text{)}]$	beta 0.5, 0.6, 2.21, 5.85	Based on empirical data cited in Gute, et al. (2003); see also CNWRA Scientific Notebook 410, p. 25. The use of lithophysal rock initial ground acceleration data has been used for the nonlithophysal rock because there is currently insufficient data to differentiate the properties of the two rock types. The beta distribution has a mean of 0.527 g and standard deviation of 0.015, resulting in the following probability density areas: $P(g_{init} < 0.502 \text{ g}) - 0.3 \text{ percent}$ $P(g_{init} < 0.506 \text{ g}) - 3.9 \text{ percent}$ $P(g_{init} < 0.548 \text{ g}) - 89.5 \text{ percent}$ $P(g_{init} < 0.567 \text{ g}) - 99.0 \text{ percent}$
	TypeTwoSubarea_1[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_2[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_3[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_4[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_5[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_6[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_7[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_8[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_9[pga]			
	GroundAccelerationInitialRock			
	TypeTwoSubarea_10[pga]			

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	GroundAccelerationMaximum	g_{max} Acceleration value that will cause drift to collapse and fill up with rubble for lower lithophysical rock unit [g] ($1g = 9.81 \text{ m/s}^2$)	beta 1.0, 2.0, 2.79, 17.15	Based on empirical data cited in Gute, et al. (2003); see also CNWRA Scientific Notebook 410, p. 25. The beta distribution has a mean of 1.14 g and standard deviation of 0.076, resulting in the following probability density areas: $P(g_{max} < 1.013 \text{ g}) - 0.3 \text{ percent}$ $P(g_{max} < 1.035 \text{ g}) - 3.9 \text{ percent}$ $P(g_{max} < 1.238 \text{ g}) - 89.5 \text{ percent}$ $P(g_{max} < 1.361 \text{ g}) - 99.0 \text{ percent}$
	RockTypeOneSubarea_1[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_2[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_3[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_4[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_5[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_6[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_7[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_8[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_9[pga]			
	GroundAccelerationMaximum			
	RockTypeOneSubarea_10[pga]			

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	GroundAccelerationMaximum RockTypeTwoSubarea_1[pga] GroundAccelerationMaximum RockTypeTwoSubarea_2[pga] GroundAccelerationMaximum RockTypeTwoSubarea_3[pga] GroundAccelerationMaximum RockTypeTwoSubarea_4[pga] GroundAccelerationMaximum RockTypeTwoSubarea_5[pga] GroundAccelerationMaximum RockTypeTwoSubarea_6[pga] GroundAccelerationMaximum RockTypeTwoSubarea_7[pga] GroundAccelerationMaximum RockTypeTwoSubarea_8[pga] GroundAccelerationMaximum RockTypeTwoSubarea_9[pga] GroundAccelerationMaximum RockTypeTwoSubarea_10[pga]	g_{max} Acceleration value that will cause drift to collapse and fill up with rubble for middle nonlithophysal rock unit [g ($1g = 9.81 \text{ m/s}^2$)]	beta 1.0, 2.0, 2.79, 17.15	Based on empirical data cited in Gute, et al. (2003); see also CNWRA Scientific Notebook 410, p. 25. The use of lithophysal rock maximum ground acceleration data has been used for the nonlithophysal rock because there is currently insufficient data to differentiate the properties of the two rock types. The beta distribution has a mean of 1.14 g and standard deviation of 0.076, resulting in the following probability density areas: $P(g_{max} < 1.013 \text{ g}) - 0.3 \text{ percent}$ $P(g_{max} < 1.035 \text{ g}) - 3.9 \text{ percent}$ $P(g_{max} < 1.238 \text{ g}) - 89.5 \text{ percent}$ $P(g_{max} < 1.361 \text{ g}) - 99.0 \text{ percent}$
DRIFTFAIL	TrapezoidBaseAngle	Angle used in the definition of trapezoidal degraded shape [degree]	constant 50.7	Based on geometrical calculation described in CNWRA Scientific Notebook 760E.
DRIFTFAIL	FractionDriftDegradationOccurs ByChimney	Fraction of drifts assigned a chimney-shaped degraded configuration [unitless]	constant 0.75	Based on information described in Ibarra, et al. (2007).
DRIFTFAIL	SeismicMinimumBulkingFactor	Threshold for decreasing the bulking factor parameter due to compaction [unitless]	constant 1.15	Based on information calculated by DOE for lithophysal rock (Bechtel SAIC Company, LLC, 2004a) and an analysis described by Ibarra, et al. (2007).

Table 6-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DRIFTFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DRIFTFAIL	DriftDegradationGeometry SelectionValue	Random value used for comparison to <i>tpa.inp</i> parameter FractionDrift DegradationOccurs ByChimney to select drift geometry	uniform 0.0, 1.0	
Disruptive Scenario Flags	SeismicDisruptiveScenario Flag(yes=1,no=0)	Seismic disruptive scenario	iflag 0	Activates the seismic scenario.
Disruptive Scenario Flags	DriftDegradationScenario Flag(yes=1,no=0)	Drift degradation scenario	iflag 1	Activates the drift degradation scenario.
MECHFAIL	Seismic_MAPE_PGV_PGAm_ PGAsd_CFmin_CFmax [1/yr,m/s,m/s ² ,_,_,_]	$PGA_{seismic\_event}$ Array of seismic parameters associated with discrete points of the selected hazard curve [1/hr, m/s, s ² , unitless, unitless, unitless]	hazardcurve 5 1.0e-4 0.47 0.38 0.64 0.10 0.20 1.0e-5 1.05 1.85 0.64 0.20 0.40 1.0e-6 2.44 4.13 0.53 0.30 0.60 1.0e-7 5.35 11.04 0.53 0.40 0.60 1.0e-8 5.35 11.04 0.53 0.40 0.60	The natural number of the first row is a table link controlling the number of entries in the array. The first value of each subsequent row is the mean annual frequency of exceedance. The rest of the values are associated with the corresponding mean annual frequency of exceedance and refer to the mean peak ground velocity in the horizontal direction, median peak ground acceleration in the vertical direction, standard deviation of the natural logarithm of the peak ground acceleration, lower boundary for compaction factor, and upper boundary for compaction factor. Values are consistent with Ibarra, et al. (2007b).

Table 6-2. Intermediate Output Files Created During Execution of DRIFTFAIL	
Output File	Description
<i>dsfail.res</i>	Number of drip shields failed by corrosion and mechanical failure including time of failure for each realization.
<i>driftfail.inp</i>	This is a copy of the input file for DRIFTFAIL. It defines the drift geometries, engineered barrier geometries, and rock properties. This file is overwritten each time a subarea calculation is performed. At the end of a simulation, the file contains the input information for the drift degradation calculation for the last subarea evaluated.
<i>driftfail.dat</i>	This is a copy of the output file produced by DRIFTFAIL during the drift degradation calculations. This file contains the time-dependent values for vertical pressures exerted by the degraded drift and geometries of the degraded drift. At the end of a simulation, the file contains the output for the drift degradation calculation for the last subarea evaluated.
<i>driftfail.dbg</i>	This is a copy of screen output produced by DRIFTFAIL during the drift degradation calculations when the debug flag set in <i>driftfail.inp</i> has been set to 1. This file contains a list of the timesteps, and the seismic event properties: time of events, peak ground acceleration and rubble compaction factor. The file is overwritten each time a subarea calculation is performed.

Table 6-3. Optional Intermediate Output Files Created During Execution of DRIFTFAIL	
Output File	Description
<i>driftfail.ech</i>	This file contains the characteristic values of seismic events used to evaluate drift degradation. Seismic events are evaluated on a potential repository scale. At the end of a simulation, this file contains the seismic histories for all realizations performed during the simulation.
<i>driftfail.rlt</i>	This file contains the outputs generated by DRIFTFAIL for all subareas in each realization evaluated during the stimulation. The output includes times at which drifts fill with rubble, vertical pressures at the time of seismic events, and the drift geometries and vertical pressures resulting from drift degradation.

compare starting conditions (rock properties, seismic events, etc.) with end results (rubble heights, pressures, etc.). However, these files show only the results for the last subarea calculation. For more detailed evaluation of drift degradation for each subarea, the user may examine the optional output file *driftfail.ech*, which contains the characteristic properties of seismic events evaluated during drift degradation, and *driftfail.rlt*, which contains the times at which drifts fill with rubble (based on the initial bulking factor), drift geometries and vertical

pressures resulting from drift degradation for TPA Version 5.1 simulation timesteps for each subarea evaluated in each realization.

The effects of individual parameters with respect to particular subsystem processes can be examined by repetitively varying an input parameter and analyzing results from relevant output and intermediate-output files. A single-parameter importance analysis may be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distributions specified for all parameters. Alternatively, single parameter importance analyses may be performed by repetitively specifying smaller ranges within the parameter's original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges; the user should exercise care in interpreting results from simulations in which input data are altered beyond their intended ranges.

Key input parameters that may significantly influence DRIFTFAIL results include the parameters BulkingFactorRockTypeOneSubarea_#[] and BulkingFactorRockTypeTwoSubarea_#[], which provide the bulking factors for the two types of rocks evaluated in drift degradation analyses, and SeismicMinimumBulkingFactor, which controls the minimum bulking factor of the rock considering seismically induced compaction of rubble.

Several DRIFTFAIL user options to examine the effect of various processes involve adjusting parameter values in *tpa.inp* to implement block-specific processes in the abstraction, including the following:

- To force the drift degradation geometry to be either chimney or trapezoidal, the *tpa.inp* parameter FractionDriftDegradationOccursByChimney can be set to 1.0 or 0.0, respectively.
- To examine the effect of drift degradation geometry on vertical pressures and rubble geometries, the degraded drift geometry can be forced to trapezoidal shape. The width of the rubble column above the drift can be varied by altering the *tpa.inp* parameter TrapezoidBaseAngle. By varying the angle (θ) from 90° to 45°, the width of the rubble column can be varied from the width of the drift diameter (basic chimney degradation) to twice the drift diameter [$\text{width} = 2r(1 + \cotan(\theta))$, where r is the drift radius].
- To understand the level of contribution of drift degradation to system performance, drift degradation can be disabled from the reference case by setting the SeismicDisruptiveScenarioFlag(yes=1,no=0) to zero and ensuring DriftDegradationScenarioFlag(yes=1,no=0) is set to zero. Under these conditions, rubble accumulation is not evaluated.
- To evaluate the individual behavior of the two rock types found within the potential repository footprint (i.e., lithophysal and nonlithophysal), the fraction of rock type as specified by *tpa.inp* as FractionRockTypeOneInSubarea_#[] can be changed to zero or one, resulting in nonlithophysal (zero) or lithophysal (one) rock assigned to the entire subarea.
- To more readily evaluate the impact of low probability seismic events on modeled drift degradation, the hazard curve Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_] can be

altered by changing the frequency of seismic events or the characteristics of these events.

Caution should be used when modifying *tpa.inp* parameter distributions. The underlying reasoning for parameter distributions should be well understood prior to these types of investigations.

6.8 References

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7 NEAR-FIELD ENVIRONMENT (NFENV)

The Near-Field Environment module (NFENV)¹ contains model abstractions for (i) heat transfer and temperature distribution on a mountain and drift scale, (ii) thermally perturbed percolation, and (iii) chemical composition of seepage water in the vicinity of the potential repository drift. The flow of information into, through, and out of these three distinct module components is presented in Figure 7-1. NFENV receives as input (i) the time-varying amount of rubble accumulation from the Drift Degradation module (DRIFTFAIL);² (ii) the time-varying deep percolation rate from the Climate and Infiltration module (UZFLOW);³ and (iii) the time of drip shield failure from the Drip Shield and Waste Package Mechanical Failure module (MECHFAIL).⁴ NFENV calculates the time-dependent temperature of the drip shield, flux of seepage water approaching the drift, and chemistry of the seepage water and passes them to DRIFTFAIL, the Engineered Barrier System Radionuclide Release module (EBSREL),⁵ and the Waste Package Corrosion Failure module (EBSFAIL),⁶ respectively. NFENV is executed for each subarea in every realization.

7.1 Conceptual Model

The movement of heat, fluids, and dissolved chemical species in the vicinity of the potential repository is conceptualized as a coupled process of heat transfer (convection, conduction, and radiation), fluid movement (evaporation, condensation, and reflux), and chemistry (dissolution, precipitation, and deliquescence). The heat from radioactive decay is expected to dry out the near-field and in-drift components (Figure 7-2) during the peak thermal pulse. The dryout zone formed above the drift may keep liquid water from entering the drift and contacting the waste package, except by transient pulses of water that flow through fractures that could penetrate the above-boiling temperature zone. In the abstracted model, the thermal, hydrological, and chemical processes are simplified by uncoupling. The heat transfer model is composed of a three-dimensional, mountain-scale, conduction-only analytic model for the host rock and a multimode heat transfer model for the in-drift thermal conditions. Relative humidity in the drift is derived from temperature estimates. The conduction model by itself cannot estimate near-field drying and rewetting in the host rock. The Abstracted Reflux model (REFLUX3),⁷ described in Section 7.1.2, represents fluid flow in the near-field environment, but uses the temperature history from the heat transfer abstraction. The seepage water chemistry is abstracted using temperature and relative humidity inputs from the heat transfer model to describe the chemistry based on equilibrium chemical processes. Jointly, these models provide temperature, relative

¹The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

²The Drift Degradation module is referenced frequently throughout this chapter. The abbreviation DRIFTFAIL will be used.

³The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

⁴The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAIL will be used.

⁵The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

⁶The Waste Package Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

⁷The Abstracted Reflux model is referenced frequently throughout this chapter. The abbreviation REFLUX3 will be used.

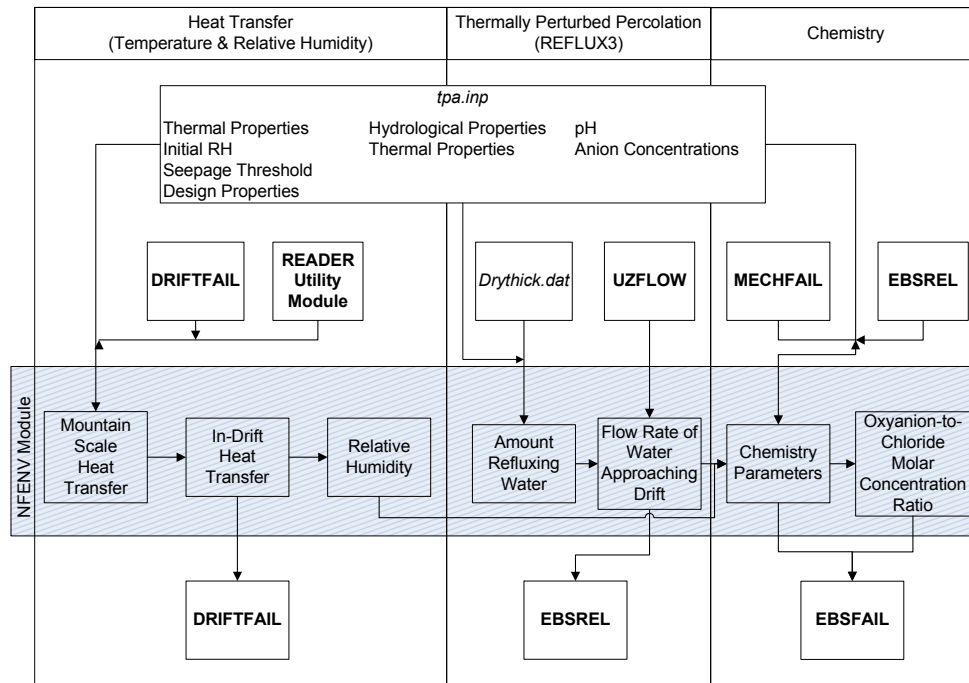


Figure 7-1. Information Flow Diagram for NFENV

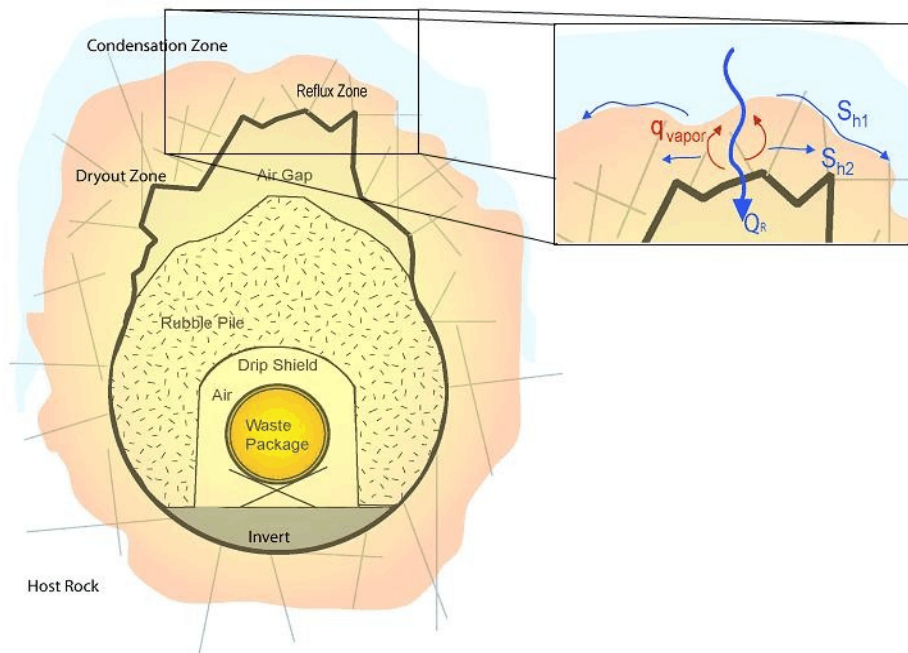


Figure 7-2. A Schematic Representation of the Thermal Hydrologic Processes in the Near-Field Environment. Insert Shows the Processes Related to REFLUX3 Abstraction (Section 7.3.2).

humidity, the amount and chemical composition of water moving toward and into a drift, and changes in liquid saturation and temperature at the drift wall as a function of time. The details of the three models are discussed separately in the following subsections.

7.1.1 Heat Transfer

The conceptual model description for heat transfer is divided into three portions: (i) heat transfer on a mountain scale that determines the temperature distribution of the drift wall; (ii) heat transfer on a drift scale that determines the temperature of the in-drift components (e.g., waste package and drip shield); and (iii) calculation of relative humidity from the derived in-drift temperatures. The mountain-scale heat transfer model calculates the temperature at the drift wall, which is then used to calculate the temperatures of the in-drift components.

The effect of drift degradation on heat transfer uses information generated by DRIFTFAIL. An alternate case conceptualizes an intact drift where the geometry of the drift remains constant for the nondegraded drift duration of the simulation. Specific approaches for these alternate conceptualizations are described in detail in the following sections.

7.1.1.1 Mountain-Scale Heat Transfer

The thermal perturbation at the mountain scale caused by emplaced waste is conceptualized as a transfer of heat (i.e., thermal energy in transit) resulting from a temperature difference between the waste package surface and the surrounding host rock. The dominant mode of heat transfer at the mountain scale is conduction in the host rock (a solid medium). The abstraction determines the temperature evolution at the drift wall using an analytical conduction-only model for mountain-scale heat transfer. The analytical model accounts for the time-dependent potential repository heat flux from the emplaced waste. It also accounts for the reduction in the heat load because of forced ventilation during the preclosure period. The drift wall temperature is calculated at the center of each subarea. For the degraded drift case, the analytical model accounts for the temporal variation of the location of the drift wall as determined by DRIFTFAIL.

7.1.1.2 In-Drift Heat Transfer

A multimode (i.e., conduction, convection, and radiation) heat-transfer model is used for modeling heat transfer inside the drift. The temperature gradient between the hot waste package and cool drift wall is the driver for the thermal energy transfer. The in-drift temperature distribution depends on (i) the geometry of in-drift components that include the waste package, drip shield, ground support systems, and invert; (ii) the temperature of the drift wall; (iii) the thermal energy released from the waste package; and (iv) the presence of rubble because of drift degradation.

A simplified thermal network using an electrical analog estimates the temperatures at different locations such as waste package, drip shield, and rubble. The theoretical basis of the thermal network analysis can be found in Holman (2001) and Incropera and Dewitt (2002). The temperature at various locations is calculated using a steady-state conduction heat transfer approach. The dominant heat transfer in the solid components is conduction, while radiative and convective heat transfer dominate in the air gaps (Kuehn and Goldstein, 1978, 1976). Convection varies with the configuration of the engineered barrier system and is driven by the three-dimensional temperature gradient in the air space. Thermal radiation is a function of the absolute temperatures and temperature differences across the air gap. Conduction through the air gaps is assumed negligible. The effects of convection and radiation are indirectly implemented using equivalent thermal conductances in the thermal network. The complex geometry of the in-drift components [Figure 7-3(a)] is simplified using a radial approach as shown in Figure 7-3(b). The in-drift components that are explicitly represented in the abstraction are the waste package, drip shield, invert, and rubble along with the air gap.

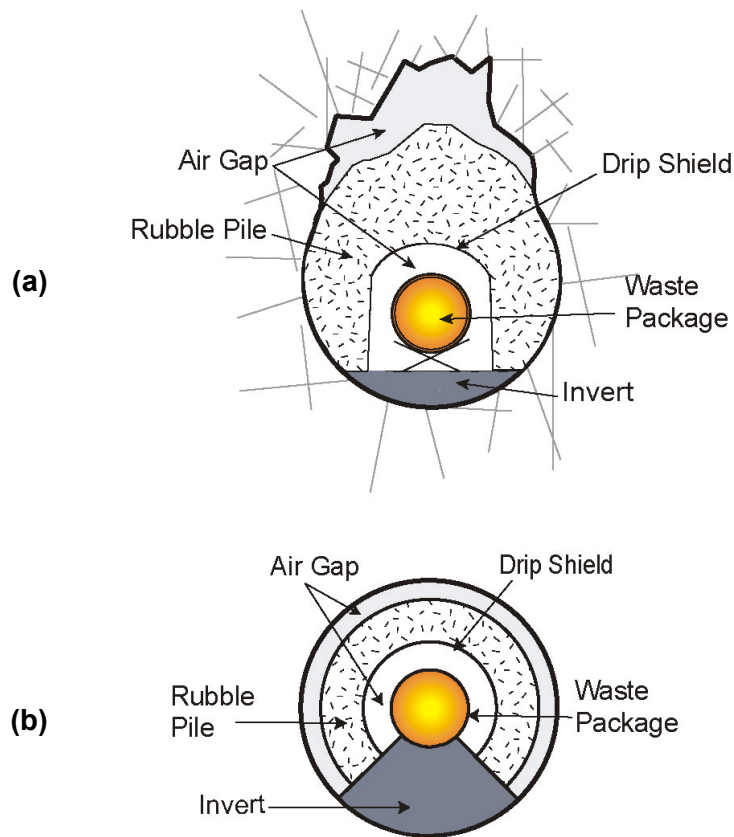


Figure 7-3. (a) Schematic of the Drift Cross Section; (b) Simplified Radial Geometrical Representation of In-Drift Components

Other components such as the ground support system are not explicitly represented in the abstraction. The effect of drift degradation is represented using two modes of the abstraction. Thermal Mode 1 accounts for rubble piling up on the sides of the drip shield and then accumulating in the vertical direction. Thermal Mode 2 represents the uniform filling up of the drift in the simplified radial geometrical representation used in the abstraction. The rate of degradation is calculated in DRIFTFAIL.

7.1.1.3 Relative Humidity

The relative humidity at the waste package surface is calculated based on the temperature at the surface of the waste package and drift wall. Relative humidity is required for the calculations related to chemistry, corrosion, and radionuclide transport and release processes. The calculation of relative humidity for both below- and above-boiling conditions is based on the mole fraction definition found in thermodynamic textbooks (e.g., Moran and Shapiro, 1992; van Wylen and Sonntag, 1978).

7.1.2 Thermally Perturbed Percolation—REFLUX3

The conceptual model for thermally perturbed percolation includes the concept that during the thermal period, water near the drift evaporates and the vaporized water moves toward the

cooler regions away from the drift. Further, the conceptual model includes the idea that when the vaporized water reaches cooler regions where the temperatures are below boiling, it condenses and leaves a dry zone between the condensate zone and the heat source (Figure 7-2). The thickness of the dryout zone can vary for degraded and intact drift cases. The conceptual model considers that the water above the boiling isotherm reaches the drift when the potential penetration depth of the water in the condensate zone exceeds the dryout zone thickness. REFLUX3 calculates the potential penetration depth of the water in the condensate zone and the water flux rate across the dryout zone during the thermal period. In the conceptual model, the water volume in the condensate zone contains the vaporized matrix pore water from the dryout zone, infiltration from the ground surface, and the residual water in the condensate zone.

7.1.3 Seepage Water Chemistry

In the NFENV conceptual model, the chemistry of water contacting the engineered barrier system can be influenced by temperature, interaction with the rocks and the engineered materials, evaporation, and deliquescence. To simplify the identification and evaluation of various processes influencing the water chemistry, Browning, et al. (2004) defined four environments that are distinguished by the temperature at the drift wall and in-drift relative humidity for the abstraction of the near-field environments (Figure 7-4). These environments are referred to as the dry environment and Environments I, II, and III. The dry environment occurs when there is insufficient water to support aqueous corrosion of the waste package, and no seepage chemistry is considered. Dry air oxidation and humid air corrosion are considered as part of the dry environment in the conceptual model for EBSFAIL (Chapter 8 contains additional information). The remaining three environments are considered to be capable of supporting aqueous corrosion of the waste package and have water chemistries associated with them. A description of all four environments follows.

The conceptual model includes the effect of ventilation prior to closure of the potential repository. For the period after the potential repository closure, the conceptual model includes the effect of heat generated from the radioactive decay of waste inside the waste packages on water movement to the drifts and consequent effects of humidity within the drifts.

The conceptual model incorporates the process of deliquescence by using the temperature and relative humidity in the drifts. In NFENV, the period during which the drift wall temperature remains at or above the boiling point of water but the in-drift relative humidity increases above the deliquescence relative humidity is referred to as Environment I. In this environment, the only feasible source of water to initiate waste package corrosion is the deliquescence of salts on the waste package surface.

In NFENV, Environment II begins when the drift wall temperature drops below the boiling point of water such that water can seep from the overlying rocks and drip onto the waste packages. The conceptual model incorporates the evaporative concentration of seepage water to form brines and mineral precipitates by using residual heat from the waste package.

In NFENV, Environment II ends and Environment III begins when the seepage rate becomes equal to or greater than the evaporation rate, such that the evaporation of water leading to concentrated solutions or brines is no longer expected to be significant. During Environment III, the temperature and chemistry of the seepage water returns to ambient conditions.

In TPA Version 5.1, Environments II and III waters can only interact with waste packages if the drip shield has failed and no longer prevents seepage water from contacting the waste package. During Environment I, potentially corrosive chemistries can contact the waste package even when the drip shield is intact if brines form on the waste package surface by salt deliquescence.

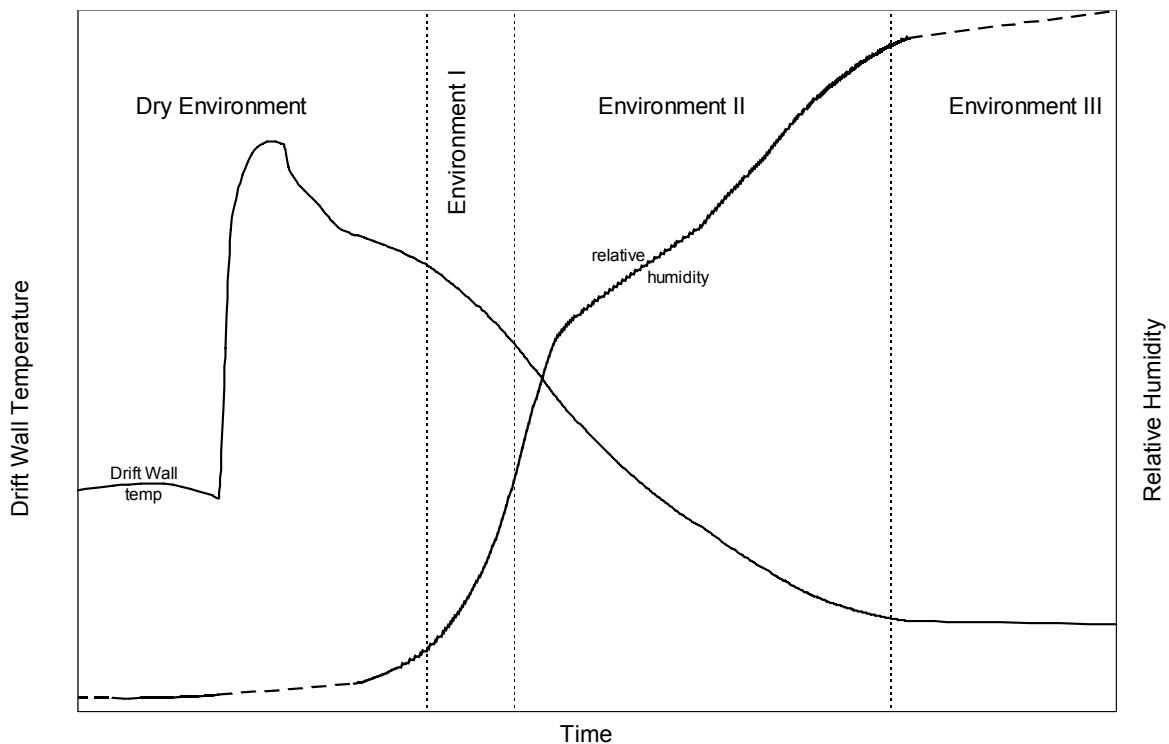


Figure 7-4. Plot of Calculated Drift Wall Temperature and Relative Humidity and the Four Near-Field Environments Abstracted into TPA Version 5.1

7.2 Model Support and Assumptions

NFENV abstracts the following processes in the vicinity of the potential repository drift: (i) heat transfer and temperature on a mountain and drift scale, (ii) thermally perturbed percolation of groundwater, and (iii) chemical composition of seepage water. The model support and assumptions for each of these areas are described separately in the following subsections.

7.2.1 Heat Transfer

7.2.1.1 Mountain-Scale Heat Transfer

The main assumption made in the determination of the temperature at the drift wall is that conduction is the dominant mode for heat transfer. This is a reasonable assumption at the mountain scale where the heat transfer in the host rock predominantly controls the temperature at the drift wall. This assumption is consistent with process model results (Bechtel SAIC Company, LLC, 2005a; Manepally, et al., 2004; Painter, et al., 2001). Temperatures measured in the drift-scale heater test at Yucca Mountain (TRW Environmental Safety Systems, Inc., 2000) and a laboratory-scale heater test (Green and Painter, 2002) support the conceptualization of the mountain-scale heat-transfer abstraction.

7.2.1.2 In-Drift Heat Transfer

A thermal network approach (Incropera and DeWitt, 2002) is used to calculate in-drift temperature using a simplified radial geometry. The main assumption of the temperature calculation is that drift wall temperature is not affected by in-drift heat transfer, because the thermal response time for the in-drift heat transfer process is significantly less than mountain-scale heat transfer. The thermal response time depends on the heat capacity of the material, and the heat capacity of air is an order of magnitude lower than that of host rock (Incropera and DeWitt, 2002). The host rock is treated as a sink due to its high thermal capacity, and the in-drift heat transfer process is assumed to be in quasi-steady state. The heat output from the waste package is also required for temperature calculation and is obtained from constitutive relationships described in Section 7.3. A detailed process-level study (Manepally, et al., 2004) indicates that the nature of the rubble accumulation around the drip shield significantly affects the temperature evolution of the engineered barrier system, which supports the two Thermal Modes implemented to address the effect of drift degradation.

7.2.1.3 Relative Humidity

For the preclosure period, the relative humidity at the waste package is set to the relative humidity of the ventilated air as specified by the *tpa.inp* parameter `RelativeHumidityForVentilatedAir[]`. The ventilation intake is the outside air, which varies in both temperature and relative humidity. The underground drift system is expected to modulate the temperature, and relative humidity changes sufficiently. A constant value of relative humidity is chosen based on field measurements (Bechtel SAIC Company, LLC, 2004c). For the postclosure period, the calculation of relative humidity is based on the mole fraction definition frequently found in thermodynamic textbooks (e.g., Moran and Shapiro, 1992). Relative humidity is generally defined as the ratio of the actual mole fraction of water vapor in the air to the maximum or saturation mole fraction of water vapor in the air at the same temperature and pressure. For below boiling conditions, mole fractions are related to the vapor partial pressures. For temperatures above boiling, the partial vapor pressure cannot exceed the atmospheric pressure within the drift, even in the presence of rubble, because of its high porosity. When the waste package surface temperature exceeds the boiling point, relative humidity is defined as a ratio of the two vapor pressures specified previously based on the temperature at boiling, which is consistent with the technical literature (Fyfe, 1994; Hartman, 1991; Bejan, 1988). The partial vapor pressure is calculated as a function of temperature based on the relationship described by Reid, et al. (1987).

To calculate relative humidity on the waste package surface, the partial pressure of water vapor in the drift is assumed to be uniform. This is the equivalent of saying that the absolute humidity in the drift is the same as that at the drift wall. This assumption recognizes that the gas in the drift (which consists of air and water vapor) is well mixed as a result of turbulent mixing (driven by buoyant gas-phase convection) and binary vapor diffusion of air and water. This mixing causes the absolute humidity to be uniform inside the emplacement drift at a given location along the drift. This assumption is supported by the analysis given in Bechtel SAIC Company, LLC (2005a).

7.2.2 Thermally Perturbed Percolation—REFLUX3

Evidence of thermal refluxing has been documented during heater tests performed at the laboratory scale (Green and Prikryl, 1998), small field scale (Lin, et al., 2001), and large field scale (Bechtel SAIC Company, LLC, 2002). This evidence was in the form of temperature excursions, corrosion of engineered materials, and liquid water dripping into air voids.

Time-series dryout zone thickness data for the nominal (degraded) and intact drift geometries were generated from process level simulations using MULTIFLO™ as described in Manepally, et al. (2004) and supplied in *drythick.dat*. A single representative rubble volume versus time

curve was used as input to the MULTIFLO simulations to compute the dryout zone thickness as a function of time (Manepally, et al., 2004). Therefore, there is no consideration to the contribution of uncertainty in the dryout zone thickness to the REFLUX3 simulations. The main output of REFLUX3 is the time at which seepage develops in the drifts, as well as water flow rates per waste package. Consideration of uncertainty in the dryout zone thickness is likely to have only a limited effect on the onset of seepage.

7.2.3 Seepage Water Chemistry

NFENV specifies the pH value and the fluoride, chloride, nitrate, carbonate, and sulfate concentrations of water contacting the waste package for Environments I, II, and III for the potential repository.

In Environment I the entire repository is assigned a pH or concentration of fluoride, chloride, nitrate, carbonate, and sulfate. This approach is appropriate because the molar ratio of corrosion-inhibiting oxyanions (sulfate and nitrate) to chloride present in dust samples taken from the Yucca Mountain vicinity is high (Juckett, 2006; Reheis, 2003; Peterman, et al., 2003), consequently the initiation of localized corrosion of the Alloy 22 waste package outer barrier, under brines that form by salt deliquescence, is unlikely.

In Environment II each subarea is assigned a pH or concentration of fluoride, chloride, nitrate, carbonate, and sulfate. The stochastic variability in water chemistry for the repository as a whole during Environment II is accounted for by sampling each chemical parameter individually for every subarea in each realization. This approach attempts to capture the range of potential water chemistries while maintaining computational efficiency.

In Environment III the entire repository is assigned a pH or concentration of fluoride, chloride, nitrate, carbonate, and sulfate. This approach is appropriate because the relative humidity is assumed to be high (95–98 percent). The solution compositions are assumed to be comparable to existing ambient pore water samples, with typical ionic concentrations on the order of 10^{-3} mol/L (Yang, et al., 2003; 1998; 1996). The initiation and propagation of localized corrosion of Alloy 22, in the form of crevice corrosion, require concentrated solutions (Dunn, et al., 2005). Consequently, localized corrosion of the Alloy 22 waste package outer barrier by dilute pore waters is unlikely.

The following assumptions were used in developing NFENV:

- Regarding deliquescence, it is assumed that the Yucca Mountain dust samples have similar compositions to dusts that could deposit on the waste package surface.
- It is assumed that seepage water in Environment II will have chemical characteristics similar to Yucca Mountain unsaturated zone pore waters and that the effects of seepage water interaction with natural and engineered materials in the vicinity of the drift can be neglected.
- It is assumed that the range in chemistry of water contacting the waste package, which was calculated for a temperature of 110 °C [230 °F], is applicable for the whole period of Environment II, when temperatures vary from about 130 to 25 °C [266 to 77 °F].
- The range in water chemistry that can contact the waste package is assumed to be the same for the degraded drift and the nondegraded drift. However, because the in-drift relative humidity is calculated as a function of temperature in TPA Version 5.1 and the temperature histories of the two cases are different, the onset of the different environments is expected to be different for the degraded drift and nondegraded drift.

- The chemistry of seepage water in Environment III is assumed to be dilute and is not expected to initiate localized corrosion of the waste package.

7.3 Implementation of Conceptual Model in TPA Version 5.1

NFENV is called once for each subarea in every realization (Chapter 2 contains a description of subareas and realizations). NFENV describes the (i) heat transfer and temperature on a mountain and drift scale, (ii) thermally driven refluxing of groundwater, and (iii) chemical composition of seepage water in the vicinity of the potential repository drift. The general flow of information into, out of, and within NFENV is illustrated in Figure 7-1. The implementation of each of these module components is described separately in the following subsections.

7.3.1 Heat Transfer

7.3.1.1 Mountain-Scale Heat Transfer

The potential repository-horizon average rock temperature is computed using an analytic conduction-only model for mountain-scale heat transfer. The drifts are represented as an array of parallel-linear heat sources of varying length, in a semi-infinite medium with specified rock properties (Figure 7-5). Because more than one line source (i.e., drift) exists, the temperature increase in the semi-infinite medium is the sum of contributions from each line source based on the principle of superposition. The model is based on thermal line sources representing drifts separated by the drift spacing, as specified by the *tpa.inp* parameter EmplacementDriftSpacing[m], residing in a semi-infinite medium. The model consists of parallel line sources that cover the potential repository footprint (Figure 7-5). Waste is assumed to be emplaced in waste packages, sufficiently close to each other in drifts that there is no spatial variation in the heat output along the drift (a linear heat load is assumed), but there is significant variation in heat output between the drifts. Because of this variation in heat output, the temperature varies significantly between drifts (i.e., between the line sources). Each line source is at a depth of H below the ground surface and is represented as a high aspect ratio rectangular element with a length of 2L and width of 2B (the drift diameter). The general solution for the temperature increase at any point in space and time is given by Claesson and Proberts (1996) and Carslaw and Jaeger (1959)

$$\Delta T(x, y, z, t) = \int_0^t \frac{\alpha q''_{\text{rep}}(t')}{4k\sqrt{\pi}} \frac{1}{\sqrt{4\alpha(t-t')}} \left[\operatorname{erf}\left(\frac{L-x}{\sqrt{4\alpha(t-t')}}\right) + \operatorname{erf}\left(\frac{L+x}{\sqrt{4\alpha(t-t')}}\right) \right] \left[\operatorname{erf}\left(\frac{B-y}{\sqrt{4\alpha(t-t')}}\right) + \operatorname{erf}\left(\frac{B+y}{\sqrt{4\alpha(t-t')}}\right) \right] \left[\exp\left(\frac{-z^2}{4\alpha(t-t')}\right) - \exp\left(\frac{-(z-2H)^2}{4\alpha(t-t')}\right) \right] dt' \quad (7-1)$$

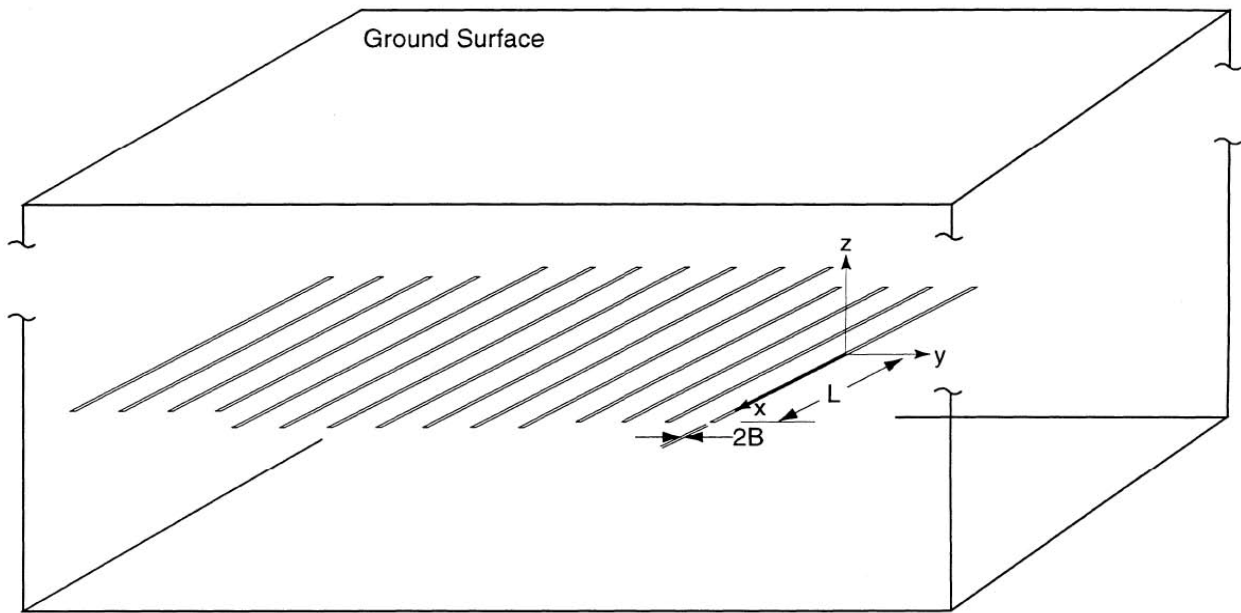


Figure 7-5. Mountain-Scale Heat Transfer Model With Line Sources

where

$\Delta T(x,y,z,t)$	— increase in temperature at time t at a point (x, y, z) in the semi-infinite medium due to one line source [C]
$q''_{rep}(t)$	— time-dependent potential repository heat flux [W/m^2] calculated using Eq. (7-2)
α	— thermal diffusivity of the semi-infinite medium [m^2/s] calculated using Eq. (7-3)
k	— thermal conductivity of the semi-infinite medium [$\text{W}/(\text{m}\cdot\text{K})$] as specified by the <i>tpa.inp</i> parameter ThermalConductivityofYMRock[$\text{W}/(\text{m}\cdot\text{K})$]
L	— half-length of a line source [m]
B	— half-width of a line source [m]
H	— depth of a line source below the ground surface [m]
t	— actual time after activation of heat flux [s]
t'	— variable of integration [s]
x,y,z	— location of interest [m]

The time-dependent potential repository heat flux [$q''_{rep}(t)$] is calculated as follows

$$q''_{rep}(t) = q_{permtu} AML U_{conv} \quad (7-2)$$

where

q_{permtu}	—	heat load for a representative waste package (given in Chapter 2) [W/MTU]
AML	—	areal mass loading for the area occupied by the drifts (given in Chapter 2) [MTU/acre]
U_{conv}	—	factor used to implement unit conversion [1/4047] [acre/m ²]

The thermal diffusivity (α) is calculated as follows (Incopera and DeWitt, 2002)

$$\alpha = \frac{k}{\rho(c_p)} \quad (7-3)$$

where

ρ	—	density of the semi-infinite medium as specified by the <i>tpa.inp</i> parameter MassDensityofYMRock[kg/m ³]
C_p	—	specific heat at constant pressure of the semi-infinite medium as specified by the <i>tpa.inp</i> parameter SpecificHeatofYMRock[J/kg-K]

The heat flux $q''_{rep}(t)$ is also adjusted for heat losses due to ventilation during the preclosure period using (i) FactorForActiveVentilationHeatLosses[] for the forced ventilation period defined by the TimeActiveVentilationEnds[yr] and (ii) FactorForPassiveVentilationHeatLosses[] for the passive ventilation period that is between the forced ventilation and time of potential repository closure defined by TimeOfRepositoryClosure[yr].

The half-length of the line source (L) is calculated as the midpoint of the drift. The depth of the line source below the ground surface (H) is calculated based on the difference between ElevationOfRepositoryHorizon[m] and ElevationOfGroundSurface[m]. The values for both of these *tpa.inp* parameters are intended to be representative of the entire potential repository. The value of z is updated at every timestep based on the height of the drift crown as calculated by DRIFTFAIL. The location of the temperature calculation (i.e., x, y, z) in Eq. (7-1) for the reference case is the centroid of the subarea. The ground surface is assumed to be exposed to atmospheric conditions and has a constant temperature. It is assumed that the ground temperature is not affected by climate change. Equation (7-1) is valid below the ground surface, $z < H$.

7.3.1.2 In-Drift Heat Transfer

A radial thermal network approach with a constant heat flux is used to calculate temperature inside the drift. The presence of in-drift components such as invert, drip shield, air gap, and rubble are represented as thermal conductance elements in the network model. The network is solved to calculate the total effective thermal conductance in the drift. The thermal network approach used in the linear model to calculate the temperatures of the in-drift components is represented as

$$Q_{wp} = (T_{wp} - T_{Wall})G_{Total} \quad (7-4)$$

where

- Q_{wp} — time-dependent total thermal output for a waste package adjusted for ventilation during the preclosure period [W] [Eq. (7-2)]
- T_{Wall} — drift wall temperature [°C]
- T_{wp} — waste package surface temperature [°C]
- G_{Total} — effective thermal conductance for the total network [W/°C]

Two modes are available to calculate G_{Total} : Thermal Mode 1 and Thermal Mode 2. These modes differ in conceptualizing the rubble-accumulation process around the drip shield. Thermal Mode 1 adopts a two-step approach where the rubble initially accumulates on the side of the drip shield. Once the sides are filled up, accumulation occurs on the top of the drip shield. Thermal Mode 2 assumes that the rubble accumulates uniformly around the drip shield. Two different conceptualizations are incorporated in TPA Version 5.1 to enable the user to investigate different accumulation patterns and resulting temperature evolutions and are described next, with additional details on their implementation provided in Appendix B.

7.3.1.2.1 Thermal Mode 1

Thermal Mode 1 accounts for rubble accumulation first on the side of the drip shield followed by the accumulation on top of the drip shield. In this mode, the zone between the drip shield and drift wall is divided into three separate concurrent pathways or legs for heat transfer. The invert leg represents the waste package and invert. The vertical segment (Leg A) represents heat transfer across the area between waste package and drift crown. The horizontal segment (Leg B) represents heat transfer across the area between the waste package and the drift sidewall. The outer extent of the horizontal segment is limited by the drift wall radius, whereas the outer extent of the vertical segment is constrained by the degraded drift ceiling. The relative extent of different segments along the periphery of the drip shield is controlled using the *tpa.inp* parameter FractionAllowedToDegrade[].

The process of time-dependent rubble accumulation and the changing rubble thickness for the vertical and horizontal segments are illustrated in Figure 7-6(a) through (c). Initially, the area represented by the horizontal segment is filled with air. As rockfall occurs, the area between the drip shield and drift sidewall starts to fill with rubble. The conceptualization of the horizontal segment at this stage is shown in Figure 7-6(a), where it contains a layer of rubble followed by an air gap between the wall rock and rubble outer boundary. This process continues until the entire area represented by the horizontal segment is filled with rubble. Any subsequent rubble accumulation takes place in the vertical segment as shown in Figure 7-6(b) and (c). The vertical extent of the vertical segment is determined by the degraded drift crown and could extend beyond the original drift wall location as shown in Figure 7-6(c).

7.3.1.2.2 Thermal Mode 2

Thermal Mode 2 conceptualizes the rubble accumulation on the drip shield surface as a uniform thickness in the radial direction. In this mode, heat transfer from the waste package to the drift wall takes place in two concurrent pathways. The first pathway is the invert leg that represents the invert and waste package in simplified radial geometry. The second pathway consists of the drip shield, accumulated rubble, and the air gap.

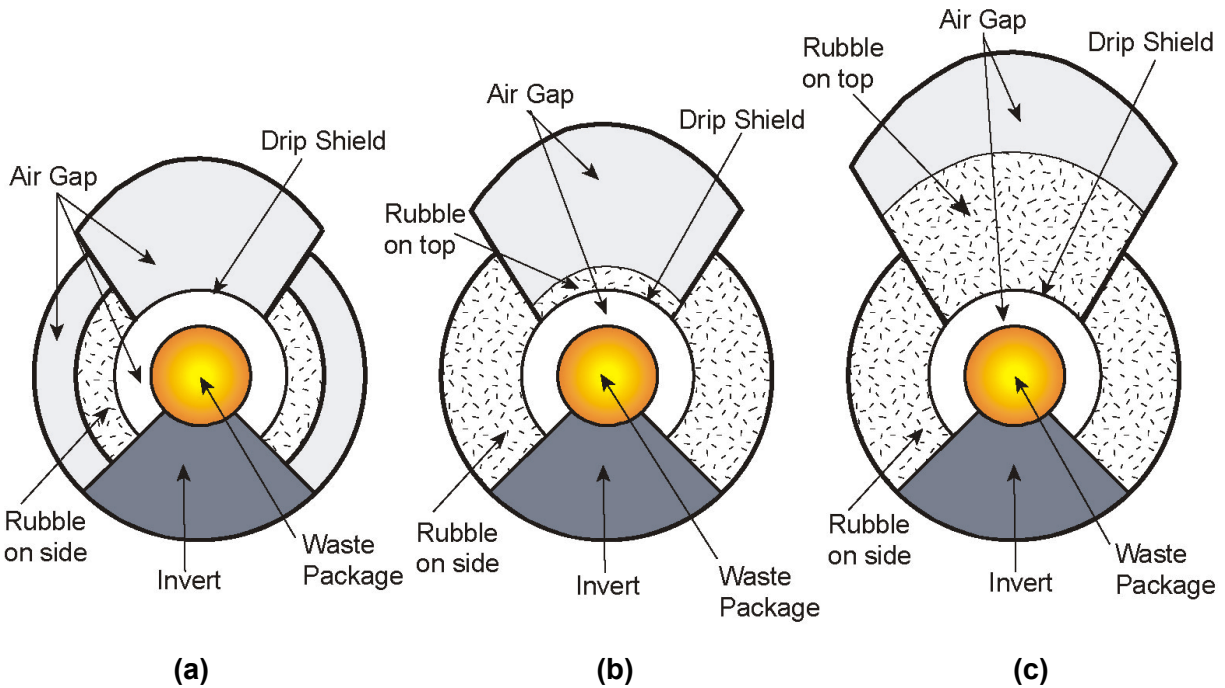


Figure 7-6. Time-Dependent Pattern of Rubble Accumulation Thermal Mode 1

7.3.1.2.3 Selection of Thermal Mode

TPA Version 5.1 uses Thermal Mode 1 or Thermal Mode 2 depending on the user-specified values for the following two *tpa.inp* parameters: `CircumferentialFractionNotCoveredByFloor[]` and `FractionAllowedToDegrade[]`. The first parameter stipulates the fraction of the drift periphery that will not be covered by the invert and is susceptible to degradation. The second parameter stipulates the fraction of a drift wall that is allowed to degrade and form rubble.

When `CircumferentialFractionNotCoveredByFloor[]` is greater than `FractionAllowedToDegrade[]`, only a fraction of the drift wall degrades and forms a wedge-shaped ceiling with the degraded materials filling up the side of the drift before vertical accumulation occurs on top of the drip shield (Mode 1). When `CircumferentialFractionNotCoveredByFloor[]` is less than `FractionAllowedToDegrade[]`, then the whole drift wall uniformly degrades, and the rubble accumulates on the drip shield as a mass of rubble with uniform thickness (Mode 2).

7.3.1.2.4 Implementation

The equivalent thermal conductance G_{Total} in Thermal Mode 1 and 2 is obtained using a thermal network approach that is discussed in Appendix B. The waste package temperature is calculated using the following equation

$$T_{WP} = T_{Wall} + \frac{Q_w}{G_{Total}} \quad (7-5)$$

where

Q_w	—	time-dependent total thermal output adjusted for ventilation for a waste package during the preclosure period [W]
T_{Wall}	—	drift wall temperature [°C]
T_{WP}	—	waste package surface temperature [°C]
G_{Total}	—	effective thermal conductance for the total network [W/°C], where the calculational approach is described in Appendix B

Equations for temperature and heat flux values at the drip shield and rubble outer surface are also described in Appendix B.

TPA Version 5.1 has options for building thermal networks for different scenarios such as an intact drift, fully filled the horizontal segment with partially filled vertical segment, and partially filled the horizontal segment with no rubble accumulation in the vertical segment. These scenarios are determined internally in TPA Version 5.1 depending on the drift configuration, and no specific user input is needed. Development of the network is based on the physical configuration of the drift. NFENV receives geometric parameters such as the rubble radius and equivalent drift radius from DRIFTFAIL and builds the network accordingly. Thermal networks for different scenarios for Thermal Mode 2 are similar to those for Thermal Mode 1. As described before, TPA Version 5.1 internally modifies the network segments and parameters for a particular scenario. This variation depends on the modeling requirement for a given thermal mode. No user specification is needed.

One approach that is not currently supported, but is preserved in TPA Version 5.1 for flexibility, models heat transfer through the accumulated rubble as conduction with an equivalent conductivity to account for conduction, convection, and radiation through the porous rubble. The user can use this approach by setting the *tpa.inp* parameter flag `SelectThermalModel(1=linear,2=iterative)` to 2. Details of the iterative model that accounts for conduction and convection in rubble is presented in Mohanty, et al. (2006) and Mohanty and Adams (2005). The iterative model for heat transfer through the rubble is not supported in TPA Version 5.1, but is preserved to add flexibility for alternative models.

7.3.1.3 Relative Humidity

The approach for calculating the relative humidity is described in Mohanty, et al. (2004). The relative humidity at the waste package is calculated based on the temperature on the waste-package surface and temperature at the drift wall. The partial pressure of water vapor in the drift is uniform, is the same as that at the drift wall at any location, and is used to calculate the relative humidity. The relative humidity at the waste package is defined as the ratio of the actual vapor pressure to the vapor pressure at the waste package surface

$$RH = \frac{P_v \left[\min(T_b, T_w) \right]}{P_v(T_{wp})} \quad (7-6)$$

where

RH	—	relative humidity [unitless]
P_v	—	vapor pressure calculated as a function of temperature [Pa]
$\min(T_b, T_w)$	—	minimum of T_b and T_w [K]
T_b	—	boiling point temperature of water as specified by the <i>tpa.inp</i> parameter BoilingPointofWater[C]
T_w	—	drift wall temperature [K]
T_{wp}	—	waste package surface temperature [K]

The vapor pressure is calculated as a function of temperature based on the relation (Reid, et al., 1987)

$$\ln\left(\frac{P_v}{P_c}\right) = \left[v_{pa} \left(1 - \frac{T}{T_c}\right) + v_{pb} \left(1 - \frac{T}{T_c}\right)^{1.5} + v_{pc} \left(1 - \frac{T}{T_c}\right)^3 + v_{pd} \left(1 - \frac{T}{T_c}\right)^6 \right] \left[\frac{T}{T_c} \right]^{-1} \quad (7-7)$$

where

$v_{pa}, v_{pb}, v_{pc}, \text{ and } v_{pd}$	—	reference values or coefficients (Reid, et al., 1987)
T_c	—	critical Temperature {assumed 647 K [705 °F]}
P_c	—	critical Pressure {assumed 221 atm [3,247 psi]}

7.3.2 Thermally Perturbed Percolation—REFLUX3

In REFLUX3, the water volume in the condensate zone above the boiling isotherm contains (i) water vaporized from below the boiling isotherm surrounding the waste packages prior to the penetration of the reflux water into the dryout zone (thermal component); (ii) infiltration from the ground surface (isothermal component); and (iii) the residual water volume in the condensate zone from the previous timestep.

The maximum available volume of matrix pore water that could vaporize below the boiling isotherm and migrate to the condensate zone above the boiling isotherm is calculated as

$$V_p(t) = D(t)\theta(S_w - S_r)A_c \quad (7-8)$$

where

$V_p(t)$	—	maximum available volume of pore water below the boiling isotherm that can contribute to the condensate zone above the boiling isotherm [m ³]
$D(t)$	—	thickness of the fractured porous domain between the boiling isotherm and the drift [m] specified in <i>drythick.dat</i> (auxiliary input file)

- θ — porosity of the potential repository horizon [dimensionless] as specified by the *tpa.inp* parameter Reflux3Porosity
- S_w — initial pore water saturation of the potential repository matrix [dimensionless] as specified by the *tpa.inp* parameter Reflux3SatInit
- S_r — residual pore water saturation in potential repository matrix [dimensionless] as specified by the *tpa.inp* parameter Reflux3SatResid
- A_c — area of a unit cell holding one waste package [m²]

The temporal variations in the dryout zone thickness, $D(t)$, for both degraded and intact drift cases are read from an external file *drythick.dat*. These data files are based on process-level simulations using MULTIFLO and are described in Manepally, et al. (2004). In TPA Version 5.1 simulations, the dryout zone thickness data for the degraded drift scenario are used only when the drift degradation period is shorter than the thermal pulse period. The thermal pulse period is an input parameter (timePulseEnd) in *drythick.dat*. For the intact drift case, the dryout zone thickness data extend until the end of the thermal pulse period. The area occupied by a single waste package (A_c) is calculated by multiplying the cell diameter, as specified by the *tpa.inp* parameter WPDiameter[m], by the length, as specified by the *tpa.inp* parameter WPLength[m].

Subarea-average net infiltration rates are calculated by UZFLOW. These values are multiplied by A_c to calculate the additional water volume supplied to the condensate zone by the percolating water from ground surface. Hence, the total water volume in the condensate zone in the first timestep ($t = 1$)

$$V_c(1) = I(1) + V_p(1) \quad (7-9)$$

and the subsequent timesteps ($t > 1$) is written as

$$V_c(t) = V_c(t-1) + I(t) + V_p(t) - V_L(t) \quad (7-10)$$

where

- $V_c(t)$ — available water volume in the condensate zone for the reflux at time t after removing the water loss due to shedding and lateral flows [m³]
- $V_c(t-1)$ — available water volume in the condensate zone at time $t-1$ (in the previous timestep) [m³]
- $I(t)$ — water volume added to the condensate zone by the water percolating from ground surface [m³]
- $V_L(t)$ — total water loss due to shedding in the condensate and dryout zones, vaporization in the dryout zone, and water arriving at the drift [m³]

Equation (7-9) indicates that water accumulation in the condensate zone starts after the first timestep, and there is no water loss in the first timestep. Water loss calculations will be explained next.

The water volume in the condensate zone above the boiling isotherm represents the maximum water volume available for reflux. The actual reflux volume, however, is less than the maximum because of lateral flows of condensate and shedding around the edges of the potential repository prior to reflux (Hughson, 2000). Implementation details are shown in Figure 7-2. Water loss in the condensate zone due to shedding and lateral flow and the potential volumetric flow from the condensate zone are computed as

$$V_{L1}(t) = V_C(t-1) S_{h1} \quad (7-11)$$

and

$$Q_C(t) = \frac{V_C(t-1)}{\Delta t} (1 - S_{h1}) Q_F \quad (7-12)$$

where

- V_{L1} — total water loss due to shedding and lateral flow in the condensate zone [m³]
- S_{h1} — shedding factor due to lateral flows of the condensate and shedding around the edges of the potential repository prior to reflux [dimensionless] as specified by the *tpa.inp* parameter FractionOfCondensateRemoved[]
- $Q_C(t)$ — volumetric flow rate from the condensate zone at time t after removing the water loss due to shedding and lateral flow [m³/s]
- Q_F — fraction of the water volume in the condensate zone that flows toward the potential repository [dimensionless] as specified by the *tpa.inp* parameter FractionOfCondensateTowardRepository[]
- Δt — timestep length [s]

In TPA Version 5.1, the necessary condition for the reflux water to reach the drift is determined by the relative lengths of the penetration depth of the reflux water in the dryout zone and the dryout zone thickness. The former can be computed using a modified form of the O.M. Phillips solution (Phillips, 1996)

$$L(t) = \sqrt{\frac{Q_C(t) h \rho_w}{k \nabla T}} \quad (7-13)$$

where

- $L(t)$ — penetration distance of the refluxed water [m]
- ρ_w — density of the boiling water as specified by the *tpa.inp* parameter DensityOfWaterAtBoiling[kg/m³]
- h — enthalpy of phase change for water [J/kg] as specified by the *tpa.inp* parameter EnthalpyOfPhaseChangeForWater[J/kg]
- k — thermal conductivity of rock [W/m-K] as specified by the *tpa.inp* parameter ThermalConductivityofYMRock[W/(m-K)]
- ∇T — temperature gradient in vicinity of boiling isotherm [K/m] as specified by the *tpa.inp* parameter TemperatureGradientInVicinityOfBoilingIsotherm[K/m]

If the penetration distance is shorter than the dryout zone thickness, the reflux water vaporizes and migrates back to the condensate zone. Otherwise, the reflux water can reach the drift. In this case, as the water flows through the dryout zone, a fraction of the reflux water is shed and vaporized (Hughson, 2000). The water losses due to the shedding and vaporization in the dryout zone and the corresponding volumetric reflux rate in the dryout zone near the drift are computed as

$$V_{L2}(t) = Q_C(t) S_{h2} \Delta t + Q_C(t) \frac{D(t)}{L(t)} (1 - S_{h2}) \Delta t \quad (7-14)$$

$$Q_R(t) = Q_C(t) (1 - S_{h2}) \left(1 - \frac{D(t)}{L(t)} \right) \quad (7-15)$$

where

- $V_{L2}(t)$ — total water loss due to shedding and vaporization in the dryout zone after refluxing [m³]
- $Q_R(t)$ — volumetric flow rate of the reflux water near the drift at time t [m³/s]
- S_{h2} — shedding factor in the dryout zone [dimensionless] as specified by the *tpa.inp* parameter FractionOfCondensateTowardRepositoryRemoved[]

The first term on the right-hand side of Eq. (7-14) accounts for losses due to shedding, and the second term accounts for losses due to vaporization, both in the dryout zone. The second term in Eq. (7-14) is used only when $L(t) > D(t)$. When $L(t) < D(t)$, $Q_R(t) = 0$ (i.e., the reflux water will not reach the drift). At the first timestep, $S_{h1} = S_{h2} = 0$, and $Q_R(t) = 0$ (i.e., no shedding and no flow to drift).

The total water losses, V_{L2} , in Eq. (7-14) will then be

$$V_{L2}(t) = V_{L1}(t) + Q_C(t) \Delta t S_{h2} + Q_R(t) D t \quad (7-16)$$

The quantity of refluxing deep percolation as well as that obtained from UZFLOW is passed to EBSREL (Chapter 10) after accounting for shedding in the condensate and dryout zones to calculate the quantity of water that could contact the waste package surface.

A user-specified option is available to set the percolation rate to zero whenever the temperature at the drip shield is above a threshold temperature. This option is based on the approach described in Basagaoglu, et al. (2007). The seepage threshold temperature is defined using the sampled *tpa.inp* parameter SeepageThresholdT[C], as indicated in Section 7.4. Setting FlagSeepageThreshold[] to one in *tpa.inp* enables the temperature threshold modification. Setting the flag to zero passes REFLUX3 output to the seepage abstraction without modification. The likelihood of thermal reflux decreases as temperatures rise significantly above the boiling temperature of water in the host rock. Capillarity is expected to retain some water in the rock at temperatures slightly above boiling, with the amount retained dependent on the hydrologic properties of the unsaturated zone rock. Using a higher temperature threshold implies that water breaching the dryout zone is more common across the potential repository. The *tpa.inp* parameter SeepageThresholdT[C] (Table 7-1, Section 7.4) controls the timing when water could initially contact the drip shield or the waste package. For the intact drift scenario, when the drift wall temperature is above SeepageThresholdTemperature, the flux across the dryout zone is 0, even if the penetration depth of the condensed water exceeds the dryout zone thickness. Similarly, for the degraded drift scenario, the flux across the dryout zone can occur when the drip shield temperature cools below SeepageThresholdTemperature.

7.3.3 Seepage Water Chemistry

One function of NFENV is to pass chemistry parameters to EBSFAIL for calculating waste package corrosion rates for both welded and mill-annealed portions of the outer container. These parameters include time-varying concentrations of fluoride, chloride, nitrate, sulfate, and

carbonate ions, along with the values of pH and the change in critical potential, ΔE_{crit}^{NFENV} . In addition, NFENV calculates the oxyanion-to-chloride molar concentration ratio (r) defined as

$$r = \frac{[NO_3^-]}{[Cl^-]} + \frac{r_n}{r_s} \frac{[SO_4^{2-}]}{[Cl^-]} + \frac{r_n}{r_c} \frac{[CO_3^{2-}] + [HCO_3^-]}{[Cl^-]} \quad (7-17)$$

where

- r_n — nitrate inhibitor constant [unitless], as specified by the *tpa.inp* parameters OuterInhibitingNitrateToCl and WeldInhibitingNitrateToCl
- r_c — carbonate inhibitor constant [unitless], as specified by the *tpa.inp* parameters OuterInhibitingCarbonateToCl and WeldInhibitingCarbonateToCl
- r_s — sulfate inhibitor constant [unitless], as specified by the *tpa.inp* parameters OuterInhibitingSulfateToCl and WeldInhibitingSulfateToCl
- $[Cl^-]$ — chloride ion concentration [M]
- $[NO_3^-]$ — nitrate ion concentration [M]
- $[SO_4^{2-}]$ — sulfate ion concentration [M]
- $[CO_3^{2-}]$ — carbonate ion concentration [M]
- $[HCO_3^-]$ — bicarbonate ion concentration [M]

which is passed to EBSFAIL.

As discussed previously, seepage chemistry is abstracted into TPA Version 5.1 using four distinct environments defined by temperature, relative humidity, and seepage flux approaching the drift (Figure 7-4). The implementation of each environment in TPA Version 5.1 is described next.

7.3.3.1 Dry Environment

The dry environment is in effect when the relative humidity is less than the *tpa.inp* parameter CriticalRelativeHumidityAqueousCorrosion. The dry environment is described mathematically as

$$RH < \text{CriticalRelativeHumidityAqueousCorrosion}$$

The conceptual model for EBSFAIL divides the dry environment in a region of dry air oxidation and a region of humid air corrosion. Chapter 8 discusses corrosion and the *tpa.inp* parameter CriticalRelativeHumidityAqueousCorrosion.

7.3.3.2 Environment I (Deliquescence)

Environment I is in effect when the relative humidity is greater than the *tpa.inp* parameter CriticalRelativeHumidityAqueousCorrosion and the drip shield is intact or the volumetric flow rate of water approaching the drift (Q_R) is zero. The flow of water contacting the waste package (Chapter 10) is proportional to the flow of water approaching the drift, Q_R {described by Eq. (7-15)}. Therefore, the flow of water contacting the waste package is greater than zero only if Q_R is zero. This environment is described mathematically as

$$\{Q_R = 0\} \text{ and } \{RH > \text{CriticalRelativeHumidityAqueousCorrosion}\} \text{ or } \{\text{time } (t) < \text{time of drip shield failure}\}$$

7.3.3.3 Environment II (Seepage Evaporation)

Environment II is in effect when the relative humidity is greater than the *tpa.inp* parameter CriticalRelativeHumidityAqueousCorrosion, but less than the *tpa.inp* parameter RewettingHumidity, the drip shield has failed, and the volumetric flow rate of seepage approaching the drift (Q_R) is greater than zero. The flow of water contacting the waste package (Chapter 10) is proportional to the flow of water approaching the drift, Q_R {described by Eq. (7-15)}. Therefore, the flow of water contacting the waste package is greater than zero only if Q_R is greater than zero. These conditions are described mathematically as

$\{CriticalRelativeHumidityAqueousCorrosion < RH < RewettingHumidity[]\}$ and $\{t > \text{time of drip shield failure}\}$ and $\{Q_R > 0\}$

The time of drip shield failure is supplied to NFENV by MECHFAIL.

7.3.3.4 Environment III (Seepage)

Environment III is in effect when the relative humidity is greater than the *tpa.inp* parameter RewettingHumidity[], the drip shield has failed, and the seepage flux approaching the drift (Q_R) is greater than zero. The flow of water contacting the waste package (Chapter 10) is proportional to the flow of water approaching the drift, Q_R {described by Eq. (7-15)}. Therefore, the flow of water contacting the waste package is greater than zero only if Q_R is greater than zero. These conditions are described mathematically as

$\{RH > RewettingHumidity[]\}$ and $\{t > \text{time of drip shield failure}\}$ and $\{Q_R > 0\}$

7.4 Input Parameters in *tpa.inp*

Table 7-1 lists the input parameter values relevant to NFENV in *tpa.inp* that are included in the reference data set for TPA Version 5.1.

7.5 Auxiliary Input Data and External Process Models

Auxiliary input data files used by NFENV provide (i) dryout zone thickness data used in REFLUX3; and (ii) user-defined temperature and relative humidity values at the waste package and drift wall as a function of time. Table 7-2 lists and describes the auxiliary input data files for NFENV. NFENV allows the user to bypass the in-drift heat transfer abstraction calculations and use external process module results given in *tefkti.inp*. This auxiliary file can be selected by setting the *tpa.inp* parameter TabularTemperatureRHFlag(0=no,1=yes) to a value of 1. The parameter nsetUsedToPickTemp RHDDataSet selects the data set in *tefkti.inp* that has up to four sets of data (options 1 to 4).

7.6 Intermediate Outputs and Information Passed to Other Modules

Table 7-3 lists and describes the intermediate output files containing thermal hydrology and chemistry information that is created during execution of NFENV. In addition to the output files listed in Table 7-2, the user can specify that calculated information passed to and from NFENV be saved as intermediate output for specific realizations. This functionality is implemented in the *tpa.inp* input block titled <<Output Print Options>> by setting the output mode parameter, OutputMode(0=None,1=All,2=UserDefined), to a value of 1 or 2. When set to 1, all optional intermediate output for NFENV will be saved for all realizations. When set to 2, optional intermediate output selected will be saved for realizations starting from *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by *tpa.inp* parameter UserDefinedUpperRealizationAppended. The contents of NFENV intermediate output files *nfenv.rlt* and *nfenv.ech* are described in Table 7-4.

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	Cond_EqvForNaturalConvection[W]/(m-C)]	$K_{n,c}$ Equivalent conductance representing natural convection [W/m-C]	constant 0.9	Thermal conductance equivalence value based on a thermal conductivity approximately 30 times that of air.
NFENV	TimeOfRepositoryClosure[yr]	Used to determine when the potential repository is closed and ventilation stops and potentially when backfill may be emplaced [yr]	constant 100.0	Value based on DOE proposal for length of preclosure period [Williams (2003) cited in Bechtel SAIC Company, LLC (2004a)].
NFENV	TimeActiveVentilationEnds[yr]	The year in which active ventilation ends and passive ventilation may begin [yr]	constant 50.0	Length of preclosure period [Williams (2003) cited in Bechtel SAIC Company, LLC (2004a)].
NFENV	TotalWasteEmplacedInRepository[MTU]	Total waste emplaced in repository in metric tons of uranium [MTU]	uniform 70040.0	The Nuclear Waste Policy Act of 1982 (Section 114) sets a limit for the Yucca Mountain potential repository of 70,000 metric tons of heavy metal or a quantity of solidified high-level radioactive waste resulting from reprocessing of such a quantity of spent fuel. A number slightly exceeding 70,000 tons is specified in TPA Version 5.1. This ensures that the tracked mass is close (actually slightly above) the 70,000-ton limit in case the number of waste packages is rounded up. (Only an integer number of waste packages is considered in TPA Version 5.1, and some waste form mass may not be tracked due to rounding up of real numbers to integers).
NFENV	SpentFuelWastePackagePayload[MTU]	Spent fuel waste package payload in metric tons of uranium [MTU]	constant 7.89	Value based on U.S. Department of Energy (DOE) data presented in DOE (1987).
NFENV	EquivalentMTUPayloadOfGlassPackage[MTU]	Equivalent payload of glass waste in metric tons of uranium [MTU]	constant 0.258641	Value based on data presented in CRWMS M&O (2000b).
NFENV	FractionOfRepositoryWasteInGlassForm[]	The fraction of waste packages containing glass waste [unitless]	constant 0.0126	Constant value based on a range (0.0 to 0.32) of the projected fraction of waste packages containing glass (Bechtel SAIC Company, LLC, 2004b).

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	SelectThermalModel(1,2)	Models for approximating heat transfer in rubble; value of 1 enables linear model, and value of 2 enables iterative model	constant 1	Thermal Model 2 is not currently supported in TPA Version 5.1, but preserved to add flexibility.
NFENV	SelectParticleModel(1,2)	Used only in Thermal Model 2; selects a particle model in which backfill/rubble parameters are calculated in particle Model 1 or directly substituted in particle Model 2 [unitless]	constant 2	User option. Allows the user to select between particle models. Model 1 provides the option for directly using DOE information. Model 2 is a mechanistic model that directly relates heat transfer to rockfall rubble characteristics.
NFENV	BackfillParticleDiameter [m]	Rubble Particle Diameter [m]	uniform 0.1, 0.5	Distribution based on Mohanty and Adams (2005). Note: The terms backfill and rubble are used interchangeably.
NFENV	BackfillPorosity[]	Porosity of the rubble [unitless]	uniform 0.1, 0.6	Distribution based on Mohanty and Adams (2005). Note: The terms backfill and rubble are used interchangeably.
NFENV	TortuosityOfNatural Backfill[]	Tortuosity of rubble [unitless]	uniform 1.25, 3.0	Distribution based on Mohanty and Adams (2005). Note: The terms backfill and rubble are used interchangeably.
NFENV	SortingCoefficient[]	Trask Sorting Coefficient [unitless]	constant 2.0	Value based on Mohanty and Adams (2005).
NFENV	SkewnessOfDistribution[]	Only used in particle Model 2; calculated in particle Model 1 [unitless]	uniform 0.0, 1.5	Distribution based on Mohanty and Adams (2005).
NFENV	CoefficientOfVariation[]	Only used in particle Model 2; calculated in particle Model 1 [unitless]	uniform 0.1, 0.6	Distribution based on Mohanty and Adams (2005).
NFENV	RewettingHumidity[]	Humidity at the waste package surface at which it is assumed that further evaporation is not significant [unitless]	uniform 0.95, 0.98	Distribution based on the exponential decrease in evaporation rate of pure water as a function of increasing relative humidity and decreasing temperature that is predicted using the Stefan's Law (Walton and Kam, 2003).
NFENV	EmplacementBackfill Thickness[m]	Equivalent thickness of emplaced engineered backfill [m]	constant 0.0	Value reflecting the current absence of an engineered backfill design.

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	CircumferentialFractionNotCoveredByFloor[]	f_c Fraction of the circumference of the drift not covered by floor or invert [unitless]	constant 0.75	Approximation based on average drift diameter and invert thickness (Bechtel SAIC Company, LLC, 2005a).
NFENV	DripShieldEqvIntDia[m]	D_{DS} Equivalent diameter of drip shield [m]	constant 2.75	Approximation using design specifications presented in Bechtel SAIC Company, LLC (2005a).
NFENV	WPSpacingAlongEmplacementDrift[m]	Waste package spacing [m]	constant 5.265	Approximation using design specifications presented in Bechtel SAIC Company, LLC (2005a).
NFENV	EmissivityOfDripShield[-]	ϵ_{DS} Emissivity of the drip shield internal surface [unitless]	constant 0.63	Emissivity of titanium based on Bechtel SAIC Company, LLC (2005a).
NFENV	EmissivityOfWastePackage[-]	ϵ_{wp} Emissivity of waste package surface [unitless]	constant 0.87	Emissivity of Alloy 22 based on Bechtel SAIC Company, LLC (2005a).
NFENV	NumberOfWeightsForGaussLegendreIntegration[]	Number of weights for Gauss Legendre integration for computing the potential repository scale temperature [unitless]	constant 20	Code control parameter; best estimate for numerical convergence.
NFENV	ThermalConductivityOfOuterOverpack[W/m-C]	Thermal conductivity of outer container material [W/m-°C]	constant 11.1	Value corresponds to the thermal conductivity of Titanium Grade 7 at 93.33 °C [200 °F] from data in CRWMS M&O (1999).
NFENV	ThermalConductivityOfDripShield[W/(m-C)]	Thermal conductivity of drip shield material [W/m-°C]	constant 20.77	Value corresponds to the thermal conductivity of A316 stainless steel at 100.0 °C [212 °F] (Brandes, 1983; Lyman, et al., 1960).
NFENV	ThermalConductivityOfInnerOverpack[W/m-C]	Thermal conductivity of inner container material [W/m-°C]	constant 15.0	Value corresponds to the thermal conductivity of Alloy 22 at 93.33 °C [200 °F] from data in CRWMS M&O (1999).
NFENV	WPLength[m]	L_{wp} Outer length of the waste package [m]	constant 5.165	Estimated using the range of waste package lengths presented in DOE (2002).
NFENV	WPDiameter[m]	D_{wp} Outer diameter of the waste package [m]	constant 1.659	Estimated using 21 pressurized water reactor and 44 boiling water reactor waste package diameters presented in Bechtel SAIC Company, LLC (2005a).

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EmplacementDriftDiameter[m]	D_{RW} Emplacement drift diameter [m]	constant 5.5	Value based on engineering design specification presented in CRWMS M&O (2000a).
NFENV	DripShieldThickness[m]	t_{DS} Drip shield thickness [m]	constant 0.015	Value based on engineering design specification presented in CRWMS M&O (2000a).
NFENV	EmplacementDriftSpacing[m]	Spacing between drifts [m]	constant 81.0	Value based on engineering design specification presented in CRWMS M&O (2000a).
NFENV	FractionAllowedToDegrade[]	Used only in Thermal Model 1; represents the fraction of the drift allowed to degrade and generate natural backfill [unitless]	constant 0.25	Value represents the elliptical degradation of the drift and the accumulation of rubble on the sides of the drip shield first (Manepally, et al., 2004, 2003).
NFENV	KinematicViscosityOfAir [m^2/s]	Used for iterative thermal calculations only in Thermal Model 2 [m^2/s]	constant 30.95e-6	Value from Incropera and Dewitt (2002). Based on a peak waste package temperature of 165 °C [329 °F] for an intact drift.
NFENV	VolumeOfThermalExpansionOfAir[1/K]	Volume of thermal expansion of air; used for iterative thermal calculations only in Thermal Model 2 [1/K]	constant 2.28e-3	Value determined from Incropera and Dewitt (2002). Based on the assumption that air will behave as an ideal gas.
NFENV	DensityOfAir[kg/m^3]	Used for iterative thermal calculations only in Thermal Model 2 [kg/m^3]	constant 0.797	Value from Table A.4 in Incropera and Dewitt (2002).
NFENV	SpecificHeatOfAir [kJ/kg-K]	Used for iterative thermal calculations only in Thermal Model 2 [kJ/kg-K]	constant 1.019	Value from Table A.4 in Incropera and Dewitt (2002).
NFENV	PrandtlNumberForAir[]	Used for iterative thermal calculations only in Thermal Model 2 [unitless]	constant 0.687	Value from Table A.4 in Incropera and Dewitt (2002).
NFENV	ThermalConductivityOfAir[W/(m-C)]	Thermal conductivity of air at 438 K only in Thermal Model 2 [W/(m-C)]	constant 36.5e-3	Value from Table A.4 in Incropera and Dewitt (2002).
NFENV	EmissivityOfBackfill[]	ϵ_{BF} Emissivity of backfill [unitless]	constant 0.9	Value from Table A.11 in Incropera and Dewitt (2002). Note: The terms backfill and rubble are used interchangeably.

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentI_Fl[mol/L]	Fluoride concentration during Environment I on the drip shield surface [mol/L]	constant 0.00001	Value used in an exploratory model that is available to evaluate the effect of fluoride on corrosion rates in drip shield materials. The model is no longer supported as part of TPA Version 5.1. The parameter value is a legacy from obsolete code (in the reference case, the fluoride corrosion model is not activated).
NFENV	EnvironmentI_Cl[mol/L]	Chloride concentration during Environment I on the waste package surface [mol/L]	constant 1.0	Based on the apparent abundance of corrosion inhibitor species in dusts from the Yucca Mountain vicinity (Dunn, et al., 2005; Browning, et al., 2004).
NFENV	EnvironmentI_pH[]	pH during Environment I on the waste package surface [unitless]	constant 7.0	Based on the apparent abundance of corrosion inhibitor in species dusts from the Yucca Mountain vicinity (Dunn, et al., 2005; Browning, et al., 2004).
NFENV	EnvironmentI_NO3[mol/L]	Nitrate concentration during Environment I on the waste package surface [mol/L]	constant 1.0	Based on the apparent abundance of corrosion inhibitor species in dusts from the Yucca Mountain vicinity (Dunn, et al., 2005; Browning, et al., 2004).
NFENV	EnvironmentI_CO3[mol/L]	Carbonate concentration during Environment I on the waste package surface [mol/L]	constant 0.0	Based on the apparent abundance of corrosion inhibitor species in dusts from the Yucca Mountain vicinity (Dunn, et al., 2005; Browning, et al., 2004).
NFENV	EnvironmentI_SO4[mol/L]	Sulfate concentration during Environment I on the waste package surface [mol/L]	constant 0.0	Based on the apparent abundance of corrosion inhibitor species in dusts from the Yucca Mountain vicinity (Browning, et al., 2004; Dunn, et al., 2005).
NFENV	EnvironmentI_WastePackage_DeltaECrit[VSHE]	Factor that allows for consideration of the increase in the repassivation potential due to secondary factors or unaccounted processes [V _{SHE}]	constant 0.0	Value set to zero to reflect the assumption that the action of secondary processes in increasing the repassivation potential is not considered in the reference case. Value used to construct <i>deltaec.inp</i> for EBSFAIL (Chapter 8).

Table 7-1. Reference Data for Parameters of *tpa.inp* Used by NFENV (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentII_FL Subarea_1[mol/L] EnvironmentII_FL Subarea_2[mol/L] EnvironmentII_FL Subarea_3[mol/L] EnvironmentII_FL Subarea_4[mol/L] EnvironmentII_FL Subarea_5[mol/L] EnvironmentII_FL Subarea_6[mol/L] EnvironmentII_FL Subarea_7[mol/L] EnvironmentII_FL Subarea_8[mol/L] EnvironmentII_FL Subarea_9[mol/L] EnvironmentII_FL Subarea_10[mol/L]	Fluoride concentration during Environment II on the drip shield surface [mol/L]	usersuppliedpwsecdf 25 1.68E-06, 0.0 8.14E-06, 0.041666667 1.11355E-05, 0.083333333 1.79965E-05, 0.125 5.97035E-05, 0.166666667 0.0019405, 0.208333333 0.00034545, 0.25 0.0049711, 0.291666667 0.00887261, 0.333333333 0.034946554, 0.375 0.045923167, 0.416666667 0.050417268, 0.458333333 0.062505976, 0.5 0.06994287, 0.541666667 0.07103854, 0.583333333 0.074881871, 0.625 0.078999899, 0.666666667 0.08071957, 0.708333333 0.081644782, 0.75 0.081850946, 0.791666667 0.08847118, 0.833333333 0.1238553, 0.875 0.2375897, 0.916666667 0.368547279, 0.958333333 0.509481015, 1.0	Distribution derived from process-level numerical simulations of the evaporation of Yucca Mountain pore waters at 110 °C [230 °F]. The derivation approach is detailed in Dunn, et al. (2005). Values used in an exploratory model that is available to evaluate the effect of fluoride on corrosion rates in drip shield materials. The model is no longer supported as part of TPA Version 5.1. The parameter value is a legacy from obsolete code (in the reference case, the fluoride corrosion model is not activated). The same conditional distribution function is assigned to each of the 10 individual <i>tpa.inp</i> parameters listed together here.

Table 7-1. Reference Data for Parameters of <i>tpa.inp</i> Used by NFENV (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentII_Cl Subarea_1[mol/L]	Chloride concentration during Environment II on the waste package surface [mol/L]	usersuppliedpwiseCDF	Distribution derived from process-level numerical simulations of the evaporation of Yucca Mountain pore waters at 110 °C [230 °F]. The derivation approach is detailed in Dunn, et al. (2005). The same conditional distribution function is assigned to each of the 10 individual <i>tpa.inp</i> parameters listed together here.
	EnvironmentII_Cl Subarea_2[mol/L]		25	
	EnvironmentII_Cl Subarea_3[mol/L]		3.964578, 0.0	
	EnvironmentII_Cl Subarea_4[mol/L]		4.052321471, 0.041666667	
	EnvironmentII_Cl Subarea_5[mol/L]		4.115, 0.083	
	EnvironmentII_Cl Subarea_6[mol/L]		4.263, 0.125	
	EnvironmentII_Cl Subarea_7[mol/L]		4.455, 0.167	
	EnvironmentII_Cl Subarea_8[mol/L]		4.674, 0.208	
	EnvironmentII_Cl Subarea_9[mol/L]		4.725, 0.250	
	EnvironmentII_Cl Subarea_10[mol/L]		4.852, 0.292	
	EnvironmentII_Cl Subarea_11[mol/L]		5.301, 0.333	
	EnvironmentII_Cl Subarea_12[mol/L]		5.602, 0.375	
	EnvironmentII_Cl Subarea_13[mol/L]		5.624, 0.417	
	EnvironmentII_Cl Subarea_14[mol/L]		5.745, 0.458	
	EnvironmentII_Cl Subarea_15[mol/L]		5.907, 0.500	
	EnvironmentII_Cl Subarea_16[mol/L]		6.174, 0.542	
	EnvironmentII_Cl Subarea_17[mol/L]		6.387, 0.583	
	EnvironmentII_Cl Subarea_18[mol/L]		6.393, 0.625	
	EnvironmentII_Cl Subarea_19[mol/L]		6.538, 0.667	
	EnvironmentII_Cl Subarea_20[mol/L]		6.810, 0.708	
	EnvironmentII_Cl Subarea_21[mol/L]		6.942, 0.750	
	EnvironmentII_Cl Subarea_22[mol/L]		7.039, 0.792	
	EnvironmentII_Cl Subarea_23[mol/L]		7.116, 0.833	
	EnvironmentII_Cl Subarea_24[mol/L]		7.310, 0.875	
	EnvironmentII_Cl Subarea_25[mol/L]		7.473, 0.917	
	EnvironmentII_Cl Subarea_26[mol/L]		9.088, 0.958	
	EnvironmentII_Cl Subarea_27[mol/L]		10.185, 1.000	

Table 7-1. Reference Data for Parameters of <i>tpa.inp</i> Used by NFENV (continued)				
(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentII_pH_ Subarea_1[]	pH during Environment II on the waste package surface [unitless]	usersuppliedpwisecdf	Distribution derived from process-level numerical simulations of the evaporation of Yucca Mountain pore waters at 110 °C [230 °F]. The derivation approach is detailed in Dunn, et al. (2005). The same conditional distribution function is assigned to each of the 10 individual <i>tpa.inp</i> parameters listed together here.
	EnvironmentII_pH_ Subarea_2[]		25	
	EnvironmentII_pH_ Subarea_3[]		5.8, 0.0	
	EnvironmentII_pH_ Subarea_4[]		6.14875, 0.041666667	
	EnvironmentII_pH_ Subarea_5[]		6.434, 0.083	
	EnvironmentII_pH_ Subarea_6[]		6.887, 0.125	
	EnvironmentII_pH_ Subarea_7[]		7.510, 0.167	
	EnvironmentII_pH_ Subarea_8[]		8.193, 0.208	
	EnvironmentII_pH_ Subarea_9[]		8.446, 0.250	
	EnvironmentII_pH_ Subarea_10[]		8.596, 0.292	
			9.019, 0.333	
			10.139, 0.375	
			10.519, 0.417	
			10.564, 0.458	
			10.631, 0.500	
			10.683, 0.542	
			10.714, 0.583	
			10.725, 0.625	
			10.736, 0.667	
			10.773, 0.708	
			10.803, 0.750	
			10.827, 0.792	
			10.830, 0.833	
			10.844, 0.875	
			10.900, 0.917	
			10.932, 0.958	
			10.950, 1.000	

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentII_NO3_	Nitrate concentration during Environment II on the waste package surface [mol/L]	usersuppliedpwisecdf 25 0.00265, 0.0 0.022, 0.042 0.062, 0.083 0.112, 0.125 0.152, 0.167 0.176, 0.208 0.221, 0.250 0.271, 0.292 0.294, 0.333 0.315, 0.375 0.332, 0.417 0.336, 0.458 0.351, 0.500 0.440, 0.542 0.492, 0.583 0.501, 0.625 0.796, 0.667 1.156, 0.708 1.804, 0.750 2.440, 0.792 2.795, 0.833 3.160, 0.875 3.356, 0.917 3.672, 0.958 4.109, 1.000	Distribution derived from process-level numerical simulations of the evaporation of Yucca Mountain pore waters at 110 °C [230 °F]. The derivation approach is detailed in Dunn, et al. (2005). The same conditional distribution function is assigned to each of the 10 individual tpa.inp parameters listed together here.
	Subarea_1[mol/L]			
	EnvironmentII_NO3_			
	Subarea_2[mol/L]			
	EnvironmentII_NO3_			
	Subarea_3[mol/L]			
	EnvironmentII_NO3_			
	Subarea_4[mol/L]			
	EnvironmentII_NO3_			
	Subarea_5[mol/L]			
	EnvironmentII_NO3_			
	Subarea_6[mol/L]			
	EnvironmentII_NO3_			
	Subarea_7[mol/L]			
	EnvironmentII_NO3_			
	Subarea_8[mol/L]			
	EnvironmentII_NO3_			
	Subarea_9[mol/L]			
	EnvironmentII_NO3_			
	Subarea_10[mol/L]			

Table 7-1. Reference Data for Parameters of *tpa.inp* Used by NFENV (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentII_CO3_ Subarea_1[mol/L] EnvironmentII_CO3_ Subarea_2[mol/L] EnvironmentII_CO3_ Subarea_3[mol/L] EnvironmentII_CO3_ Subarea_4[mol/L] EnvironmentII_CO3_ Subarea_5[mol/L] EnvironmentII_CO3_ Subarea_6[mol/L] EnvironmentII_CO3_ Subarea_7[mol/L] EnvironmentII_CO3_ Subarea_8[mol/L] EnvironmentII_CO3_ Subarea_9[mol/L] EnvironmentII_CO3_ Subarea_10[mol/L]	Carbonate concentration during Environment II on the waste package surface [mol/L]	usersuppliedpwisecdf 25 2.54E-09, 0.0 4.69E-08, 0.042 1.69E-07, 0.083 9.1815E-07, 0.125 3.756E-06, 0.167 1.912E-05, 0.208 0.000421, 0.250 0.000065, 0.292 0.058, 0.333 0.238, 0.375 0.324, 0.417 0.369, 0.458 0.448, 0.500 0.552, 0.542 0.690, 0.583 0.785, 0.625 0.856, 0.667 0.862, 0.708 0.868, 0.750 0.873, 0.792 0.955, 0.833 1.033, 0.875 1.077, 0.917 1.141, 0.958 1.217, 1.000	Distribution derived from process-level numerical simulations of the evaporation of Yucca Mountain pore waters at 110 °C [230 °F]. The derivation approach is detailed in Dunn, et al. (2005). The same conditional distribution function is assigned to each of the 10 individual <i>tpa.inp</i> parameters listed together here.

Table 7-1. Reference Data for Parameters of *tpa.inp* Used by NFENV (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentII_SO4_ Subarea_1[mol/L] EnvironmentII_SO4_ Subarea_2[mol/L] EnvironmentII_SO4_ Subarea_3[mol/L] EnvironmentII_SO4_ Subarea_4[mol/L] EnvironmentII_SO4_ Subarea_5[mol/L] EnvironmentII_SO4_ Subarea_6[mol/L] EnvironmentII_SO4_ Subarea_7[mol/L] EnvironmentII_SO4_ Subarea_8[mol/L] EnvironmentII_SO4_ Subarea_9[mol/L] EnvironmentII_SO4_ Subarea_10[mol/L]	Sulfate concentration during Environment II on the waste package surface [mol/L]	usersuppliedpwiseCDF 25 7.43E-06, 0.0 0.00277, 0.042 0.00117, 0.083 0.0027, 0.125 0.003, 0.167 0.0048, 0.208 0.0073, 0.250 0.0086, 0.292 0.00985, 0.333 0.011, 0.375 0.012, 0.417 0.0125, 0.458 0.013, 0.500 0.0135, 0.542 0.014, 0.583 0.015, 0.625 0.016, 0.667 0.018, 0.708 0.021, 0.750 0.071, 0.792 0.123, 0.833 0.154, 0.875 0.160, 0.917 0.166, 0.958 0.263, 1.000	Distribution derived from process-level numerical simulations of the evaporation of Yucca Mountain pore waters at 110 °C [230 °F]. The derivation approach is detailed in Dunn, et al. (2005). The same conditional distribution function is assigned to each of the 10 individual <i>tpa.inp</i> parameters listed together here.
NFENV	EnvironmentII_ WastePackage_Delta ECrit[VSHE]	Factor that allows for consideration of the increase in the repassivation potential due to secondary factors or unaccounted processes [V_{SHE}]	constant 0.0	Value set to zero to reflect the assumption that the action of secondary processes in increasing the repassivation potential is not considered in the reference case. Value used to construct <i>deltaec.inp</i> for EBSFAIL (Chapter 8).
NFENV	EnvironmentIII_FI[mol/L]	Fluoride concentration during Environment III on the drip shield surface (see page composition) [mol/L]	constant 4.08e-4	Value used in an exploratory model that is available to evaluate the effect of fluoride on corrosion rates in drip shield materials. The model is no longer supported as part of TPA Version 5.1. The parameter value is a legacy from obsolete code (in the reference case, the fluoride corrosion model is not activated).

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentIII_Cl [mol/L]	Chloride concentration during Environment III on the waste package surface (seepage composition) [mol/L]	constant 6.65e-3	Constant value based on the dilute porewater concentrations presented in Yang, et al. (2003, 1998, 1996).
NFENV	EnvironmentIII_pH[]	pH during Environment III on the waste package surface (seepage composition) [unitless]	constant 8.37e0	Constant value based on the dilute porewater concentrations presented in Yang, et al. (2003, 1998, 1996).
NFENV	EnvironmentIII_NO3 [mol/L]	Nitrate concentration during Environment III on the waste package surface (seepage composition) [mol/L]	constant 6.65e-3	Constant value based on the dilute porewater concentrations presented in Yang, et al. (2003, 1998, 1996).
NFENV	EnvironmentIII_CO3 [mol/L]	Carbonate concentration during Environment III on the waste package surface (seepage composition) [mol/L]	constant 2.11e-3	Constant value based on the dilute porewater concentrations presented in Yang, et al. (2003, 1998, 1996).
NFENV	EnvironmentIII_SO4 [mol/L]	Sulfate concentration during Environment III on the waste package surface (seepage composition) [mol/L]	constant 0.0	Constant value based on the dilute porewater concentrations presented in Yang, et al. (2003, 1998, 1996).
NFENV	EnvironmentIII_Wastepackage_Delta ECrit[VSHE]	Factor that allows for consideration of the increase in the repassivation potential due to secondary factors or unaccounted processes [V_{SHE}]	constant 0.0	Value set to zero to reflect the assumption that the action of secondary processes in increasing the repassivation potential is not considered in the reference case. Value used to construct <i>deltaec.inp</i> for EBSFAIL (Chapter 8).
NFENV	SeepageThresholdT[C]	Temperature threshold for seepage for breaching the dryout zone; used to impart a temperature dependence on REFLUX3 results [C]	triangular 100.0, 105.0, 125.0	From information in Basagaoglu, et al. (2007).

Table 7-1. Reference Data for Parameters of *tpa.inp* Used by NFENV (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	FlagSeepageThreshold[]	A flag to activate use of the SeepageThreshold[T][C]; the intent of this flag is to recover previous code computations when desired [unitless]	iflag 1	User option. The seepage threshold temperature is used to introduce a temperature dependence into the REFLUX3 model and avoid the presence of seepage at high temperatures (higher than the seepage threshold temperature). A flag value equal to one is used to activate the seepage threshold temperature concept and a flag equal to zero to activate REFLUX3 without temperature correction as in previous versions of the TPA code (Mohanty, et al., 2002).
NFENV	RelativeHumidityTransitionTimeAfterClosure[yr]	Number of years over which to smooth the transition from preclosure to postclosure relative humidity calculations to avoid abrupt increases caused by change in methodology for estimating relative humidity [yr]	constant 30.0	Control parameter to smooth a spurious peak in the relative humidity curve that is expected to occur 5–10 years after closure. Relative humidity values are expected to be low during the preclosure period, and will drop during the initial part of the postclosure, prior to attainment of peak temperatures. The value of 30 years was determined iteratively to adequately smooth the peak, created by the change in methodology for estimating the preclosure and postclosure relative humidity values.
NFENV	RelativeHumidityForVentilatedAir[]	Constant value of relative humidity for preclosure period with forced ventilation [unitless]	constant 0.3	Constant value set to the approximate annual average relative humidity of air at the ground surface, based on values provided in Bechtel SAIC Company, LLC (2005a).
NFENV	TabularTemperatureRHFlag(yes=1,no=0)	Flag to use <i>tefkti.inp</i> containing four sets of temperature and relative humidity data computed external to TPA Version 5.1 [unitless]	iflag 0	User option. Program control parameter used to select <i>tefkti.inp</i> auxiliary input; see also <code>nsetUsedToPickTempRHDataSet</code> , which selects a particular set within <i>tefkti.inp</i> . When TPA Version 5.1 is run in Monte Carlo mode, use of the external data sets (val=1 setting) makes temperature and relative humidity deterministic.
NFENV	nsetUsedToPickTempRHDataSet	Selects the data set in <i>tefkti.inp</i> that has up to four sets of data (options 1 to 4), when TabularTemperatureRHFlag=1 [unitless]	constant 1	User option. Enables TPA Version 5.1 to bypass the temperature calculation and use an externally generated temperature and relative humidity data set. Temporal output from MULTIFLO (Painter, et al., 2001) is typically used in <i>tefkti.dat</i> .

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	FractionOfCondensate Removed[]	S_{n1} Fraction of water condensate removed in each REFLUX3 timestep (parameter specific to REFLUX3 model) [unitless]	uniform 0.0, 0.25	Distribution representing the fraction of water collecting in reflux zone above drift that is shed laterally and is no longer available for preferential breaching of the dryout zone. The distribution is presented in Hughson (2000).
NFENV	FractionOfCondensate TowardRepository[]	Q_F Fraction of condensate moving toward the potential repository (parameter specific to REFLUX3 model) [unitless]	uniform 0.05, 1.0	Distribution representing the fraction of the water collected in the reflux zone that drains toward the drift opening during the timestep. Distribution based on Hughson (2000).
NFENV	FractionOfCondensate TowardRepository Removed[]	Fraction of condensate moving toward the potential repository but escaped before entering the potential repository (parameter specific to REFLUX3 model) [yr]	constant 0.0	Constant value based on recommended value in Hughson (2000).
NFENV	DensityOfWaterAt Boiling[kg/m^3]	ρ_w Density of water at the boiling point temperature at the potential repository (kg/m ³) (parameter specific to REFLUX3 model) [kg/m ³]	constant 961.0	Value consistent with the potential repository elevation of 1,072–1,101 m [3,517–3,612 ft] and a boiling temperature of 96–97 °C [205–207 °F] using National Institute of Standards and Technology Steam Table Version 2.2 (U.S. Department of Commerce, 1996).
NFENV	EnthalpyOfPhase ChangeForWater[J/kg]	h Enthalpy of phase change for water [J/kg] (parameter specific to REFLUX3 model)	constant 2.67e6	Value consistent with the potential repository elevation of 1,072–1,101 m [3,517–3,612 ft] and a boiling temperature of 96–97 °C [205–207 °F] using National Institute of Standards and Technology Steam Table Version 2.2 (U.S. Department of Commerce, 1996).
NFENV	TemperatureGradientIn VicinityOfBoilingIsotherm [K/m]	∇T Temperature gradient in the vicinity of the boiling isotherm (parameter specific to REFLUX3 model) [K/m]	uniform 1.0, 20.0	Based on MULTIFLO (Painter, et al., 2001) analyses and laboratory-scale experiments. Details are provided in Basagaoglu, et al. (2007).

Table 7-1. Reference Data for Parameters of <i>tpa.inp</i> Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	AmbientRepository Temperature[C]	Ambient potential repository temperature interpolated from estimates of ground surface and water table temperature values used in thermal hydrology models for initial conditions [C]	constant 23.5	Constant value based on information in CRWMS M&O (2001) and Manepally, et al. (2004).
NFENV	MassDensityofYMRock [kg/m ³]	ρ Mass density of rock [kg/m ³]	constant 2166	Average of two values for the <i>tpa.inp</i> parameters RockMassDensityForRockTypeOne[kg/m ³] = 2,139 and RockMassDensityForRockTypeTwo[kg/m ³] = 2,322 (15 percent). Both of these input parameter values are specified in DRIFTFAIL section of <i>tpa.inp</i> .
NFENV	SpecificHeatofYMRock [J/(kg-K)]	Specific heat of rock as in Eq. (7-3) [J/kg-K]	constant 930	Value represents predominant potential repository horizon (Tptpl) and was taken from Bechtel SAIC Company, LLC (2004a).
NFENV	EmissivityOfDriftWall[-]	ϵ_{Wall} Emissivity of drift wall [unitless]	constant 0.9	Value based on data from Incropera and DeWitt (2002) and Bechtel SAIC Company, LLC (2003b).
NFENV	ThermalConductivityOf Floor[W/(m-C)]	k_{inert} Thermal conductivity of floor [W/m-°C]	constant 0.2	Value based on measured values from the Yucca Mountain Program, supported by Incropera and DeWitt (2002) and Bechtel SAIC Company, LLC (2003b).
NFENV	FactorForActive VentilationHeatLosses[]	A factor for reducing the heat load caused by preclosure forced ventilation [unitless]	constant 0.83	Value representing the integrated 50-year average based on Painter, et al. (2001) and Bechtel SAIC Company, LLC (2005b, 2004b).
NFENV	FactorForPassive VentilationHeatLosses[]	Heat loss factor for passive ventilation [unitless]	constant 0.00	Passive ventilation is disabled by using a value of 0.
NFENV	ThermalConductivityOf BackfillModelOne [W/(m-C)]	k_{BF} Effective thermal conductivity of rubble associated with drift degradation; used to approximate conductive, convective, and radiative heat transfer through the rubble in Thermal Model 1 calculations [W/m-°C]	triangular 0.19, 0.27, 1.0	Distribution based on information provided in Bechtel SAIC Company, LLC (2004a), Green, et al. (1997), and Mohanty and Adams (2005).

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	ThermalConductivityOfBackfillModelTwo [W/(m-C)]	Thermal conductivity of the natural rubble associated with drift degradation; used to calculate the heat transfer through the rubble in Thermal Model 2 calculations [W/m-°C]	constant 0.27	Value representing heat transfer solely caused by the heat conduction process within the rubble pile based on Mohanty and Adams (2005).
NFENV	ElevationOfRepository Horizon[m]	Elevation of the potential repository horizon above sea level [m]	constant 1087.0	Value based on information documented in Fedors, et al. (2004).
NFENV	ElevationOfGround Surface[m]	Elevation of ground surface above sea level [m]	constant 1381.0	Value based on information documented in Fedors, et al. (2004).
NFENV	Reflux3Porosity	θ Porosity of rock in dryout zone (TSw) [unitless]	constant 0.14	Value is consistent with calibrated hydrological properties in the Bechtel SAIC Company, LLC (2005a).
NFENV	Reflux3SatInit	S_w Initial saturation of dryout zone rock (TSw) [unitless]	constant 0.9	Value is consistent with representative saturation of matrix in MUTLIFLO models using properties in Bechtel SAIC Company, LLC (2003a).
NFENV	Reflux3SatResid	S_r Residual saturation of dryout zone rock (TSw) [unitless]	constant 0.0	Constant value representing the entire dryout zone based on modeling presented in Manepally, et al. (2004) and Fedors and Painter (2004).
NFENV	ThermalConductivityofYMRock[W/(m-K)]	k Thermal conductivity of rock [W/m-K]	uniform 1.90, 2.30	Value based on Basagaoglu, et al., 2007.
NFENV	OneTemperatureCell PerWP(yes=1,no=0)	Allows user to specify one temperature cell for each waste package rather than for each drift; (0=one cell per drift; 1=one cell per waste package)	constant 0	User option. Each emplacement drift is considered as a line source in the mountain-scale calculation. Computation time will increase exponentially when one cell per waste package is selected (yes =1). The reference case scenario considers one temperature cell per drift.
NFENV	TemperatureReference Point(1=Subarea Centroid,2=UserDefined)[J]	Point at which subarea temperature is calculated	constant 1	User option. Reference case is defined as having subarea centroids as the temperature reference points.

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	UserTemperature ReferencePoint_x[U TM]	Point at which the potential repository temperature is calculated using Universal Transverse Mercator units [m]	constant 548325.0	Value used to represent the center of the large northern portion of the potential repository for heat load determinations—primarily subareas 1, 2, and 3. Only used for user-defined case and when only one subarea has been selected or when one point is representing the entire potential repository midpoint.
NFENV	UserTemperature ReferencePoint_y[U TM]	Point at which the potential repository temperature is calculated using Universal Transverse Mercator units [m]	constant 4080145.0	Value used to represent the center of the large northern portion of the potential repository for heat load determinations—primarily subareas 1, 2, and 3. Only used for user-defined case and when only one subarea has been selected or when one point is representing the entire potential repository midpoint.
NFENV	UserTemperature ReferencePoint_z[m]	Point at which the potential repository temperature is calculated; based on a single quadrilateral approximation to the potential repository footprint; corresponds to a point in the rock matrix above the waste package center line [m]	constant 2.75	Value used to represent the center of the large northern portion of the potential repository for heat load determinations—primarily subareas 1, 2, and 3. Only used for user-defined case and when only one subarea has been selected or when one point is representing the entire potential repository midpoint.
NFENV	BoilingPointOfWater[C]	T _b Boiling point of water °C	constant 97.0	Value consistent with the repository elevation of 1,072–1,101 m [3,517–3,612 ft] using National Institute of Standards and Technology Steam Table 110 °C [230 °F] Version 2.2 (U.S. Department of Commerce, 1996). Used in calculation of the relative humidity.
EBSFAIL	OuterInhibitingNitrateToCl	r _n Nitrate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential of the mill-annealed region of the outer container [unitless]	constant 0.1	Below this parameter value, the repassivation potential is assumed to increase linearly with the ratio of nitrate-to-chloride molar concentration up to OuterDeltaECritln[mV]. Above this parameter value, the increase in the critical potential is assumed to remain constant equal to OuterDeltaECritln[mV]. The parameter value is given based on the critical potential model described in Dunn, et al. (2006, 2005).

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	OuterInhibitingCarbonateToCl	r_c^c Carbonate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential of the mill-annealed region of the outer container [unitless]	constant 0.2	Below this parameter value, the repassivation potential is assumed to increase linearly with the ratio of carbonate-to-chloride molar concentration up to OuterDeltaEcritInh[mV]. Above this parameter value, the increase in the critical potential is assumed to remain constant equal to OuterDeltaEcritInh[mV]. The parameter value is given based on the critical potential model described in Dunn, et al. (2006, 2005).
EBSFAIL	OuterInhibitingSulfateToCl	r_s^s Sulfate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential of the mill-annealed region of the outer container [unitless]	constant 0.5	Below this parameter value, the repassivation potential is assumed to increase linearly with the ratio of sulfate-to-chloride molar concentration up to OuterDeltaEcritInh[mV]. Above this parameter value, the increase in the critical potential is assumed to remain constant equal to OuterDeltaEcritInh[mV]. The parameter value is given based on the critical potential model described in Dunn, et al. (2006, 2005).
EBSFAIL	WeldCritChlorideConc [mol/L]	Critical chloride concentration for the localized corrosion initiation for the welded region of the outer container [mol/L]	constant 1.0e-3	Dunn, et al. (2005, Figure 4-6) reported localized corrosion in solutions containing chloride at a concentration as low as 1.0×10^{-3} mol/L at 95 °C [203 °F] in welded plus solution annealed material. Because critical chloride threshold does not appear to be well defined, a low value of the critical chloride concentration is adopted.
EBSFAIL	WeldInhibitingNitrateToCl	r_n^n Nitrate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential for the welded region of the outer container [unitless]	constant 0.3	The parameter value is based on the critical potential model described in Dunn, et al. (2006, 2005).

Table 7-1. Reference Data for Parameters of tpa.inp Used by NFENV (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	WeldInhibitingCarbonateToCl	r_c^c Carbonate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential for the welded region of the outer container [unitless]	constant 0.2	The parameter value is based on the critical potential model described in Dunn, et al. (2006, 2005).
EBSFAIL	WeldInhibitingSulfateToCl	r_s^s Sulfate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential for the welded region of the outer container [unitless]	constant 0.5	The parameter value is based on the critical potential model described in Dunn, et al. (2006, 2005).
EBSFAIL	CriticalRelativeHumidityAqueousCorrosion	Critical relative humidity above which aqueous corrosion will initiate [unitless]	constant 0.2	This parameter controls the onset of aqueous corrosion. Recent studies show that aqueous corrosion can take place in elevated temperature and low relative humidity systems (Yang, 2006). Deliquescent multicomponent salt systems have been reported that can form liquid solutions at temperatures as high as 200 °C [392 °F] or above (Rard, et al., 2006). The parameter CriticalRelativeHumidityAqueousCorrosion indirectly controls the maximum extrapolation temperature for corrosion rates of the waste package. The parameter value of 0.2 is consistent with experimental data by Rard, et al. (2006) and high enough to avoid extrapolation of aqueous corrosion rates to extreme temperatures, where long-term corrosion rates are highly uncertain.
EBSFAIL	CritChlorideConcForFirstLayer[mol/L]	$[Cl^-]_{crit}$ Critical chloride concentration for localized corrosion initiation for the mill-annealed region of the outer container [mol/L]	constant 1.0e-3	Dunn, et al. (2005, Figure 4-6) reported localized corrosion in solutions containing chloride ions at a concentration of 0.05 mol/L at 95 °C [203 °F] in mill-annealed Alloy 22. Because critical chloride threshold does not appear to be well defined, a low value of critical chloride concentration is adopted.

Table 7-2. Auxiliary Input Data Files Used by NFENV

File	Contents
<i>drythick.dat</i>	The reference data set in TPA Version 5.1 defines the time-series dryout zone thickness data for the nominal (degraded) and intact drift geometries. This auxiliary input file contains information organized by sections. The end of thermal pulse section contains the end of the thermal pulse in years which is used to determine whether the degraded scenario dryout zone thicknesses are used {for periods before timePulseEnd[]} or the nondegraded zone thicknesses are used {for periods after timePulseEnd[]}. It also contains the number of entries for the time-dependent dryout zone thickness. The dryout zone thickness for a degraded drift section contains the time-dependent dryout zone thickness for a degraded drift based on process-level model results. The nondegraded drift section contains the number of entries for the nondegraded drift dryout thickness and the dryout zone thickness for an intact drift section contains the time-dependent dryout zone thickness for an intact drift based on process-level model results.
<i>tefkti.inp</i>	The <i>tefkti.inp</i> file contains user-defined temperature and relative humidity data at the waste package and drift wall as a function of time. The number of entries for each data set is specified at the beginning of each data set. Current values in <i>tefkti.inp</i> are based on detailed process-level model results for a degraded drift and intact drift described in Manepally, et al. (2004).

Table 7-3. Intermediate Output Files Created During Execution of NFENV

Output File	Contents
<i>nearfld.res</i>	Reports waste package temperature, relative humidity, and chloride concentration averaged for all subareas for every 10 th timestep. See Chapter 19 for further details.
<i>fluoride.dat</i>	NFENV contributes to this primary output file (Chapter 19), which reports fluoride concentration for all times.
<i>reflux3.out</i>	Reports output from NFENV module including infiltrated water volume from ground surface per unit waste package area, thickness and the equivalent thickness of the fractured porous medium between the boiling isotherm and the drift, penetration distance of the reflux water, water volume available in the condensate zone for reflux, the total water losses in the dryout zone, and the volumetric flow rate per unit waste package area from the condensate zone after removing the water losses due to shedding and lateral flows.
<i>thermal.dbg</i>	Reports time, drip shield temperature, waste package temperature, rubble temperature, rubble thickness, and conductance of different legs modeled in Thermal Mode 1 and 2 for a subarea at the end of each realization. For simulations involving more than one realization, the results for the last subarea of the last realization is recorded in this file.

Table 7-4. Optional Intermediate Output Files Created During Execution of NFENV

Output File	Contents
<i>nfenv.ech</i>	This optional output file gives timestep and flow rate approaching the drift per waste package length for each subarea at all times.
<i>nfenv.rlt</i>	This optional output file gives rock wall temperature, drip shield temperature, waste package temperature, relative humidity, pH value, and chloride, carbonate, nitrate, and sulfate concentrations for each subarea at all times.

The user should be aware that setting OutputMode(0=Name,1=All,2=UserDefined) to 1 will also cause intermediate output files to be written for numerous other modules when the parameter SelectAppendFiles remains set at the default value of 0. Some of these files can be very large and can quickly fill up available storage if all intermediate outputs are specified for all realizations. Therefore, when the user is interested only in NFENV intermediate outputs, the SelectAppendFiles parameter in the <<Output Print Options>> input block should be set to a value of 2 for just *nfenv.ech* and *nfenv.rlt*.

7.7 Techniques for Understanding Module Performance

While there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of processes modeled by NFENV. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques may be useful to understand the effects of near-field processes on system-level performance.

In addition, pinch-point techniques, wherein output or intermediate results produced from NFENV can be understood in combination with output or intermediate results from other modules (e.g., DRIFTFAIL) may help to better evaluate subsystem processes. Key output files and intermediate result files useful for these comparisons include *nfenv.rlt* and *thermal.dbg*. These files provide values calculated by NFENV that include (i) temperature at the waste package, drip shield, and outer and inner surfaces of the rubble; (ii) relative humidity at the waste package; (iii) quantity of water that could contact the engineered barrier system; and (iv) seepage water chemistry (a detailed discussion follows).

Further, single parameter importance analyses can be performed by repetitively varying input parameters associated with particular subsystem processes and analyzing output and intermediate results from various consequence modules, as mentioned previously. Single parameter importance analyses could be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, a single parameter importance analysis could be performed by repetitively specifying smaller ranges within the parameter's original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges. The user should exercise care in interpreting results from simulations in which input is altered beyond its intended range. A key NFENV parameter that can influence dose calculations is ThermalConductivityofYMRock[W/m-K].

The effect of drift degradation on the temperature field can be examined by changing the DriftDegradationScenarioFlag[] in *tpa.inp*. The resulting output files could help the user understand the effect of degradation on temporal variation of temperature. Temperature variation of the waste package with different rubble thickness can be investigated by varying the fraction of the drift that is allowed to degrade. The rate of degradation is determined in DRIFTFAIL. The *tpa.inp* parameter FractionAllowedToDegrade[] can be varied to change the amount of rubble that accumulates on the drip shield.

Some of the user options available in calculation of the drift wall temperature include

- The thermal line sources in the analytical model (Eq. 7-1) can be used to represent each waste package instead of a drift by selecting a value of one for the *tpa.inp* parameter OneTemperatureCellPerWP(yes=1,no=0). Note that the computation time will increase exponentially when one cell per waste package is selected (yes=1).
- Alternate locations of the temperature calculation (i.e., x, y, and z) in Eq. (7-1) for the reference case can be specified by selecting a value of 2 for the *tpa.inp* parameter TemperatureReferencePoint(1=SubareaCentroid,2=UserDefined). The new location is specified by UserTemperatureReferencePoint_x[UTM],

UserTemperatureReferencePoint_y[UTM], and UserTemperatureReferencePoint_z[m]. This option is available when only one subarea has been selected or when one point represents the entire potential repository midpoint.

Further parametric study can be conducted by varying physical properties using the *tpa.inp* parameters ThermalConductivityofYMRock[W/m-K], ThermalConductivityofAir[W/(m-C)], and ThermalConductivityofFloor[W/(m-C)]. These parameters have a direct impact on the calculated drift wall, waste package, and drip shield temperatures. The temperature and relative humidity values in the auxiliary file *tefkti.inp* (Section 7.5) can also be modified to investigate the effect of temperature on chemistry and corrosion processes.

The abstraction of the chemistry of water in contact with the waste package was developed to support the corrosion model described in Chapter 8. Therefore, changes in chemical compositions directly affect the onset of localized corrosion of the waste package. Localized corrosion can be deactivated by reducing the chloride concentrations in Environment II {e.g., *tpa.inp* parameter EnvironmentII_Cl_Subarea_1[mol/L]} to concentrations less than *tpa.inp* parameters CritChlorideConcForFirstLayer[mol/L] and WeldCritChlorideConc[mol/L]. These parameters represent minimal chloride concentrations for the onset of localized corrosion on the mill-annealed and welded areas of the waste package, respectively, and are explained in Chapter 8. Similarly, localized corrosion can be deactivated by setting the *tpa.inp* parameters CritChlorideConcForFirstLayer[mol/L] and WeldCritChlorideConc[mol/L] to a high value (a value of 100 is sufficiently high). Alternatively, localized corrosion can be disabled by selecting high concentrations of the oxyanions nitrate and bicarbonate {e.g., EnvironmentII_NO3_Subarea_1[mol/L], EnvironmentII_CO3_Subarea_1[mol/L]}. By comparing runs of the reference case to runs in which localized corrosion is deactivated, insight can be gained on the effects of seepage chemistry in determining the significance of localized corrosion.

It is difficult to define a single water composition (i.e., a feasible combination of pH, chloride, and oxyanion concentrations) as representative of possible water compositions contacting waste packages in a single realization. To overcome this difficulty, water compositions for Environment II (compositions potentially conducive to localized corrosion) are sampled independently per subarea to incorporate expected stochastic variability. The effect of stochastic variability on TPA Version 5.1 results can be studied, to a limited extent, by correlated sampling among subareas. For example, if the user wants to define a single water pH for the whole potential repository in a realization, correlations such as the following can be defined in *tpa.inp*:

```
correlateinputs
EnvironmentII_pH_Subarea_1[]
EnvironmentII_pH_Subarea_3[]
0.9999
**

correlateinputs
EnvironmentII_pH_Subarea_1[]
EnvironmentII_pH_Subarea_4[]
0.9999
**
```

For the correlation algorithm of TPA Version 5.1 to properly function, all of the binary correlations among subareas must be specified. For example, if pH_1 , pH_2 , and so on, are pH values per subarea, and if it is desired to sample similar values for all subareas, then all of the entries above the diagonal in the matrix in Figure 7-7 must be specified as correlations in *tpa.inp*.

	pH_1	pH_2	pH_3	...	pH_N
pH_1	1	0.9999	0.9999	...	0.9999
pH_2		1	0.9999	...	0.9999
pH_3			1	...	0.9999
$\vdots$				$\ddots$	$\vdots$
pH_N					1

Figure 7-7. Correlations That Must Be Specified in *tpa.inp* for Similar Values of the pH To Be Sampled for All Subareas

7.8 References

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8 DRIP SHIELD AND WASTE PACKAGE CORROSION FAILURE (DSFAIL AND EBSFAIL)

The Drip Shield Corrosion Failure module (DSFAIL)¹ is used to calculate the time-dependent drip shield thickness and the failure time of the drip shield due to corrosion. The calculated output from DSFAIL is passed to the Drip Shield and Waste Package Mechanical Failure module (MECHFAIL)² (Chapter 9) for calculating mechanical failure of the drip shield and mechanical interactions between the drip shield and waste package. DSFAIL also passes calculated outputs to the Engineered Barrier System Radionuclide Release module (EBSREL)³ (Chapter 10) for source term computations. DSFAIL is executed for each subarea in each realization of the reference case simulation.

The Engineered Barrier System Corrosion Failure module (EBSFAIL)⁴ is used to calculate the time-dependent waste package thickness and the failure time of the waste packages caused by various modes of corrosion. EBSFAIL receives time-dependent in-drift environmental conditions as calculated in the Near-Field Environment module (NFENV)⁵ (Chapter 7). EBSFAIL passes the time of breaching of the waste package to EBSREL for source term computations. In addition, EBSFAIL provides the remaining waste package thickness as a function of time to MECHFAIL to compute of waste package and drip shield mechanical interactions. EBSFAIL is executed for each subarea in each realization of the reference case simulation.

8.1 Conceptual Model

Two components of the expected engineered barrier system are the drip shield and the waste package. In conjunction with the natural barriers, this system can contain the release of radionuclides to the biosphere from the potential repository. In the potential repository in-drift environment, the waste package and drip shield can degrade and fail as a result of various corrosion processes that are triggered by material, environmental, and electrochemical conditions. The conceptual models of these corrosion processes for the drip shield and the waste package are described as follows.

¹The Drip Shield Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation DSFAIL will be used.

²The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAIL will be used.

³The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

⁴The Engineered Barrier System Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

⁵The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

8.1.1 Drip Shield Corrosion

The drip shield is expected to be an inverted U-shaped metallic structure made of titanium alloys and designed to protect the waste packages from water seepage and rockfall (DOE, 2002). The drip shields extend over the length of the emplacement drift, enclosing the top and sides of the waste packages. In DSFAIL, general corrosion under passive conditions, established by the existence of a protective titanium oxide film on the metal surface, is modeled as the only corrosion mode affecting the integrity of drip shield.

8.1.2 Waste Package Corrosion

The waste package design in the U.S. Department of Energy (DOE) site recommendation (DOE, 2002) consists of an outer container made of mill-annealed Alloy 22, a corrosion-resistant nickel-chromium-molybdenum alloy, and an inner container made of Type 316 nuclear grade stainless steel. Because welds are expected to be used for fabrication and closure of the outer container (Bechtel SAIC Company, LLC, 2001a,b), EBSFAIL allows two different materials with different metallurgical parameters to be modeled in the outer container. In the reference case, these two metallurgical conditions correspond to mill-annealed and welded Alloy 22. Corrosion of the welded material is treated in parallel with corrosion of the mill-annealed Alloy 22 in EBSFAIL. The waste package is considered to be breached when either the welded or mill-annealed regions of the outer container are thin enough to meet the user-specified failure criterion. Corrosion of the inner container material is not considered in TPA Version 5.1.

The following corrosion processes for the waste package outer container are modeled in EBSFAIL: dry-air oxidation, humid-air corrosion, aqueous corrosion in the form of general (uniform) corrosion or localized (crevice) corrosion, thermal embrittlement, radiolysis, and galvanic coupling. Both general corrosion and localized corrosion are treated separately and counted as two separate modes of corrosion under the aqueous corrosion process. In EBSFAIL, the initiation time of a corrosion model is determined by the relative humidity of the in-drift environment, which is provided by NFENV. The last three corrosion models—thermal embrittlement, radiolysis, and galvanic coupling—are legacy models and are no longer supported in TPA Version 5.1.

8.2 Model Support and Assumptions

8.2.1 Drip Shield Corrosion

In DSFAIL, general corrosion under passive conditions, established by the presence of a protective oxide layer on the metal surface, is considered to be the only corrosion mode for the drip shield. It is assumed that both the outer and underside of the drip shield are in contact with the same environment and, therefore, undergo general corrosion at the same rate. DSFAIL applies a time-invariant general corrosion rate under passive conditions (i.e., the surface is assumed to be protected with a corrosion-resistant oxide film). DSFAIL assumes that the corrosion rate remains unchanged for the entire simulation. The corrosion front is assumed to advance perpendicularly to the drip shield surface. DSFAIL assumes that the corrosion mode and corrosion rate are independent of the environment surrounding the drip shield, and corrosion initiates immediately after repository closure.

Several studies suggest that hydrogen embrittlement, stress corrosion cracking, and localized corrosion are expected to have a negligible influence on the drip shield integrity in the repository drift environment (Fix, et al., 2004; Qin and Shoesmith, 2004; Schutz, 2005, 1992). Therefore, localized corrosion, hydrogen embrittlement, and stress corrosion cracking are not included in DSFAIL.

A demonstration model for enhanced drip shield corrosion caused by fluoride ions was developed after TPA Version 4.0 (Mohanty, et al., 2000). However, it is not supported in TPA Version 5.1. The presence of calcium in seepage water is likely to cause precipitation of fluoride at high temperature due to evaporation. Thus, amounts of soluble fluoride are expected to be too small to enhance corrosion of the drip shield (Lin, et al., 2003; Codell and Leslie, 2006). Furthermore, fluoride ion concentrations do not appear to alter the crevice corrosion resistance of titanium alloys. Schutz and Grauman (1986) suggested that at low concentrations, fluoride did not affect the repassivation potentials for different titanium alloys.

8.2.2 Waste Package Corrosion

In EBSFAIL, dry-air oxidation, humid-air corrosion, and aqueous corrosion in the form of general corrosion under passive conditions and localized corrosion are considered to be the predominant chemical degradation models for the waste package outer container. EBSFAIL assumes that the rate of different corrosion processes (i.e., dry-air oxidation, humid-air corrosion, general and localized corrosion) is the same for both mill-annealed and welded Alloy 22. It also assumes that all corrosion processes propagate in the direction perpendicular to the waste package surface.

EBSFAIL assumes that aqueous corrosion of the waste package outer container initiates above a humidity threshold and at temperatures above the boiling point of seepage water. Therefore, the abstraction assumes a low value of relative humidity, marking a transition from humid-air to aqueous corrosion. Recent studies suggest that salt mixtures containing nitrate anions could deliquesce (Rard, et al., 2006) in a low humidity environment. Experimental studies have suggested that deliquescence brines formed at higher temperatures ranging from 140 to 180 °C [284 to 356 °F] could induce general corrosion on the Alloy 22 (Yang, 2006).

Spatial and temporal variations in the chemistry of the water exist that may affect the general corrosion rate. EBSFAIL assumes that the general corrosion rate is independent of the in-drift chemical environment, but is dependent on the waste package surface temperature.

EBSFAIL assumes that the corrosion potential of the mill-annealed and welded Alloy 22 is affected by the waste package surface temperature, the concentration of dissolved oxygen, and the pH of in-drift water contacting the waste package surface. The corrosion potential of mill-annealed and welded Alloy 22 is computed using a semi-empirical equation derived using electrochemical kinetic rate models for anodic and cathodic reactions. The corrosion potential model is consistent with measurements up to 95 °C [203 °F] in a fully immersed electrolyte (Dunn, et al., 2005). The semi-empirical equation for the corrosion potential model is used to extrapolate the corrosion potential at temperatures higher than 95 °C [203 °F]. It is assumed that as long as there is an aqueous phase, the kinetic rate models for anodic and cathodic reactions remain valid.

The predominant cathodic reaction expected to affect the corrosion potential is the oxygen reduction reaction. In acidic solutions, it is assumed that the contribution of the hydrogen evolution reaction is negligible compared to the oxygen reduction contribution. This is justifiable because the equilibrium potential of the hydrogen evolution reaction is expected to be much lower than that of the oxygen reduction reaction (Bard and Faulkner, 1980, Table C.I). Similarly, the contribution of the water reduction reaction to the cathodic current is neglected in neutral-to-alkaline solutions in the reference case.

EBSFAIL does not account for variations in the corrosion potential due to changes in the dissolved oxygen concentration. The presence of dissolved salts in the seepage water is likely to reduce the dissolved oxygen concentration compared to that in pure water under the same pressure and temperature (Tromans, 2000). This phenomenon is known as the salting-out effect. The reduced quantity of dissolved oxygen is likely to lower the corrosion potential compared to the values estimated by the model implemented in TPA Version 5.1. The inclusion of the salting-out effect can decrease the likelihood of localized corrosion.

In EBSFAIL, the corrosion potential model can account for the presence of a thin water film or salt scale that can form on the waste package surface during seepage. It is assumed that salt scales are porous, and seepage water is present in the pores of the salt scale. It is further assumed that the dissolved oxygen in seepage water solution diffuses through the pores of salt scales and reacts at the metal–film interface. Therefore, water film or salt scale act as a diffusion barrier for the oxygen reduction reaction.

Localized corrosion of metals and alloys can occur in the form of pitting or crevice corrosion. Pitting corrosion of the waste package is not considered in EBSFAIL due to the low propensity of highly corrosion-resistant materials such as Alloy 22 to experience this form of corrosion (Cragnolino, et al., 1999; Gdowski, 1991). EBSFAIL assumes that localized corrosion (in the form of crevice corrosion) instantaneously initiates when the corrosion potential exceeds the critical potential for localized corrosion. Once initiated, crevice corrosion is assumed to propagate (He and Dunn, 2005) unless the condition for initiation is reversed. EBSFAIL assumes that the crevice corrosion penetration rate is a linear function of time for both mill-annealed and welded Alloy 22. The experimentally determined crevice growth rate of mill-annealed Alloy 22 (He and Dunn, 2005) suggests that the penetration rate decreases with time. Therefore, the crevice penetration rate implemented in the module is expected to overestimate the penetrated depth of the waste package due to localized corrosion. The general corrosion of the outer container is suppressed when localized corrosion is activated. The possibility of repassivation of the crevice region is not taken into account in EBSFAIL unless conditions for initiation are reversed (e.g., the corrosion potential drops below the critical potential).

Three additional corrosion models—thermal embrittlement, radiolysis, and galvanic coupling—are also available in EBSFAIL. Mechanical failure caused by thermal embrittlement is not expected to be a feasible mode of failure for Alloy 22 because of the high ductility of this material (ASME, 1995). Similarly, radiation levels are expected to be too low to have any effect on the corrosion potential of Alloy 22 (Shoesmith and King, 1999; CRWMS M&O, 2001a,b). In addition, the galvanic coupling of the Alloy 22 outer container and the Type 316 nuclear grade stainless steel inner container does not occur because corrosion of the inner container is not modeled, and therefore, the inner container does not exist in EBSFAIL.

In EBSFAIL, stress corrosion cracking of outer container materials, mill-annealed and welded Alloy 22, is not considered. The rationale for neglecting this corrosion mode is provided in Chiang, et al. (2007).

Only one waste package per subarea is simulated in EBSFAIL using the corrosion modes described here. When the representative waste package is breached by corrosion, an ensemble of intact waste packages in a subarea is also assumed to breach, potentially allowing water to contact the waste form. The number of waste packages affected by corrosion that releases radionuclides is determined by EBSREL.

8.3 Implementation of Conceptual Model in TPA Version 5.1

The implementation of abstracted corrosion models for the drip shield and the waste packages is described in this section. The abstracted general corrosion model for the drip shield is implemented in the DSFAIL and the abstracted corrosion models for the waste package are implemented in EBSFAIL.

8.3.1 Drip Shield Corrosion

DSFAIL obtains the general corrosion rate, DripShieldCorrosionRate[m/yr], from *tpa.inp*. DSFAIL calculates the remaining thickness of the drip shield as a function of emplacement time and the breaching time. The breaching time corresponds to the emplacement time when the penetrated depth normalized with respect to initial thickness exceeds the *tpa.inp* parameter DSFractionThicknessPenetratedForFailureByCorrosion[]. The flow of information through DSFAIL is illustrated in Figure 8-1. DSFAIL obtains the drip shield corrosion-related input parameters from *tpa.inp*. DSFAIL integrates the corrosion rate with elapsed time until the end of realization. The remaining (uncorroded) drip shield thickness as a function of emplacement time and the breaching time is provided to MECHFAIL. The drip shield breaching time is provided to EBSREL.

8.3.2 Waste Package Corrosion

The abstracted corrosion models for the waste packages are described in this section. The abstracted models of dry-air oxidation, humid-air corrosion, and aqueous corrosion in the form of general and localized corrosion were developed for mill-annealed and welded Alloy 22. EBSFAIL calculates the outer container remaining thickness and breaching time for both mill-annealed and welded regions of the outer container. The breaching time is defined when the fractions of the waste package outer container wall thickness and weld thickness penetrated by the corrosion front exceed the *tpa.inp* parameters WPFractionThicknessPenetratedForFailureByCorrosion[] and WPWeldFractionThicknessPenetratedForFailureByCorrosion[] for mill-annealed and welded regions, respectively.

In the potential repository environment, the waste package surface temperature is expected to initially increase after repository closure and decrease thereafter due to decay of the waste form heat source. As a result, the relative humidity in the in-drift environment is expected to increase as the waste package surface temperature decreases. When the relative humidity is less than the critical relative humidity for humid-air corrosion (denoted by RH1 in Figure 8-2 and defined by the *tpa.inp* parameter CriticalRelativeHumidityHumidAirCorrosion), the waste package

surface is dry and the dry-air oxidation is the only corrosion process considered. When the in-drift environment relative humidity becomes greater than the critical relative humidity for humid-air corrosion (denoted by RH1 in Figure 8-2) but less than the critical relative humidity for aqueous corrosion (denoted by RH2 in Figure 8-2 and defined by the *tpa.inp* parameter CriticalRelativeHumidityAqueousCorrosion), the humid-air corrosion is the only corrosion mode considered. When the relative humidity in the in-drift environment exceeds the critical relative humidity for aqueous corrosion (denoted by RH2 in Figure 8-2), aqueous corrosion is the dominant corrosion mode. Aqueous corrosion is either general or localized corrosion. Other in-drift environmental conditions, which include the waste package surface temperature, pH,

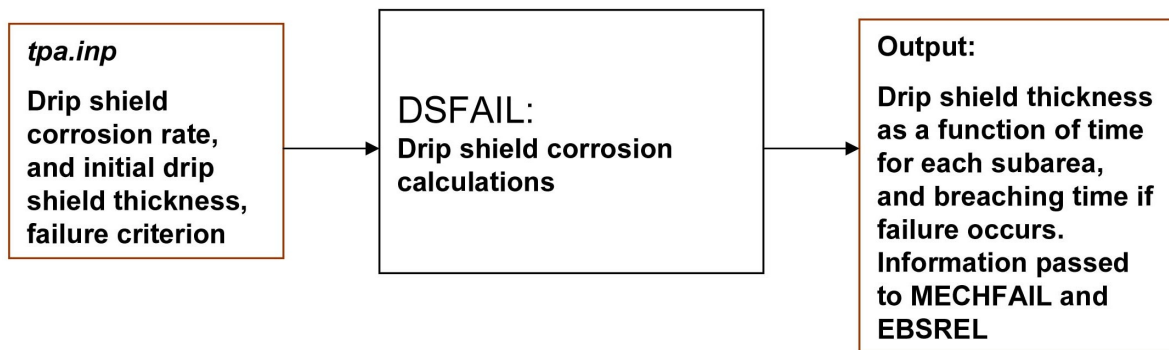


Figure 8-1. Information Flow Diagram for DSFAIL

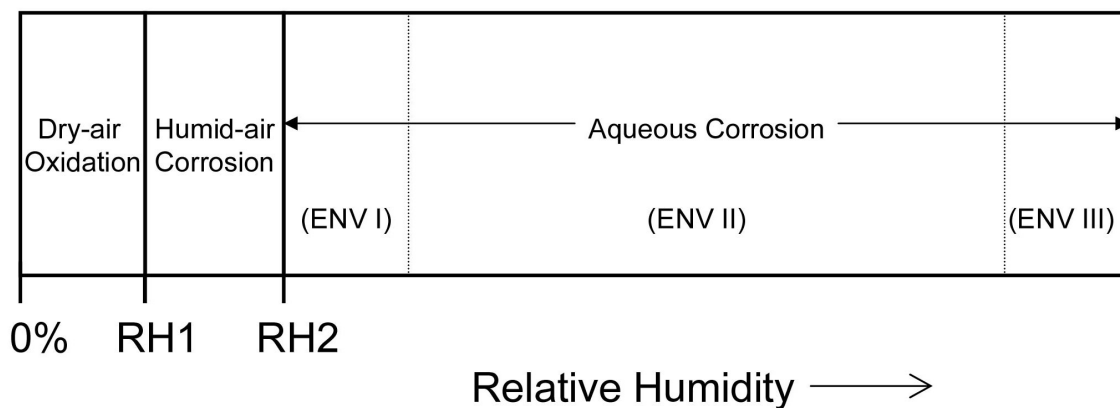


Figure 8-2. Implementation of Different Corrosion Modes in EBSFAIL

and the chemical composition of the water contacting the waste package, are used to compute the initiation condition for the occurrence of localized corrosion and the rate of aqueous corrosion. Localized corrosion is possible in the environment classified as ENV II (as shown in Figure 8-2) by NEFNV. The necessary conditions for localized corrosion initiation require that chloride concentration be greater than a critical value in the seepage water and the corrosion potential be higher than the critical potential for localized corrosion. If such conditions exist, localized corrosion is activated; otherwise, general corrosion is the predominant aqueous corrosion process degrading the waste package.

The corrosion rate of various corrosion modes (dry-air oxidation, humid-air corrosion, general and localized aqueous corrosion) is integrated over the elapsed time to compute the penetration depth of the corrosion front as a function of emplacement time. The flow of information through EBSFAIL is illustrated in Figure 8-3. EBSFAIL obtains the waste package corrosion-related input parameters from *tpa.inp* and near-field environment conditions from NFENV. EBSFAIL integrates the corrosion rate with elapsed time. Three outputs are generated by EBSFAIL: (i) the uncorroded thickness (initial thickness minus corroded depth) of the mill-annealed Alloy 22 waste package surface excluding localized corrosion, (ii) the uncorroded thickness of the mill-annealed Alloy 22 waste package surface including localized corrosion, and (iii) the uncorroded thickness of the weld areas of the waste package. If the ratio of penetrated depth to the initial thickness of the mill-annealed Alloy 22 outer container wall {OuterWPThickness[m]} and welded region thickness {WPWeldThickness[m]} exceeds user-defined fractions {WPFractionThicknessPenetratedForFailureByCorrosion[]} (for the mill-annealed region) or WPWeldFractionThicknessPenetratedForFailureByCorrosion[] (for the welded region) the waste package is considered to be breached. The time of failure corresponding to the three outputs is passed to EBSREL. In addition, the uncorroded outer container thickness as a function of emplacement time from output (i) is passed to MECHFAL.

The abstracted corrosion models for dry-air oxidation, humid-air corrosion, general corrosion, and localized corrosion are discussed in following four sections. In addition, three other potential waste package degradation processes—thermal embrittlement, radiolysis, and galvanic coupling—are also briefly described in Section 8.3.2.5. These are legacy models and

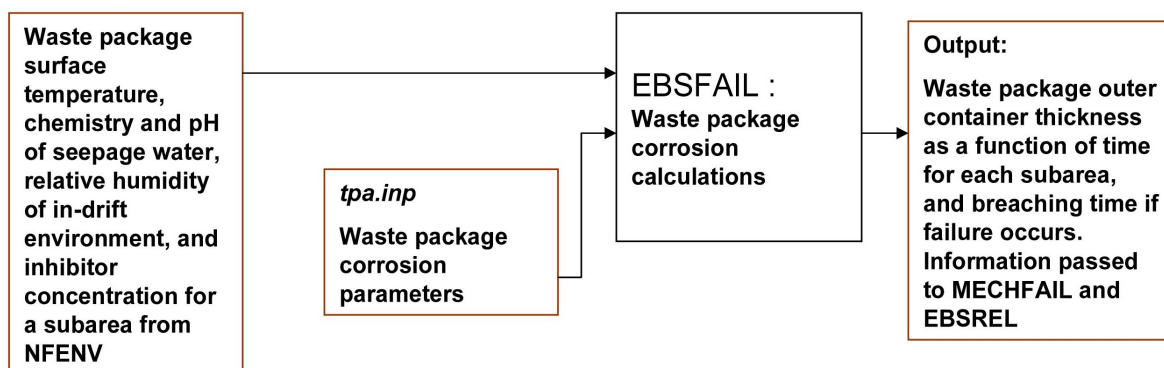


Figure 8-3. Information Flow Diagram for EBSFAIL

are no longer supported in TPA Version 5.1. A brief description of these three models and associated parameters is provided in this chapter, and additional details can be found in TPA Version 4.0 (Mohanty, et al., 2000).

8.3.2.1 Dry-Air Oxidation

EBSFAIL applies the dry-air oxidation to waste packages by considering interaction with gaseous oxygen present in air at the high temperatures and low relative humidity environment prevailing initially in the repository drift. The dry-air oxidation abstraction is implemented when the relative humidity of the air surrounding the waste packages is less than the value specified by the parameter CriticalRelativeHumidityHumidAirCorrosion (denoted by RH1 in Figure 8-2) in *tpa.inp*. The penetration depth of the oxidation front in the metal along grain boundaries at time, t , is computed by the following expression

$$Y_p = \left[\frac{4D_l}{r_g \delta D_g} \sum_{n=1}^{\infty} \exp\left(-\frac{D_l n^2 \pi^2 t}{r_g^2}\right) \right]^{-1/2} \quad (8-1)$$

where

- Y_p — penetration depth by intergranular oxidation [cm]
- D_l — matrix diffusivity [cm²/s]
- D_g — grain boundary diffusivity [cm²/s]
- δ — the thickness of grain boundary [cm], as specified by the *tpa.inp* parameter GrainBoundaryThickness[micrometer]
- r_g — the grain radius [cm], as specified by the *tpa.inp* parameter MetalGrainRadius[micrometer]
- t — time [s]

The following equation is used to calculate D_l in TPA Version 5.1

$$D_l = 5.75 \times 10^{-6} \exp\left(-\frac{169}{RT}\right) \quad (8-2)$$

where

- T — waste package surface temperature [K] as provided by NFENV
- R — universal gas constant = 8.3145 J/K/mol

In TPA Version 5.1, D_l/D_g is specified as DryOxidationConstant in *tpa.inp*. The value of D_g is internally calculated using Eq. (8-2) and the ratio D_l/D_g , which is then used in Eq. (8-1) to calculate the dry-air oxidation rate. Additional information on the dry-air oxidation model abstraction can be found in Mohanty, et al. (2000).

8.3.2.2 Humid-Air Corrosion

The humid-air corrosion model is activated when the relative humidity of the repository in-drift environment is above a critical value (denoted by RH1 in Figure 8-2), defined by the *tpa.inp* parameter CriticalRelativeHumidityHumidAirCorrosion. The corrosion rate is set by the *tpa.inp*

parameter HumidAirCorrosionRate[m/yr]. The humid-air corrosion rate is assumed to be independent of temperature and time, and is applied to both mill-annealed and welded Alloy 22.

8.3.2.3 General Corrosion

EBSFAIL considers that aqueous corrosion of the waste package initiates when the relative humidity of the near-field environment is greater than the specified value of *tpa.inp* parameter CriticalRelativeHumidityAqueousCorrosion (defined by RH2 in Figure 8-2). Two forms of aqueous corrosion, general and localized, are expected to take place under different material and environmental conditions. In the absence of the conditions required for localized corrosion initiation, the general corrosion rate is computed as a function of passive current density according to the following equation derived from the Faraday charge conservation principle

$$CR = \frac{i_a(T)E_w}{F\rho} \quad (8-3)$$

where

- CR — general corrosion rate [m/yr]
- $i_a(T)$ — passive current density [C/m²/yr] at temperature T [K]
- E_w — equivalent weight of Alloy 22 [kg/mol], as specified by the *tpa.inp* parameter EquivalentWeightOuterOverpack[kg/mol]
- F — Faraday constant = 96486.7 C/mol
- ρ — density of Alloy 22 [kg/m³], as specified by the *tpa.inp* parameter DensityOuterOverpack[kg/m³]

At a given temperature, the passive current density is calculated in EBSFAIL for both mill-annealed and welded materials using the following Arrhenius equation

$$i_a(T) = i_a^0 \exp \left[- \frac{E_a}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}^a} \right) \right] \quad (8-4)$$

where

- $i_a(T)$ — passive current density [C/m²/yr] at temperature T [K]
- T — waste package surface temperature as provided by NFENV
- i_a^0 — passive current density [C/m²/yr] at temperature T_{ref}^a [K], as specified by the *tpa.inp* parameter AA_1_1[C/m2/yr]
- E_a — effective activation energy [J/mol] for the anodic current density, as specified by the *tpa.inp* parameter OuterActivationEnergyPassiveCurrDens[J/mol]
- R — universal gas constant = 8.3145 J/K/mol
- T_{ref}^a — reference temperature [K] for passive current density, as specified by the *tpa.inp* parameter RefTemperaturePassiveCurrDens[K]

8.3.2.4 Localized Corrosion

EBSFAIL considers that aqueous corrosion in the form of either general or localized corrosion corrodes the waste package when the relative humidity of the in-drift environment is more than

that specified by CriticalRelativeHumidityAqueousCorrosion in *tpa.inp*. The activation of localized corrosion also requires that water of appropriate chemical composition contacts the waste package surface. NFENV determines the chemical composition of the water with time.

EBSFAIL assumes that localized corrosion initiates and propagates when both of the following conditions are satisfied: (i) the waters contacting the waste package surface have a concentration of chloride ions above a critical value and (ii) the critical potential for localized corrosion, E_{crit} , exceeds the corrosion potential, E_{corr} .

For both mill-annealed and welded Alloy 22, the critical value of chloride ion concentration is specified by the *tpa.inp* parameters CritChlorideConcForFirstLayer[mol/L] and WeldCritChlorideConc[mol/L], respectively. In EBSFAIL, the abstracted corrosion potential model for Alloy 22 is used to calculate the corrosion potential of mill-annealed and welded regions of the outer container. The abstracted critical potential model is used to separately calculate E_{crit} for mill-annealed and welded regions of the outer container. Once localized corrosion initiates, the penetration of the waste package is calculated using the localized-corrosion penetration model. The three components of the localized corrosion model—the corrosion potential model, the critical potential model for localized corrosion, and the localized-corrosion penetration model—are described below.

8.3.2.4.1 Corrosion Potential Model

The corrosion potential is the potential difference across the metal/solution interface when a metal is immersed in an aqueous solution, and it is measured against a reference electrode (e.g., the standard hydrogen electrode). The sum of currents associated with the anodic dissolution reactions must be equal to the sum of currents associated with the cathodic reactions at the corrosion potential. Hence, the net external current generated by the corrosion processes is equal to zero at the corrosion potential to preserve charge neutrality.

The corrosion potential model is constructed from analytical expressions for anodic and cathodic reactions at the metal/solution interface based on fundamental electrochemical kinetic laws. Then, the sum of currents from anodic and cathodic reactions are set equal to zero. The resulting equation is solved for the corrosion potential, E_{corr} .

In the corrosion potential model, it is assumed that the dominant cathodic reaction under the mild oxidizing conditions in neutral-to-alkaline aerated water is the oxygen reduction reaction expressed as



In acidic solutions, the dissolved oxygen molecules are reduced by the following expression



In TPA Version 5.1, the transition point between acidic and neutral-to-alkaline solutions is specified by the *tpa.inp* input parameter TransitionLowHighpH. If water pH is less than TransitionLowHighpH, it is treated as acidic, otherwise; water is treated as neutral-to-alkaline.

Assuming that oxygen is transported to a distance either through a water film or through a precipitated salt scale film before being reduced at the metal–film interface and assuming steady-state conditions, Dunn, et al. (2005) proposed the following equation for the cathodic current density due to the oxygen reduction reaction in neutral-to-alkaline and in acidic solutions

$$i_r(T) = \frac{-i_r^{ref} \frac{C_{O_2}^{bulk}(T)}{C_{O_2}^{bulk}(T_{ref})} \exp\left[-\frac{E_a^{ef}}{RT}\right] \exp\left[-\frac{Z_r \beta_r^{ef}}{RT} E_{corr}\right] \left(\frac{[H^+]}{c_o}\right)^{n_H} \left(\frac{pO_2}{p_o}\right)^{n_o}}{1 + i_r^{ref} \exp\left[-\frac{E_a^{ef}}{RT}\right] \exp\left[-\frac{Z_r \beta_r^{ef} F}{RT} E_{corr}\right] \left(\frac{[H^+]}{c_o}\right)^{n_H} \left(\frac{pO_2}{p_o}\right)^{n_o} \frac{\max(\delta_{water-film}, \delta_{scale})}{Z_r F \phi \tau D_r(T) C_{O_2}^{bulk}(T)}} \quad (8-7)$$

where

- $i_r(T)$ — oxygen reduction reactions current density [C/m²/yr] at temperature T [K]
- E_{corr} — corrosion potential [volts vs. standard hydrogen electrode]
- E_a^{ef} — effective activation energy [J/mol], as specified by the *tpa.inp* parameter OuterActivationEnergyReductionReactLowpH[J/mole] for pH < TransitionLowHighpH and OuterActivationEnergyReductionReactHighpH[J/mole] for pH > TransitionLowHighpH
- Z_r — number of electrons per molecule of oxygen in the cathodic reduction reaction [unitless], 4
- i_r^{ref} — reference current density [C/m²/yr], as specified by the *tpa.inp* parameter OuterReferenceCurrReductionReactLowpH[C/(m2*yr)] for pH < TransitionLowHighpH and OuterReferenceCurrReductionReactHighpH[C/(m2*yr)] for pH > TransitionLowHighpH
- F — Faraday constant = 96,486.7 C/mol
- $C_{O_2}^{bulk}(T)$ — dissolved oxygen concentration [mol/kg] in solution as a function of temperature T [K]
- $C_{O_2}^{bulk}(T_{ref})$ — dissolved oxygen concentration [mol/kg] in solution at the reference temperature T_{ref} [K]
- T_{ref} — reference temperature = 298.15 K
- β_r^{ef} — effective charge transfer coefficient [unitless], as specified by the *tpa.inp* parameter OuterChargeTransferCoefReductionReactLowpH for pH < TransitionLowHighpH, and OuterChargeTransferCoefReductionReactHighpH for pH > TransitionLowHighpH
- T_{ref}^a — reference temperature [K] for anodic current density, as specified by the *tpa.inp* parameter RefTemperaturePassiveCurrDens[K]
- T — waste package surface temperature [K] as provided by NFENV

n_H	— constant [unitless], as specified by the <i>tpa.inp</i> parameter OuterEffectiveReactionOrderHLowpH for pH <TransitionLowHighpH and OuterEffectiveReactionOrderHHighpH for pH >TransitionLowHighpH
n_o	— constant [unitless], as specified by the <i>tpa.inp</i> parameter OuterChargeTransferCoefReductionReactLowpH for pH <TransitionLowHighpH and OuterChargeTransferCoefReductionReactHighpH for pH >TransitionLowHighpH
pO_2	— partial pressure of oxygen = 0.21 atm
p_o	— atmospheric pressure = 1.0 atm
R	— universal gas constant = 8.3145 J/K/mol
$[H^+]$	— hydrogen ion concentration [M], 10^{-pH} , where pH is provided by NFENV
c_o	— constant = 1M
$\delta_{water-film}$	— thickness of the water film [m], as specified by the <i>tpa.inp</i> parameter ThicknessOfWaterFilm[m]
δ_{scale}	— thickness of the salt scales [m], as specified by the <i>tpa.inp</i> parameter WPSurfaceScaleThickness[m]
ϕ	— porosity of scales of various precipitated solids [unitless], as specified by the <i>tpa.inp</i> parameter PorosityOfScaleWP
τ	— tortuosity of the scales of various precipitated solids [unitless], as specified by the <i>tpa.inp</i> parameter TortuosityOfScaleonWP
$D_r(T)$	— diffusivity of the dissolved oxygen [m ² /sec] in solution as a function of temperature

The dissolved oxygen concentration in the aqueous solutions is calculated using the following equation (Battino, 1981)

$$C_{O_2}^{bulk}(T) = pO_2 \exp \left[-0.2984 - \frac{5.5961 \times 10^3 K}{T} + \frac{1.04967 \times 10^6 K^2}{T^2} \right] \quad (8-8)$$

where

$C_{O_2}^{bulk}(T)$	— dissolved oxygen concentration [mol/kg] in aqueous solution at temperature T [K]
T	— waste package surface temperature [K] as provided by NFENV
pO_2	— partial pressure of oxygen = 0.21 atm

The kinetic rate model for oxygen reduction reaction represented by Eq. (8-7) is valid only for oxygen concentration estimated by Eq. (8-8) at a given temperature and at $pO_2 = 0.21$ atm. The numerical constants in Eq. (8-8) are internally programmed to avoid any inadvertent change by the user in TPA Version 5.1.

The diffusivity of the dissolved oxygen is given by

$$D_r(T) = 0.063 \exp \left[-\frac{14612 \text{ J mol}^{-1}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right] \quad (8-9)$$

where

- $D_r(T)$ — diffusivity of oxygen concentration [m^2/sec] in aqueous solution at temperature T [K]
- T — waste package surface temperature [K] as provided by NFENV
- T_{ref} — reference temperature = 298.15 K
- R — universal gas constant = 8.3145 J/K/mol

The numerical constants in Eq. (8-9) are internally programmed to avoid any inadvertent change by the user in TPA Version 5.1.

The water reduction reaction, expressed as



is also thermodynamically possible in neutral-to-alkaline solutions. The equation implemented in the TPA Version 5.1 to compute the current density due to water reduction reaction is given by

$$i_w(T) = -i_w^{ref} \exp \left[-\frac{E_a^w}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right] \exp \left[-\frac{\beta_w Z_w F}{RT} E_{corr} \right] \quad (8-11)$$

where

- $i_w(T)$ — water reduction reaction current density [$\text{C}/\text{m}^2/\text{yr}$] at temperature T [K]
- i_w^{ref} — reference current density [$\text{C}/\text{m}^2/\text{yr}$] for water reduction reaction, as specified by the *tpa.inp* parameter OuterWPRateConstantforWaterReduction[$\text{coulomb}/\text{m}^2/\text{yr}$]
- E_a^w — effective activation energy [J/mol] for the water reduction reaction, as specified by the *tpa.inp* parameter OuterWPAActivationEnergyforWaterReduction[J/mole]
- R — universal gas constant = 8.3145 J/K/mol
- T — waste package surface temperature [K] as provided by NFENV
- T_{ref} — reference temperature = 298.15 K
- β_w — charge transfer coefficient for water reduction reaction [unitless], as specified by the *tpa.inp* parameter OuterWPBetaKineticsParameterforWater
- F — Faraday constant = 96,486.7 C/mol
- E_{corr} — corrosion potential [volts vs. standard hydrogen electrode]
- Z_w — number of electrons per molecule of water involved in the water reduction reaction [unitless], 1

The total current due to anodic and cathodic reactions are give by the following equation

$$i_{total}(T) = i_r(T) + i_w(T) + i_a(T) \quad (8-12)$$

where

- $i_{total}(T)$ — total current density [C/m²/yr] due to anodic and cathodic reactions at temperature T [K]
- $i_r(T)$ — oxygen reduction reaction current density [C/m²/yr] at temperature T [K] as given by Eq. (8-7)
- $i_w(T)$ — water reduction reaction current density [C/m²/yr] at temperature T [K] as given by Eq. (8-11)
- $i_a(T)$ — passive current density [C/m²/yr] at temperature T [K] as given by Eq. (8-4)

The total current is zero at the corrosion potential due to dynamic equilibrium between anodic and cathodic process. In TPA Version 5.1, the corrosion potential E_{corr} is calculated by numerically solving the Eq. (8-12) when the total current $i_{total}(T)$ is equal to zero.

In EBSFAIL, the variability in the corrosion potential obtained by solving Eq. (8-12) at a given temperature and pH is assumed to be due to the variability in the Alloy 22 passive current density, i_a^o , which corresponds to the single anodic oxidation reaction considered in the model.

The capability of Eq. (8-12) to predict the corrosion potential at partial pressures other than $pO_2 = 0.21$ atm has not been experimentally verified. In TPA Version 5.1, EBSFAIL models mill-annealed and welded Alloy 22 at the same corrosion potential under the environmental conditions prevailing in the repository drift. The same set of parameters is used to calculate the corrosion potential for both metallurgical conditions.

8.3.2.4.2 Critical Potential Model

In TPA Version 5.1, localized corrosion of mill-annealed and welded Alloy 22 occurs when the corrosion potential, E_{corr} , exceeds critical potential for localized corrosion, E_{crit} . This critical potential corresponds to the crevice corrosion repassivation potential to account for the possibility of extremely long crevice corrosion initiation times. E_{crit} is calculated by the following expression (Dunn, et al., 2005) in TPA Version 5.1

$$E_{crit}(T) = A_1 + A_2T + (B_1 + B_2T)\log_{10}\left(\frac{[Cl^-]}{c_0}\right) + \Delta E_{crit} + \Delta E_{crit}^{NFENV} \quad (8-13)$$

where

- $E_{crit}(T)$ — critical potential [mV_{SHE}] for localized corrosion initiation at temperature T [°C]
- T — waste package surface temperature [°C] as provided by NFENV
- A_1 — intercept constant [mV_{SHE}], as specified by the *tpa.inp* parameter OuterOverpackErpIntercept or ErpInterceptWeld[mVSHE]
- A_2 — intercept slope constant [mV_{SHE}/°C], as specified by the *tpa.inp* parameter TempCoefOfOuterPackErpIntercept or TemperatureCoefficientOfErpInterceptWeld[mVSHE/C]

B_1	—	chloride concentration intercept constant [mV_{SHE}], as specified by the <i>tpa.inp</i> parameter OuterOverpackErpSlope or ErpSlopeWeld
B_2	—	chloride concentration intercept slope constant [$\text{mV}_{\text{SHE}}/^\circ\text{C}$], as specified by the <i>tpa.inp</i> parameter TempCoefOfOuterPackErpSlope or TemperatureCoefficientOfErpSlopeWeld [$\text{mV}_{\text{SHE}}/\text{C}$]
$[\text{Cl}^-]$	—	chloride ion concentration of water [M] as provided by NFENV
c_o	—	constant = 1 M
ΔE_{crit}	—	correction for inhibiting effect of oxyanions on critical potential [mV_{SHE}]
$\Delta E_{\text{crit}}^{\text{NFENV}}$	—	change in critical potential [mV_{SHE}] as calculated through the input parameters of NEFNV

In parameter definitions, the acronym SHE stands for standard hydrogen reference electrode. In EBSFAIL, both the corrosion potential (E_{corr}) and critical potential (E_{crit}) are calculated in volts in reference to the standard hydrogen reference electrode. Values and distribution for the coefficients A_1 , A_2 , B_1 , and B_2 used in TPA Version 5.1 are listed in Table 8-1 of Section 8-4 for mill-annealed and welded Alloy 22. All four parameters appear with two denominations: one for mill-annealed and another for welded material. The values of these parameters are different for both metallurgical conditions of Alloy 22, and therefore, the computed values of E_{crit} are also different.

The term ΔE_{crit} in Eq. (8-13) accounts for the effect of inhibiting oxyanions such as nitrate, sulfate, or bicarbonate on localized corrosion. Experimental results have shown that in the presence of oxyanions, E_{crit} increases sharply above a certain molar concentration ratio with respect to chloride. The term ΔE_{crit} is computed by the following expression

$$\Delta E_{\text{crit}} = \Delta E_{\text{crit}}^0 \frac{\min(r, r_n)}{r_n} \quad (8-14)$$

where

ΔE_{crit}^0 — critical potential constant [mV_{SHE}], as specified by the *tpa.inp* parameter OuterDeltaEcritInh[mV] or WeldDeltaEcritInh[mV]

The term r in Eq. (8-14) is a linear combination of oxyanion-to-chloride molar concentration ratios defined as

$$r = \frac{[\text{NO}_3^-]}{[\text{Cl}^-]} + \frac{r_n}{r_s} \frac{[\text{SO}_4^{2-}]}{[\text{Cl}^-]} + \frac{r_n}{r_c} \frac{[\text{CO}_3^{2-}] + [\text{HCO}_3^-]}{[\text{Cl}^-]} \quad (8-15)$$

where

r_n	—	nitrate inhibitor constant [unitless], as specified by the <i>tpa.inp</i> parameter OuterInhibitingNitrateToCl or WeldInhibitingNitrateToCl
r_c	—	carbonate inhibitor constant [unitless], as specified by the <i>tpa.inp</i> parameter OuterInhibitingCarbonateToCl or WeldInhibitingCarbonateToCl
r_s	—	sulfate inhibitor constant [unitless], as specified by the <i>tpa.inp</i> parameter OuterInhibitingSulfateToCl or WeldInhibitingSulfateToCl
$[\text{Cl}^-]$	—	chloride ion concentration [M] as provided by NFENV

- $[NO_3^-]$ — nitrate ion concentration [M] as calculated by NFENV
- $[SO_4^{2-}]$ — sulfate ion concentration [M] as calculated by NFENV
- $[CO_3^{2-}]$ — carbonate ion concentration [M] as calculated by NFENV
- $[HCO_3^-]$ — bicarbonate ion concentration [M] as calculated by NFENV

The values of r_n , r_s , and r_c and corresponding variable names used in *tpa.inp* are listed in Table 8-1 of Section 8-4. The value of r is calculated by NFENV and provided to EBSFAIL. TPA Version 5.1 includes ΔE_{crit}^{NFENV} to do exploratory analyses of processes (e.g., microbial action or radiolysis) that may change the repassivation potential. The user can define this value for change in critical potential for environments ENV I, ENV II, and ENV III (as shown in Figure 8-2) in *tpa.inp*. The time-dependent ΔE_{crit}^{NFENV} is added to E_{crit} [Eq. (8-13)]. In NFENV, the parameters to define ΔE_{crit}^{NFENV} are EnvironmentI_WastePackage_DeltaECrit[VSHE], EnvironmentII_WastePackage_DeltaECrit[VSHE], and EnvironmentIII_WastePackage_DeltaECrit[VSHE] in *tpa.inp*.

Equation (8-13) is used to compute E_{crit} when chloride concentration of the water contacting the waste package surface, $[Cl^-]$, exceeds a critical value. This critical chloride concentration is denoted by $[Cl^-]_{crit}$, and in TPA Version 5.1, the critical chloride concentrations for mill-annealed and welded Alloy 22 are specified by the parameters CritChlorideConcForFirstLayer and WeldCritChlorideConc, respectively.

8.3.2.4.3 Localized-Corrosion Penetration Model

Once the material, environmental, and electrochemical conditions for initiation of localized corrosion are established, the crevice corrosion rate is calculated by adopting the expression developed by Marsh and Taylor (1988), which is reported extensively in the literature (Szklaarska-Smialowska, 2004). The time-dependent penetration depth is given by

$$P = At^n \quad (8-16)$$

where

- P — crevice corrosion penetration depth [m]
- t — time [yr]
- A — experimentally determined constant [m/yr], as specified by the *tpa.inp* parameter CoefForLocCorrOfOuterOverpack
- n — constant [unitless], as specified by the *tpa.inp* parameter ExponentForLocCorrOfOuterOverpack

The parameter A and n are specified in *tpa.inp* for mill-annealed Alloy 22. The same values are used for the welded Alloy 22.

8.3.2.5 Other Waste Package Degradation Processes

Three other legacy models for corrosion are available in EBSFAIL and are briefly described in this section. Although the following three models are available to the user, these models are no

longer supported. User should exercise caution when changing the parameters associated with these models in *tpa.inp*. A detailed description of these models can be found in Mohanty, et al. (2000).

8.3.2.5.1 Thermal Embrittlement

The material toughness is defined as the ability to absorb energy in the form of plastic deformation without fracture. However, the material toughness can be affected by thermal embrittlement. In TPA Version 5.1, thermal embrittlement is evaluated by a simplified fracture model. A stress intensity factor is computed as a function of the depth of the localized corrosion front, a geometrical factor, and residual stresses according to

$$K_I = Y\sigma_s SF(\pi a)^{0.5} \quad (8-17)$$

where

- K_I — stress intensity factor [MPa m^{0.5}]
- Y — geometry factor to account for the shape of the crack and the load configuration [unitless]
- σ_s — yield strength [MPa], as specified by the *tpa.inp* parameter YieldStrength[MPa]
- SF — safety factor [unitless], as specified by the *tpa.inp* parameter SafetyFactor
- a — depth of the corrosion penetration front [m] as computed using Eq. (8-3) or Eq. (8-16)

The geometry factor Y is internally programmed in TPA Version 5.1. If the computed values of stress intensity at a timestep exceed a critical value that is specified by the parameter FractureToughness[MPa-m^{**0.5}], then thermal embrittlement of the outer container material takes place in EBSFAIL. The thermal embrittlement model is activated only when the localized corrosion model is activated. Additional details on this model are available in Mohanty, et al. (2000).

8.3.2.5.2 Radiolysis

Radiation from the high-level waste can cause the production of oxidizing species such as H₂O₂, O₂, and short-lived oxidizing radicals (i.e., HO, HO₂) in the water contacting the waste packages. The presence of these oxidizing species can cause an increase in the corrosion potential,

$$\Delta E = \Delta E_o e^{-\lambda t} \quad (8-18)$$

where

- ΔE — increase in the corrosion potential [V]
- ΔE_o — increase in the corrosion potential [V] at $t = 0$, as specified by the *tpa.inp* parameter DeltaPotentialDueToRadiolysis[V]
- λ — decaying constant [1/yr], as specified by the *tpa.inp* parameter DecayingConstantRadiolysis[1/yr]
- t — time variable [yr]

Radiolysis is neglected in the reference case because radiation levels on the waste package surface during the period when water could be in contact with the waste package are expected to be insufficient to sustain a continuous supply of radiolytic species such as H_2O_2 . Radiolysis model is activated when relative humidity of in-drift environment is greater than the *tpa.inp* parameter CriticalRelativeHumidityAqueousCorrosion. Additional discussion on the radiolysis model can be found in Mohanty, et al. (2000).

8.3.2.5.3 Galvanic Coupling

In TPA Version 5.1, waste package failure occurs when the outer container is breached and the corrosion of the inner container is not modeled. For this reason, the effect of galvanic coupling between the inner and outer containers on the breaching time of the waste package is not considered. Additional details of this model can be found in Mohanty, et al. (2000).

8.4 Input Parameters in *tpa.inp*

Table 8-1 lists the input file parameters used by DSFAIL and EBSFAIL in *tpa.inp*.

8.5 Auxiliary Input Data and External Process Models

No external process models need to be executed to generate input for DSFAIL and EBSFAIL calculations. However, DSFAIL and EBSFAIL invoke the standalone codes, DSFAILT and FAILT, respectively, to perform corrosion failure calculations. These standalone codes are located in the codes subdirectory. In DSFAIL and EBSFAIL, two auxiliary input data files (i.e., *dsfailt.def* and *ebsfail.def*) provide the parameters to calculate drip shield corrosion failure and waste package corrosion failure, respectively. The contents of these two files, located in the DATA subdirectory, are explained in Table 8-2.

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DSFAIL	DripShieldCorrosionRate[m/yr]	Drip shield corrosion rate [m/yr]	logtriangular 2.0e-8 2.98e-7 6.4e-7	A likely value of the anodic current density of Titanium Grade 7 is $1.0 \times 10^{-8} \text{ A/cm}^2$ (Brossia, et al., 2001), which is equivalent to a corrosion rate of $8.7 \times 10^{-8} \text{ m/yr}$. Based on 1-year crevice sample data by DOE (CRWMS M&O, 2004), a corrosion rate upper bound of $3.2 \times 10^{-7} \text{ m/yr}$ is assumed. The lower bound for the corrosion rate in CRWMS M&O (2004) is ignored because it is zero (actually, weight loss experiments resulted in negative corrosion rates). Instead, based on observations of long-term corrosion rates reported in the literature (Bechtel SAIC Company, LLC, 2004; Schutz, Blackwood, et al., 1988; Hua and Gordon, 2004; Schutz, 2005, 2003), it is reasonable to assume a lower bound of $1.0 \times 10^{-8} \text{ m/yr}$. The mode of the distribution, $1.49 \times 10^{-7} \text{ m/yr}$, is selected to obtain a median of $8.7 \times 10^{-8} \text{ m/yr}$. In other words, the triangular distribution is designed so that half of the realizations are sampled with a corrosion rate greater than $8.7 \times 10^{-8} \text{ m/yr}$ and the other half with a value less than $8.7 \times 10^{-8} \text{ m/yr}$. Corrosion rates are doubled to account for corrosion on both sides of the drip shield.

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	WPWeldFractionThickness PenetratedForFailureBy Corrosion[]	Fraction of the waste package outer container weld thickness penetrated by the corrosion front that defines failure [unitless]	constant 1.0	Value of 1.0 is assumed for the reference case (i.e., the entire thickness of the welded material must corrode away).
EBSFAIL	WPFractionThickness PenetratedForFailureBy Corrosion[]	Fraction of the waste package outer container wall thickness penetrated by the corrosion front that defines failure [unitless]	constant 1.0	Value of 1.0 is assumed for the reference case (i.e., the entire thickness of the mill-annealed material must corrode away).
EBSFAIL	DSFractionThickness PenetratedForFailureBy Corrosion[]	Fraction of the drip shield thickness penetrated by the corrosion front that defines failure [unitless]	constant 1.0	Value of 1.0 is assumed for the reference case (i.e., the entire thickness of the drip shield material must corrode away).
EBSFAIL	WPWeldThickness[m]	Thickness of the waste package outer container weld area [m]	constant 2.0e-2	The parameter value includes all fabrication welds that are a minimum of 2-cm thick. The inner closure lid is a fillet weld and is not a through thickness weld. Further details are described in Dunn, et al. (2003).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)					
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks	
EBSFAIL	TransitionLowHighpH	Transition pH to select low or high pH corrosion potential parameters [unitless]	constant 6.0	Empirical data obtained over pH range of 3 to 10 indicate the existence of a transition pH at about 6, above which the corrosion potential decreases (Dunn, et al., 2005).	
EBSFAIL	OuterChargeTransferCoef ReductionReactHighpH	n_o Charge transfer coefficient for oxygen reduction reaction on the outer container at high pH conditions [unitless]	constant 0.0248	The parameter value is derived from curve fitting experimental data (Dunn, et al., 2005).	
EBSFAIL	OuterChargeTransferCoef ReductionReactLowpH	n_o Charge transfer coefficient for oxygen reduction reaction on the outer container at low pH conditions [unitless]	constant 0.01287	The parameter value is derived from curve fitting experimental data (Dunn, et al., 2005).	

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	OuterReferenceCurrReduction ReactHighpH[C/(m2*yr)]	j_r^{ref} Reference current density to compute the cathodic current density due to the main reduction reaction (e.g., oxygen reduction) on the outer container for high pH conditions [C/m ² /yr]	constant 5.51e9	The parameter value is derived from curve fitting experimental data (Dunn, et al., 2005).
EBSFAIL	OuterReferenceCurrReduction ReactLowpH[C/(m2*yr)]	j_r^{ref} Reference current density to compute the cathodic current density due to the main reduction reaction (e.g., oxygen reduction) on the outer container for low pH conditions [C/m ² /yr]	constant 7.57e9	The parameter value is derived from curve fitting experimental data (Dunn, et al., 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	OuterActivationEnergy ReductionReactHighpH[J/mole]	E_a^{ef} Activation energy for Arrhenius dependence of cathodic current density on temperature at the high pH range for the outer container [J/mol]	constant 40000.0	This is an assumed value based on Calvo (1979). The value of 40,000 J/mol reproduces the temperature dependence of the corrosion potential measured in the laboratory.
EBSFAIL	OuterActivationEnergy ReductionReactLowpH[J/mole]	E_a^{ef} Activation energy for Arrhenius dependence of cathodic current density on temperature at the low pH range for the outer container [J/mol]	constant 40000.0	This is an assumed value based on Calvo (1979). The value of 40,000 J/mol reproduces the temperature dependence of the corrosion potential measured in the laboratory.
EBSFAIL	OuterEffectiveReactionOrderH LowpH	n_H Reaction order with respect to hydrogen ion for the outer container in the low pH conditions [unitless]	constant 0.0256	The parameter value is derived from curve fitting experimental data (Dunn, et al., 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>					
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks	
EBSFAIL	OuterEffectiveReactionOrderH HighpH	η_H Reaction order with respect to hydrogen ion for the outer container in the high pH conditions [unitless]	constant 0.01897	The parameter value is derived from curve fitting experimental data (Dunn, et al., 2005).	
EBSFAIL	InnerChargeTransferCoef ReductionReactHighpH	Charge transfer coefficient for oxygen reduction reaction on the inner container at high pH conditions [unitless]	constant 0.0248	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).	
EBSFAIL	InnerChargeTransferCoef ReductionReactLowpH	Charge transfer coefficient for oxygen reduction reaction on the inner container at low pH conditions [unitless]	constant 0.01287	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).	

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	InnerReferenceCurrReduction ReactHighpH[C/(m2*yr)]	Reference current density to compute the cathodic current density due to the main reduction reaction (e.g., oxygen reduction) on the inner container for high pH conditions [C/m ² /yr]	constant 5.51e9	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	InnerReferenceCurrReduction ReactLowpH[C/(m2*yr)]	Reference current density to compute the cathodic current density due to the main reduction reaction (e.g., oxygen reduction) on the inner container for low pH conditions [C/m ² /yr]	constant 7.57e9	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	InnerActivationEnergyReductionReactHighpH[J/mole]	Activation energy for Arrhenius dependence of cathodic current density on temperature at the high pH range for the inner container [J/mol]	constant 40000.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	InnerActivationEnergyReductionReactLowpH[J/mole]	Activation energy for Arrhenius dependence of cathodic current density on temperature at the low pH range for the inner container [J/mol]	constant 40000.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	InnerEffectiveReactionOrderHHighpH	Reaction order with respect to hydrogen ion for the inner container in the high pH conditions [unitless]	constant 0.01897	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued)				
(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	InnerEffectiveReactionOrderH LowpH	Reaction order with respect to hydrogen ion for the inner container in the low pH conditions [unitless]	constant 0.0256	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	InnerActivationEnergyPassive CurrDens[J/mol]	E_a^a Activation energy for Arrhenius dependence of passive current density on temperature for the inner container [J/mol]	constant 44700.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	OuterActivationEnergyPassive CurrDens[J/mol]	E_a^a Effective activation energy for Arrhenius dependence of passive current density on temperature for the outer container [J/mol]	constant 44700.00	The effective activation energy is estimated from the variation of the anodic current density as a function of temperature (Pensado, et al., 2002).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	RefTemperaturePassiveCurrDens[K]	T_{ref}^a Reference temperature to define Arrhenius dependence of passive current density on temperature [K]	constant 3.68e2	This is the reference temperature for the input values of passive current distribution specified by the parameter AA_1_1. Any other reference temperature can be selected, but the AA_1_1 parameter values must be in agreement with the reference temperature. Based on Dunn, et al. (2005), a reference temperature of 95 °C [203 °F] was selected.
EBSFAIL	OuterInhibitingNitrateToCl	r_n Nitrate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential of the mill-annealed region of the outer container [unitless]	constant 0.1	Below this parameter value, the repassivation potential is assumed to increase linearly with the ratio of nitrate-to-chloride molar concentration up to OuterDeltaEcritInh[mV]. Above this parameter value, the increase in the critical potential is assumed to remain constant equal to OuterDeltaEcritInh[mV]. The parameter value is given based on the critical potential model described in Dunn, et al. (2006, 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	OuterInhibitingCarbonateToCI	r_c Carbonate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential of the mill-annealed region of the outer container [unitless]	constant 0.2	Below this parameter value, the repassivation potential is assumed to increase linearly with the ratio of carbonate-to-chloride molar concentration up to OuterDeltaEcritInh[mV]. Above this parameter value, the increase in the critical potential is assumed to remain constant equal to OuterDeltaEcritInh[mV]. The parameter value is given based on the critical potential model described in Dunn, et al. (2006, 2005).
EBSFAIL	OuterInhibitingSulfateToCI	r_s Sulfate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential of the mill-annealed region of the outer container [unitless]	constant 0.5	Below this parameter value, the repassivation potential is assumed to increase linearly with the ratio of sulfate-to-chloride molar concentration up to OuterDeltaEcritInh[mV]. Above this parameter value, the increase in the critical potential is assumed to remain constant equal to OuterDeltaEcritInh[mV]. The parameter value is given based on the critical potential model described in Dunn, et al. (2006, 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	OuterDeltaEcritInh[mV]	Maximum increase in the critical potential due to the effect of inhibitors for the mill-annealed region of the outer container [mV]	constant 800.0	The parameter value is based on the critical potential model described in Dunn, et al. (2006, 2005).
EBSFAIL	InnerInhibitingNitrateToCl	Nitrate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential of the inner container [unitless]	constant 1.0e10	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	InnerDeltaEcritInh[mV]	Maximum increase in the critical potential due to the effect of inhibitors for the inner container [mV]	constant 0.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	WeldCritChlorideConc[mol/L]	Critical chloride concentration for the localized corrosion initiation for the welded region of the outer container [mol/L]	constant 1.0e-3	Dunn, et al. (2005, Figure 4-6) reported localized corrosion in solutions containing chloride at a concentration as low as 1.0×10^{-3} mol/L at 95 °C [203 °F] in welded plus solution annealed material. Because critical chloride threshold does not appear to be well defined, a low value of the critical chloride concentration is adopted.
EBSFAIL	WeldInhibitingNitrateToCl	r_n Nitrate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential for the welded region of the outer container [unitless]	constant 0.3	The parameter value is based on the critical potential model described in Dunn, et al. (2006, 2005).

Table 8-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	WeldInhibitingCarbonateToCl	r_c Carbonate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential for the welded region of the outer container [unitless]	constant 0.2	The parameter value is based on the critical potential model described in Dunn, et al. (2006, 2005).
EBSFAIL	WeldInhibitingSulfateToCl	r_s Sulfate-to-chloride molar concentration ratio used to compute the effect of inhibitors on the critical potential for the welded region of the outer container [unitless]	constant 0.5	The parameter value is based on the critical potential model described in Dunn, et al. (2006, 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	WeldDeltaEcritInh[mV]	Maximum increase in the critical potential due to the effect of inhibitors for the welded region of the outer container [mV]	constant 800.0	The parameter value is based on the model described in Dunn, et al. (2006, 2005).
EBSFAIL	ErpInterceptWeld[mVSHE]	A_1 E_{rp} intercept in mV for the waste package outer container welds [mV _{SHE}]	triangular 991.2 1041.2 1091.2	The central value of 1041.2 mV _{SHE} is derived from curve fitting of the repassivation potential and is consistent with values reported in Dunn, et al. (2006, 2005). The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984). Based on judgment from visualization of experimental data, it is considered that uncertainty in the repassivation potential is bounded by a 100-mV envelope around the most likely value.
EBSFAIL	TemperatureCoefficientOfErpInterceptWeld[mVSHE/C]	A_2 Temperature coefficient of E_{rp} intercept for the waste package outer container welds [mV/°C]	constant -10.0	This parameter value is derived from curve fitting (Dunn, et al., 2006, 2005) of the repassivation potential for thermally aged Alloy 22, which is assumed to bound the repassivation potential for weld material. The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued)				
(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	ErpSlopeWeld[mVSHE]	B ₁ E _{rp} slope in mV for the waste package outer container welds [mV _{SHE}]	constant -584.2	This parameter value is derived from curve fitting (Dunn, et al., 2006, 2005) of the repassivation potential data for thermally aged Alloy 22, which is assumed to bound the repassivation potential for weld material. The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984).
EBSFAIL	TemperatureCoefficientOfErpSlopeWeld[mVSHE/C]	B ₂ Temperature coefficient of E _{rp} slope for the waste package outer container welds [mV/°C]	constant 3.7	This parameter value is derived from curve fitting (Dunn, et al., 2006, 2005) of the repassivation potential data for thermally aged Alloy 22, which is assumed to bound the repassivation potential for weld material. The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984).
EBSFAIL	OuterWPTickness[m]	Thickness of the waste package outer container [m]	constant 0.02	This is the design data from DOE (2002).
EBSFAIL	InnerWPTickness[m]	Thickness of the waste package inner container [m]	constant 0.05	This is the design data from DOE (2002).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	MetalGrainRadius[micrometer]	r_g Average radius of the metal grains of the waste package outer container material [μm]	constant 13.75	This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000) and is used to estimate the propagation rate for a dry-air oxidation front (Lobnig, et al., 1992). Based on experimental data at high temperatures, it is assumed that dry-air oxidation is a negligible process for the waste package outer container (Dunn, et al., 2005). TPA Version 5.1 results are independent from this parameter value if the DryOxidationConstant is equal to a large enough value.
EBSFAIL	GrainBoundaryThickness [micrometer]	δ Thickness of grain boundary used in the model for calculating coupled oxygen diffusion along grain boundaries in metal [μm]	constant 7.0e-4	This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000) and is used to estimate the propagation rate for a dry-air oxidation front (Lobnig, et al., 1992). Based on experimental data at high temperatures, it is assumed that dry-air oxidation is a negligible process for the waste package outer container (Dunn, et al., 2005). TPA Version 5.1 results are independent from this parameter value if the DryOxidationConstant is equal to a large enough value.

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	DryOxidationConstant	Constant relating the diffusivity of oxygen along matrix and grain boundary in metal [unitless]	constant 1.0e20	The rate of dry-air oxidation for the waste package outer container material can be neglected if the waste package temperature is low {e.g., less than 400 °C [752 °F]}. Based on experimental data at high temperatures, it is assumed that dry-air oxidation is a negligible process in the waste package outer container material (Dunn, et al., 2005). In the potential repository environment, the waste package surface temperatures are expected to be lower than 300 °C [572 °F] (Manepally and Fedors, 2003; Fedors, et al., 2004). This parameter is set to a large value to emulate the expected negligible dry-air oxidation on Alloy 22. Hence, penetration of the waste package due to this corrosion mode is not expected.
EBSFAIL	CriticalRelativeHumidityHumidAirCorrosion	Critical relative humidity above which humid-air corrosion will initiate [unitless]	constant 0.15	It is assumed that the rate of humid-air oxidation is negligible in the waste package outer container material in the reference case. TPA Version 5.1 results are independent from the parameter value of CriticalRelativeHumidityHumidAirCorrosion, but this parameter must not exceed the CriticalRelativeHumidityAqueousCorrosion parameter.

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	CriticalRelativeHumidity AqueousCorrosion	Critical relative humidity above which aqueous corrosion will initiate [unitless]	constant 0.2	This parameter controls the onset of aqueous corrosion. Recent studies show that aqueous corrosion can take place in elevated temperature and low relative humidity systems (Yang, 2006). Deliquescent multicomponent salt systems have been reported that can form liquid solutions at temperatures as high as 200 °C [392 °F] or above (Rard, et al., 2006). The parameter CriticalRelativeHumidityAqueousCorrosion indirectly controls the maximum extrapolation temperature for corrosion rates of the waste package. The parameter value of 0.2 is consistent with experimental data by Rard, et al. (2006), and high enough to avoid extrapolation of aqueous corrosion rates to extreme temperatures, where long-term corrosion rates are highly uncertain.
EBSFAIL	ThicknessOfWaterFilm[m]	$\delta_{\text{water-film}}$ Thickness of water film on the waste package surface [m]	constant 0.0	Setting this parameter equal to zero is equivalent to assuming negligible diffusion control on the cathodic current density to determine the corrosion potential. The assumption is reasonable in the range of possible corrosion potentials. Corrosion potential computations employing this assumption produced trends consistent with experimental data (Dunn, et al., 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	OuterOverpackErpIntercept	A_1 E_{rp} intercept in mV for the waste package for the mill-annealed region of the outer container [mV _{SHE}]	triangular 1025.04 1180.76 1336.49	The central value of 1180.76 mV _{SHE} is consistent with values reported in Dunn, et al. (2006). The confidence bound was derived from fitting to upper and lower bounds in the repassivation potential in temperatures ranging from 60 to 105 °C [140 to 221 °F] (Dunn, et al., 2006). The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984). It is assumed that the parameter follows a triangular distribution. In TPA Version 5.1 computations, the repassivation potential is extrapolated up to a temperature defined by the NFENV parameter SeepageThresholdT[C].
EBSFAIL	TempCoefOfOuterPackErpIntercept	A_2 Temperature coefficient of E_{rp} intercept for the mill-annealed region of the outer container [mV/°C]	constant -9.35026	This parameter value is derived from curve fitting the repassivation potential data for mill-annealed Alloy 22 (Dunn, et al., 2006). The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984).
EBSFAIL	OuterOverpackErpSlope	B_1 E_{rp} slope in mV for the mill-annealed region of the outer container [mV]	constant -752.034	This parameter value is derived from curve fitting the repassivation potential data for mill-annealed Alloy 22 (Dunn, et al., 2006). The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued)				
(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	TempCoefOfOuterPackErp Slope	B_2 Temperature coefficient of E_{rp} slope for the mill-annealed region of the outer container [mV/°C]	constant 5.20131	This parameter value is derived from curve fitting the repassivation potential data for mill-annealed Alloy 22 (Dunn, et al., 2006). The crevice corrosion repassivation potential has been selected as the lowest potential at which crevice corrosion is expected to initiate in extremely long exposures (Kolts and Sridhar, 1984).
EBSFAIL	InnerOverpackErpIntercept	E_{rp} intercept for the waste package inner container [mV _{SHE}]	constant -10000.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	TempCoefOfInnerPackErpIntercept	Temperature coefficient of E_{rp} intercept for the waste package inner container [mV/°C]	constant 0.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	InnerOverpackErpSlope	E_{rp} slope for the waste package inner container [mV]	constant 0.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	TempCoefOfInnerPackErp Slope	Temperature coefficient of E_{rp} slope for the waste package inner container [mV/°C]	constant 1.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	OuterWPBetaKineticsParameterforWater	Transfer coefficient for water reduction reaction for the waste package outer container [unitless]	constant 0.0	It is assumed that the partial contribution of water reduction to cathodic current density is negligible. This assumption is reasonable in the range of possible corrosion potentials. The parameter value is selected to be consistent with this assumption (Dunn, et al., 2005).
EBSFAIL	InnerWPBetaKineticsParameterforWater	Transfer coefficient for water reduction reaction for the waste package inner container [unitless]	constant 0.5	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	OuterWPRateConstantforWaterReduction[coulomb/m ² /yr]	Rate constant for water reduction for the waste package outer container [C/m ² /yr]	constant 0.0	It is assumed that the partial contribution of water reduction to cathodic current density is negligible. This assumption is reasonable in the range of possible corrosion potentials. The parameter value is selected to be consistent with this assumption. This is justifiable because the equilibrium potential of the water reduction reaction is expected to be much lower than that of the oxygen reduction reaction (e.g., Bard and Faulkner, 1980, Table C.1).
EBSFAIL	OuterWPAActivationEnergyforWaterReduction[J/mole]	E_a^w Activation energy for water reduction for waste package outer container [J/mol]	constant 25000.0	The parameter value is based on Heusler (1976). However, TPA Version 5.1 results are independent of this parameter because OuterWPRateConstantforWaterReduction [coulomb/m ² /yr] is equal to 0.0. The corrosion potential computations employing this assumption produced trends consistent with experimental data (Dunn, et al., 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	InnerWPRateConstantforWaterReduction[coulomb/m ² /yr]	Rate constant for water reduction for the waste package inner container [C/m ² /yr]	constant 0.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	InnerWPActivationEnergyforWaterReduction[J/mole]	Activation energy for water reduction reaction for the waste package inner container [J/mol]	constant 25000.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	AA_1_1[C/m2/yr]	i_a^o Passive current density for the waste package outer container [C/m ² /yr]	triangular 1600.0, 2133.33, 6400.0	This current density is used to compute the general corrosion rate under passive conditions as a function of temperature. In addition, the current density is used independently to calculate the corrosion potential. The range is based on experimental data reported in Brossia, et al. (2001); Pensado, et al. (2002); and Dunn, et al. (2005). The steady anodic current density at 95 °C [203 °F] is expected to be 1.0×10^{-8} A/cm ² [or 3200 C/(m ² ·yr)]. The mode of the distribution, 2133.33 C/(m ² ·yr), is selected to make the median 3200 C/(m ² ·yr). The triangular distribution is designed so that half of the realizations are sampled with an anodic current density greater than 1.0×10^{-8} A/cm ² and the other half with a value less than 1.0×10^{-8} A/cm ² . The mean of the proposed triangular distribution is 3377.8 C/(m ² ·yr), corresponding to 1.07×10^{-8} A/cm ² (i.e., the mean and the median of the distribution are close).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	AA_2_1[C/m2/yr]	Passive current density for the waste package inner container [C/m ² /yr]	constant 1.0e4	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	MeasuredGalvanicCouple Potential	Experimentally measured galvanic coupling potential between the inner and outer containers [V]	constant 0.0	Corrosion of the inner container is not modeled in TPA Version 5.1. For this reason, the galvanic coupling between the Alloy 22 outer container and stainless steel does not take place. Therefore, the galvanic corrosion model is not considered and parameter value is set equal to zero.
EBSFAIL	CoefForLocCorrOfOuter Overpack	A Coefficient for localized corrosion penetration depth of the waste package outer container [m/yr]	constant 2.5e-4	The time exponent (<i>n</i>) for localized corrosion penetration depth of the waste package outer container is assumed to be equal to 1 (i.e., the localized corrosion penetration rate is independent of time), and the coefficient (<i>A</i>) is assumed to be 2.5×10^{-4} m/yr. The selection of this rate is supported by the localized corrosion penetration rates reported by Dunn, et al. (1996) for Type 316L stainless steel and Cramer, et al. (1984) for Alloy 625.
EBSFAIL	ExponentForLocCorrOfOuter Overpack	<i>n</i> Exponent for localized corrosion penetration depth of the waste package outer container [unitless]	constant 1.0	This parameter is assumed to be equal to 1 (i.e., the localized corrosion penetration rate is independent of time). Because stifling tendency of localized corrosion is uncertain at longer times, the current approach does not consider stifling and repassivation in the localized corrosion model. However, stifling and repassivation has been reported in the limited term localized corrosion experimental studies (He, et al., 2005).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	CoefForLocCorrOfInner Overpack	Coefficient for localized corrosion penetration depth of the inner container [m/yr]	constant 1.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	ExponentForLocCorrOfInner Overpack	Exponent for localized corrosion penetration depth of the inner container [unitless]	constant 1.0	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).
EBSFAIL	HumidAirCorrosionRate[m/yr]	The corrosion rate of the waste package outer container in humid air [m/yr]	constant 2.5e-8	Humid-air corrosion is not a feasible corrosion process for corrosion-resistant materials such as Alloy 22 (Van Rooyen and Copson, 1968), and therefore, the outer container is minimally affected by this corrosion mode in the in-drift repository environment. The constant value is chosen based on analogous information for Alloy 825 obtained from Van Rooyen and Copson (1968). This low rate is consistent with low passive dissolution rates in Pensado, et al. (2002) and Dunn, et al. (2005).
EBSFAIL	FractionalCouplingStrength	Efficiency factor, varying from 0 to 1, representing galvanic coupling between the outer and inner containers [unitless]	constant 0.0	This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000). This parameter is used to compute the corrosion potential resulting from galvanic coupling. However, the galvanic coupling between inner and outer container materials does not occur in EBSFAIL because corrosion of the inner container is not modeled.

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>					
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks	
EBSFAIL	FactorForDefiningChoiceOfCritPotential	Factor for defining choice of critical potential (pitting or repassivation) [unitless]	constant 0.0	Versions prior to TPA Version 4.0 (Mohanty, et al., 2000) considered the critical potential for localized corrosion to be defined as either (i) the repassivation potential or (ii) the pitting potential. The user can select (i) or (ii) by setting this constant equal to 0.0 or 1.0, respectively TPA Versions 4.0 and later do not further support the pitting potential concept. Therefore, this parameter value must not be changed.	
EBSFAIL	CritChlorideConcForFirstLayer [mol/L]	$[Cr]_{crit}$ Critical chloride concentration for localized corrosion initiation for the mill-annealed region of the outer container [mol/L]	constant 1.0e-3	Dunn, et al. (2005, Figure 4-6) reported localized corrosion in solutions containing chloride ions at a concentration of 0.05 mol/L at 95 °C [203 °F] in mill-annealed Alloy 22. Because critical chloride threshold does not appear to be well defined, a low value of critical chloride concentration is adopted.	
EBSFAIL	CritChlorideConcForSecond Layer[mol/L]	Critical chloride concentration for localized corrosion initiation of the waste package inner container [mol/L]	constant 1.0e-10	Corrosion of the inner container is not modeled. The selected parameter value does not have any influence on corrosion performance of outer container. This is a legacy parameter from TPA Version 4.0 (Mohanty, et al., 2000).	
EBSFAIL	WPSurfaceScaleThickness[m]	δ_{scale} Scale deposit thickness on the waste package surface [m]	constant 0.0	It is assumed that the corrosion potential is not controlled by the diffusion of the oxidizing species through the scale deposit. This parameter value is selected to be consistent with this assumption.	

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	TortuosityOfScaleonWP	τ Tortuosity of a porous layer scale deposited on the waste package [unitless]	constant 1.0	This is an assumed value. The results are independent of the assigned value to this parameter provided that WPsurfaceScaleThickness[m] is set equal to zero.
EBSFAIL	PorosityOfScaleonWP	ϕ Porosity of the scale deposited on the waste package [unitless]	constant 1.0	This is an assumed value and does not change with time. The results are independent of the assigned value to this parameter provided that WPsurfaceScaleThickness[m] is set equal to zero.
EBSFAIL	YieldStrength[MPa]	σ Yield strength of the waste package outer container material [MPa]	constant 310.3	This is a well-established value. Uncertainties are expected to be insignificant. Data pertain to the waste package outer container. Material manufacturer specifications are from ASME Boiler and Pressure Vessel code (ASME, 1995).
EBSFAIL	SafetyFactor	SF Safety factor for residual stresses [unitless]	constant 1.0	The safety factor is used for thermal embrittlement calculations. In the reference case, the yield strength of Alloy 22 is too high for any effect of thermal embrittlement.

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued)				
(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	Fracture Toughness [MPa·m**0.5]	K_{Ic} Fracture toughness of the waste package outer container material [MPa·m ^{1/2}]	constant 304.0	The constant value is based on expert judgment, which was extracted from a correlation with limited data applicable to Ni-Cr-Mo alloys from Dunn, et al. (2004). K_{Ic} >300 MPa·m ^{1/2} for mill annealed, as welded, welded plus solution annealed; K_{Ic} = 150 MPa·m ^{1/2} for welded plus aged at 870 °C [1,589 °F] for 10 hours. The yield strength of Alloy 22 is too high to be affected by thermal embrittlement.
EBSFAIL	DensityOuterOverpack[kg/m^3]	ρ Density of the outer container material [kg/m ³]	constant 8690.0	The data is provided in an ASTM standard and is consistent with manufacturer specifications for the waste package outer container material (ASTM International, 2006a).
EBSFAIL	DensityInnerOverpack[kg/m^3]	Density of the inner container material [kg/m ³]	constant 7980.0	The data is provided in an ASTM standard and is consistent with manufacturer specifications for 316L stainless steel (ASTM International, 2006b).
EBSFAIL	EquivalentWeightOuterOverpack[kg/mol]	E_w Equivalent weight of the outer container material [kg/mol]	constant 0.02597	This is a value provided in an ASTM standard and is adopted assuming the expected oxidation states of Alloy 22 elements (ASTM International, 2006c).
EBSFAIL	EquivalentWeightInnerOverpack[kg/mol]	Equivalent weight of inner container [kg/mol]	constant 0.02494	This is a value provided in an ASTM standard and is adopted assuming the expected oxidation states (ASTM International, 2006c).

Table 8-1. Reference Data for Parameters of tpa.inp Used by DSFAIL and EBSFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
EBSFAIL	DeltaPotentialDueToRadiolysis [V]	ΔE_0 Increase in the corrosion potential due to the presence of radiolytic species [V]	constant 0.0	It is considered that in the current design (DOE, 2002), the irradiation levels near the waste package are not sufficiently high to increase the corrosion potential (Shoesmith and King, 1999; CRWMS M&O, 2001a,b); therefore, radiolysis is not considered, and the parameter value is set equal to zero.
EBSFAIL	DecayingConstantRadiolysis [1/yr]	λ Constant controlling the exponential decay of the radiolytic potential [unitless]	constant 7.0e-5	The value is selected to avoid overflow and/or underflow in the computations. The contribution of radiolysis to uncertainty in the corrosion potential should be minimal compared to other sources of uncertainty. This value has no effect on the corrosion potential when DeltaPotentialDueToRadiolysis[V] is set to zero, because radiolysis is not considered (Shoesmith and King, 1999; CRWMS M&O, 2001a,b).
NFENV	EnvironmentI_Wastepackage_DeltaECrit[V SHE]	ΔE_{crit}^{NFENV} Factor that allows for consideration of the increase in the repassivation potential due to secondary factors or unaccounted	constant 0.0	Value set to zero to reflect the assumption that secondary processes do not influence the repassivation potential in the reference case. Value used to construct input file <i>deltaec.inp</i> (Chapter 7).

Table 8-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DSFAIL and EBSFAIL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
NFENV	EnvironmentII_Wastepackage_DeltaECrit[VSHE]	ΔE_{crit}^{NFENV} Factor that allows for consideration of the increase in the repassivation potential due to secondary factors or unaccounted processes [V_{SHE}]	constant 0.0	Value set to zero to reflect the assumption that secondary processes do not influence the repassivation potential in the reference case. Value used to construct input file <i>deltaec.inp</i> (Chapter 7).
NFENV	EnvironmentIII_Wastepackage_DeltaECrit[VSHE]	ΔE_{crit}^{NFENV} Factor that allows for consideration of the increase in the repassivation potential due to secondary factors or unaccounted processes [V_{SHE}]	constant 0.0	Value set to zero to reflect the assumption that secondary processes do not influence the repassivation potential in the reference case. Value used to construct input file <i>deltaec.inp</i> (Chapter 7).

Table 8-2. Auxiliary Input Data Files Used by DSFAIL and EBSFAIL	
File	Contents
<i>dsfailt.def</i>	This file is located in the data subdirectory and contains the parameters for drip shield corrosion failure. This file contains the default parameter values for drip shield corrosion rate, drip shield thickness, failure criterion, and output file name. This is a template file for generating <i>dsfailt.inp</i> , the input file for DSFAILT. DSFAIL copies the contents of this file and replaces it with parameter values specified in the DSFAIL and EBSFAIL section of <i>tpa.inp</i> .
<i>ebsfail.def</i>	This file is located in the data subdirectory and contains the parameters for waste package corrosion failure. This is a template file for generating <i>ebsfail.inp</i> , the input file for EBSFAIL. EBSFAIL copies the contents of this file and replaces it with parameter values defined in the EBSFAIL section of <i>tpa.inp</i> . This file contains some input parameters that are not specified in <i>tpa.inp</i> {e.g., values setting numerical integration and number of terms used in the series summation for estimating the dry-air oxidation corrosion depth [see Eq. (8-1)]}.
<i>fluoride.dat</i>	This file is located in the DATA subdirectory and contains the fluoride concentration of the seepage water as a function of time. This is a legacy file and information present in this file is not used in TPA Version 5.1.

8.6 Intermediate Outputs and Information Passed to Other Modules

Tables 8-3 and 8-5 describe the intermediate output files produced by DSFAIL and EBSFAIL, respectively. In addition to the output files listed in Tables 8-3 and 8-5, the user can specify that calculated information passed to and from DSFAIL and EBSFAIL be saved as intermediate output for specific realizations. Tables 8-4 and 8-6 describe these optional output files for DSFAIL and EBSFAIL, respectively. To specify optional intermediate output files, the user can set *tpa.inp* parameter OutputMode(0=None,1=All,2=UserDefined) to a value of 1 or 2. When set to 1, all the optional intermediate output files for DSFAIL and EBSFAIL are saved for all realizations. When set to 2, optional intermediate output selected is saved for realizations starting from *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by *tpa.inp* parameter UserDefinedUpperRealizationAppended. The user can select DSFAIL optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter SelectAppendFiles to 21 for just *dsfail.rlt* and *dsfail.ech*. Alternatively, the user can select EBSFAIL optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter SelectAppendFiles to 3 for just *ebsfail.rlt* and *ebsfail.ech*, or 15 for just *failt.cum*.

Table 8-3. Intermediate Output Files Created During Execution of DSFAIL	
File	Contents
<i>dsfailt.dat</i>	This file contains the output results from the execution of DSFAIL. It contains drip shield breaching time information and drip shield thickness versus time information. Drip shield thickness versus time is passed to MECHFAIL. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.
<i>dsfailt.dbg</i>	This file contains debug information for drip shield corrosion. Information that is printed to the screen by DSFAIL is directed to this file. This file contains error messages that occur during the execution of DSFAIL of the last realization.

Table 8-3. Intermediate Output Files Created During Execution of DSFAIL (continued)	
File	Contents
<i>dsfailt.inp</i>	This file contains sampled input values for DSFAIL. This file is generated using the template file <i>dsfailt.def</i> and the input parameter values are specified in the DSFAIL and EBSFAIL sections of <i>tpa.inp</i> . This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.
<i>dsfail.res</i>	This file contains breaching time and the number of drip shields breached due to corrosion for each realization. See Chapter 19 for additional details.

Table 8-4. Optional Intermediate Output Files Created During Execution of DSFAIL	
File	Contents
<i>dsfail.rlt</i>	This file contains the results of the drip shield corrosion calculations for each subarea and realization. It displays the drip shield breaching time and the drip shield thickness versus time, which are passed to MECHFAIL.
<i>dsfail.ech</i>	This file displays the input data to DSFAIL for each subarea and realization. It displays information such as realization number, subarea, and number of timesteps.

Table 8-5. Intermediate Output Files Created During Execution of EBSFAIL	
File	Contents
<i>chlrdmf.dat</i>	This file contains chloride concentration information versus time from NFENV and is used as input to EBSFAIL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>deltaec.inp</i>	This file contains the change in critical potential versus time as calculated by NFENV and is used as input to EBSFAIL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>ebsfail.inp</i>	This file contains input parameters used by EBSFAIL. This file is generated using the template file <i>ebsfail.def</i> and the input parameter values specified in the EBSFAIL section of <i>tpa.inp</i> . This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>ebstrh.dat</i>	This file contains weld and waste package failure summary data. It also contains temperatures, relative humidity, pH, and inhibitor information versus time information from NFENV. Time, temperatures, and summary data are input to EBSREL. Within the summary data, weld corrosion breaching time and waste package surface corrosion breaching time are used by EBSREL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>ebstrhc.inp</i>	This file contains temperature, pH, and inhibitor information versus time from NFENV and is used as input to EBSFAIL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.

Table 8-5. Intermediate Output Files Created During Execution of EBSFAIL (continued)	
Files	Contents
<i>echofail.dbg</i>	Debug file showing the values read by EBSFAIL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>wpsfail.dbg</i>	Debug information for waste package failure. This file presents a table of five different waste package failure modes in time order for each realization. The subarea of failure is also noted.
<i>failt.out</i>	This file displays corrosion failure information for the waste package outer container surface and welds. This file contains the waste package surface temperature, critical potential, corrosion potential, remaining outer layer thickness, and corrosion model at each timestep for the mill-annealed region. This file also contain the remaining thickness of the mill-annealed region. If the mill-annealed region fails during the simulations, this file contains the breaching time. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>gencorrfail.out</i>	This file contains corrosion potentials versus time for general corrosion. It also contains residual thickness of the mill-annealed region versus time due to various corrosion processes excluding localized corrosion, which is an input to MECHFAL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>weldfail.out</i>	This file contains corrosion potential and critical potential versus time for the welded regions and is generated by EBSFAIL. This file also contain the residual thickness of the welded region due to various corrosion processes including localized corrosion. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.
<i>wpsfail.res</i>	This file contains the breaching time and the number of waste packages failed by corrosion processes. See Chapter 19 for additional details.

Table 8-6. Optional Intermediate Output Files Created During Execution of EBSFAIL	
File	Contents
<i>ebsfail.rlt</i>	This file displays the fraction of waste packages failed versus time and the waste package outer container wall thickness versus time for each subarea and realization.
<i>ebsfail.ech</i>	This file contains the input data to EBSFAIL for each subarea and realization. It displays information such as temperature, relative humidity, pH, and fraction of the drip shields failed versus time.
<i>failt.cum</i>	This file contains waste package outer container thickness versus time for the mill-annealed region due to various corrosion processes including localized corrosion. It also contains corrosion potential and critical potential for localized corrosion as a function of emplacement time. The information in this file is for each subarea and realization. During execution, the data contained in <i>failt.out</i> is concatenated to the end of <i>failt.cum</i> .

8.7 Techniques for Understanding Module Performance

Although there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of the corrosion processes on drip shield and waste package degradation as evaluated by

DSFAIL and EBSFAIL. Corrosion processes with significant uncertainties, such as the general corrosion of the waste package outer container, are assigned as probabilistic distributions in *tpa.inp*. A variety of parametric sensitivity analysis techniques (e.g., Mohanty, et al., 2002) may be useful to understand the effects of the various corrosion processes on system-level performance.

In addition, “pinch-point” techniques, where output or intermediate results produced by DSFAIL and EBSFAIL can be understood in combination with output or intermediate results from other modules (e.g., MECHFAIL), may help to evaluate subsystem processes. Key output files and intermediate result files useful for these comparisons include *dsfail.dat* (from DSFAIL) and files from EBSFAIL such as *weldfail.out*, *ebstrh.out*, and *gencorrfail.out*. These files contain the remaining thickness of the drip shield and outer container after corrosion. The importance of individual parameters with respect to particular subsystem processes can be examined by varying an input parameter and analyzing results from various output and intermediate result files. A single parameter analysis may be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. The output generated using the *tpameans.out* for one subarea and one realization produces a linear variation in drip shield thickness as a function of emplacement time, which is stored in *dsfail.out*. The relevance of the drip shield can be evaluated by executing TPA Version 5.1 for two conditions: first for the reference case and again for enhanced values of the corrosion rate. The enhanced corrosion rate can be implemented by assigning the higher bound to DripShieldCorrosionRate[m/yr]. The same effect can be achieved by lowering the value of the fraction DSFractionThicknessPenetratedForFailureByCorrosion to less than one. In particular, setting the parameter DSFractionThicknessPenetratedForFailureByCorrosion equal to zero simulates drip shield breaching by corrosion at the time of emplacement.

The drip shield can reduce the amount of water contacting the waste package, hence potentially limiting radionuclide releases (Chapter 10). Additionally, the drip shield can concentrate rock loads and potentially cause mechanical failure of the waste package outer container (Chapter 9). When the drip shield is fully corroded, it can neither transfer loads to the waste package nor act as an effective barrier to the contact of water with the waste package. The user is cautioned not to set the drip shield thickness equal to zero {DripShieldThickness[m]} in *tpa.inp*. This input affects thermal calculations (Chapter 7) and results in different waste package surface temperatures than estimated by setting the parameter DSFractionThicknessPenetratedForFailureByCorrosion equal to zero.

The waste package general corrosion rate in the absence of localized corrosion depends on the waste package surface temperature, which is estimated as a function of the emplacement time by NFENV (Chapter 7). The temperature- and time-dependent variation in the corrosion rate can be visualized by plotting the remaining waste package outer container thickness as a function of time.

In EBSFAIL, the general corrosion and localized corrosion of the waste package outer container are interdependent processes. For example, an increase in the passive current density for anodic dissolution of Alloy 22, i_a {AA_1_1[C/m2/yr]}, causes a decrease in corrosion potential, which decreases the likelihood of localized corrosion. The interplay between the general corrosion rate and corrosion potential can be discerned by first running TPA Version 5.1 for the reference case using the *tpameans.out* as the input file and repeating the exercise using a

higher value of AA_1_1[C/m2/yr] in *tpameans.out*. The two cases can be analyzed by examining the results in *gencorrfail.out*. A similar exercise can be repeated to understand the interplay between the general corrosion rate and the corrosion potential using the parameter OuterActivationEnergyPassiveCurrDens[J/mol]. This parameter is used to calculate the general corrosion rate and also appears in the corrosion potential model. An increase in the value of this parameter reduces the corrosion rate; however, it can either increase or decrease the corrosion potential. The corrosion potential increases with an increasing value of the parameter if the waste package surface temperature is less than T_{ref}^a . Otherwise, the corrosion potential decreases. Again, the results can be analyzed by examining the calculated values in *gencorrfail.out*.

To assess the capability of the waste package to contain waste forms, set the fraction WPFractionThicknessPenetratedForFailureByCorrosion equal to zero or to a small number to see the contribution to radionuclide release due to early failure of the waste package. Alternatively, proportional changes in the parameters AA_1_1[C/m2/yr], OuterReferenceCurrReductionReactLowpH, and OuterReferenceCurrReductionReactHighpH can be used to change the outer container general corrosion rate {because AA_1_1[C/m2/yr] is changed} without affecting the corrosion potential (because the ratio of OuterReferenceCurrReductionReactLowpH and OuterReferenceCurrReductionReactHighpH remain the same). By implementing the changes, a user will notice an increased rate of waste package degradation due to general corrosion without having a change in the likelihood of localized corrosion. The results of this change can be analyzed by noting the reported values of the corrosion rates and the corrosion potential in *weldfail.out*. An enhanced general corrosion rate causes early failure of the waste package.

The contribution of localized corrosion to radionuclide release can be studied by setting CritChlorideConcForFirstLayer and WeldCritChlorideConc to adjust the potential for initiation of localized corrosion. Localized corrosion deactivation can be accomplished by setting the parameters CritChlorideConcForFirstLayer and WeldCritChlorideConc to arbitrarily high numbers to adjust the potential for localized corrosion initiation. The result of these changes can be seen by examining the results for the welds in *weldfail.out* and *failt.cum*. The file *weldfail.out* also contains the variation in the corrosion rate as a function of time for the welds.

It is common to increase the outer container wall thicknesses {i.e., OuterWPThickness[m]} to reduce the likelihood of breaching the waste package by general and localized corrosion. However, the user is cautioned that such changes affect the waste package and drip shield mechanical interactions. On the other hand, the parameter WPWeldThickness[m] is only used in EBSFAIL, and it can be freely changed without influencing other modules of TPA Version 5.1, such as MECHFAIL.

The influence of processes such as corrosion at elevated temperatures on the engineered barrier system performance can be evaluated, for example, by setting the value of HumidAirCorrosionRate to the values found in experiments simulating corrosion by deliquescent salt mixtures (Yang, 2006). In TPA Version 5.1, a low value for the humid-air corrosion rate is used when the relative humidity falls within the bounds defined by CriticalRelativeHumidityHumidAirCorrosion and CriticalRelativeHumidityAqueousCorrosion. By adequately selecting the corrosion rate and the transition relative humidity thresholds, the effect of elevated temperature corrosion can be simulated.

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9 DRIP SHIELD AND WASTE PACKAGE MECHANICAL FAILURE (MECHFAL)

The Drip Shield and Waste Package Mechanical Failure module (MECHFAL)¹ computes mechanical failure of drip shields and waste packages subjected to static and seismic loading demands. In MECHFAL, the engineered barrier system performance is linked to the geometry, materials, and boundary conditions of the drip shield and waste package design currently considered by the U.S. Department of Energy (DOE) (Bechtel SAIC Company, LLC, 2004a,b).

MECHFAL is executed twice—once for the drip shield and once for the waste package—in each subarea of every realization when at least one of the flags `SeismicDisruptiveScenarioFlag(yes=1,no=0)` or `DriftDegradationScenarioFlag(yes=1,no=0)` is activated, leading to seismic- or thermal-induced drift degradation, respectively. Several parameters used in MECHFAL are computed in other modules and utilities. The seismic demand parameters are provided by the utility module SAMPLER (Chapter 4), whereas the Drift Degradation module (DRIFTFAIL)² (Chapter 6) computes the static vertical loading demands. The capacity of the drip shield and waste package is modified by (i) their respective temperatures provided by the Near-Field Environment module (NFENV)³ (Chapter 7) and (ii) the thinning of their plates, provided by the Drip Shield Corrosion Failure module (DSFAIL)⁴ and the Engineered Barrier System Corrosion Failure module (EBSFAIL)⁵ (Chapter 8). MECHFAL reports the number of mechanical drip shield and waste package failures and the failure time to the Engineered Barrier System Radionuclide Release module (EBSREL)⁶ (Chapter 10).

9.1 Conceptual Model

MECHFAL calculates the maximum vertical load that the drip shield and waste package can withstand (i.e., the time-dependent vertical-load-carrying capacity) and compares it to the applied loading demands. If loading demands exceed the engineered barrier system capacity, mechanical failure is reported.

¹The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAL will be used.

²The Drift Degradation module is referenced frequently throughout this chapter. The abbreviation DRIFTFAIL will be used.

³The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

⁴The Drip Shield Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation DSFAIL will be used.

⁵The Engineered Barrier Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

⁶The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

9.1.1 Drip Shield Structural Performance

The drip shield is part of the engineered barrier system currently under consideration for the potential geologic repository at Yucca Mountain, Nevada. The drip shields enclose the waste packages and protect them from seepage water and rockfall loading. The MECHFAL abstractions are based on the design currently considered by DOE (Bechtel SAIC Company, LLC, 2004a) (Figure 9-1). The drip shield consists of Titanium Grade 7 plates supported with equally spaced frames made of Titanium Grade 24 bulkhead and support beams (columns).

MECHFAL evaluates the drip shield vertical-load-carrying capacity to withstand the static and seismic loading caused by accumulated rockfall rubble. For anticipated loading conditions, drip shield failure in TPA Version 5.1 is associated with drip shield structural instability due to plastic buckling of the support beams (columns) (Figure 9-2) (Ibarra, et al., 2007a). Because lateral load variation is anticipated to have a large influence on the drip shield capacity under static loading, the first abstraction in MECHFAL correlates the drip shield vertical-load-carrying

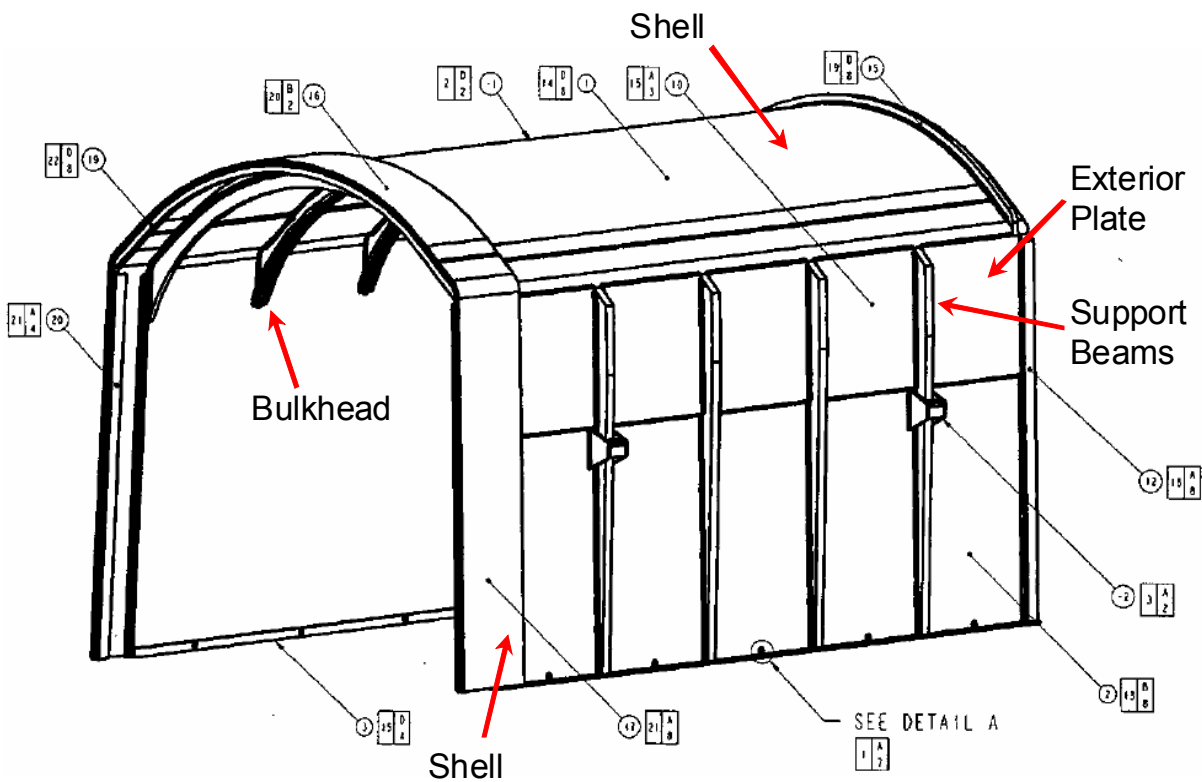


Figure 9-1. Isometric of Updated Drip Shield (Bechtel SAIC Company, LLC, 2004a)

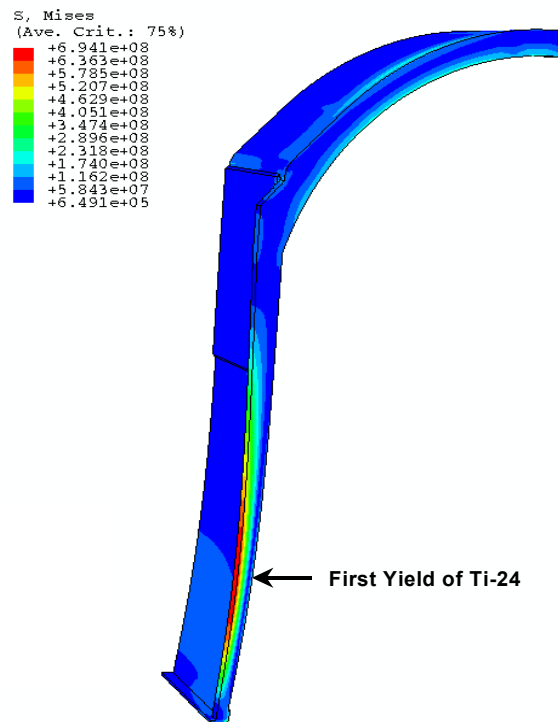


Figure 9-2. Drip Shield Von Mises Stress Distribution at Titanium Grade 24 First Yield
Units: Pa (1 Pa = 0.145×10^{-3} psi) (Ibarra, et al., 2007a)

capacity and the vertical-to-lateral load ratio (Ibarra, et al., 2007b). The drip shield capacity is further affected by other factors such as creep, temperature, and general corrosion of its component materials. For vibratory ground motions, MECHFAIL computes seismic demands as a function of the peak ground acceleration of the event and the static load applied to the drip shield.

9.1.2 Drip Shield–Waste Package Mechanical Interaction

The waste package design currently considered by DOE (Bechtel SAIC Company, LLC, 2004b) consists of two concentric cylinders separated by a gap of several millimeters. In this chapter, the 316 stainless steel internal cylinder is referred to as the waste package inner container, whereas the Alloy 22 external cylinder is named the waste package outer container. In TPA Version 5.1, waste package mechanical failure occurs when mechanical loads cause effective plastic strains in the outer container that are greater than the effective plastic strain corresponding to the ultimate tensile strength of Alloy 22. Note that the waste package inner container function is limited to providing structural support in the model abstractions.

Plastic strains in the waste package develop if the drip shield becomes structurally unstable and drip shield–waste package mechanical interaction occurs. Ibarra, et al. (2007b) indicated that stress and strain concentrations on the waste package outer container would occur only if a drip shield edge contacts the waste package at a certain angle (contact angle) that leads to a reduction in contact area (Figure 9-3). Also, the contact length between the deformed drip shield bulkhead and the waste package outer container significantly affects the contact region. The numerical analyses indicate that mechanical interaction can lead to high localized plastic stresses and strains in the waste package, although a large margin against breaching of the outer container was observed under the anticipated static loading. The static loads, however, may be amplified due to seismic ground motion accelerations, leading to waste package breaching during strong seismic events (Ibarra, et al., 2007b).

Based on the above analyses, MECHFAIL assesses the potential for waste package breaching due to drip shield–waste package mechanical interaction under static and seismic loading. In addition to these loading conditions, the abstractions consider the effects of the contact angle between the drip shield component and the waste package (Figure 9-3), the contact length, and thinning of the waste package outer container thickness due to general corrosion.

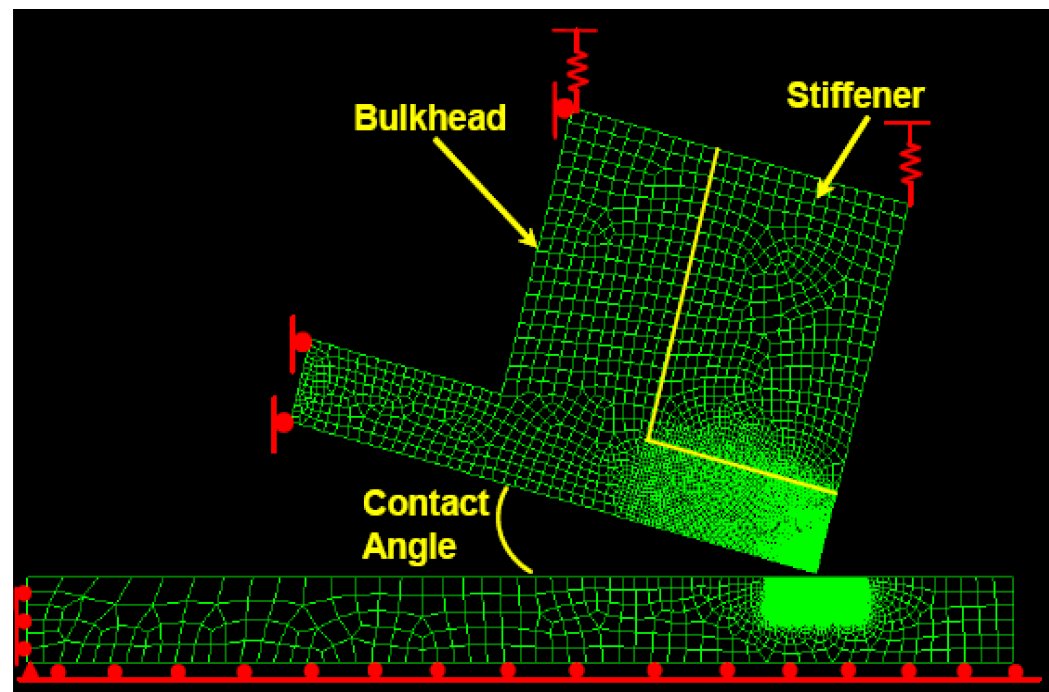


Figure 9-3. Two-Dimensional Plane Strain Finite Element Model, Bulkhead Cross Section With Longitudinal Stiffener and Waste Package Outer Shell (Ibarra, et al., 2007b)

9.2 Model Support and Assumptions

The MECHFAIL abstractions for the drip shields and waste packages were derived from structural analyses (Ibarra, et al., 2007a,b) that assume thermal-induced drift degradation causes the drifts to collapse within a few hundreds of years (Ofoegbu, et al., 2006a, 2004). Thus, TPA Version 5.1 evaluates the performance of engineered barrier system when subjected to static and dynamic (seismic) loading caused by accumulated rubble.

9.2.1 Drip Shield Structural Performance

The MECHFAIL abstractions are based on the drip shield structural performance analyses performed by Ibarra, et al. (2007a) using an ABAQUS® (ABAQUS, Inc., 2004) finite element model (Figure 9-2) and an equivalent SAP2000® (Computers and Structures, Inc., 2004) frame model. In addition, the main abstractions for static loading are consistent with the vertical-load-carrying capacity and failure mechanisms obtained by Gute, et al. (2003) for a former drip shield design and with analyses for the drip shield design currently considered by DOE with different static loading configurations (Bechtel SAIC Company, LLC, 2004b). The agreement in the structural response obtained from these drip shield structural analyses supports the resulting abstractions. The following assumptions were also made to generate the drip shield performance abstractions:

- Rockfall impact is not a critical loading scenario (Ofoegbu, et al., 2006b).
- The accumulated rubble exerts a continuous and uniform pressure around the drip shield.
- Hydrogen embrittlement, stress corrosion cracking, and localized corrosion have a negligible influence on the drip shield integrity in the potential repository environment (Section 8.2.1).
- The drip shield vertical-load-carrying capacity is not affected by variations of the rubble modulus of elasticity, the static load imbalance, stage loading, and invert degradation (Ibarra, et al., 2007a).
- The drip shield seismic performance under strong seismic events assumes initial static loading (Ofoegbu, et al., 2006b).

9.2.2 Drip Shield–Waste Package Mechanical Interaction

MECHFAIL abstractions of drip shield–waste package mechanical interaction are based on two sets of finite element models developed in ABAQUS (ABAQUS, Inc., 2004) and reported by Ibarra, et al. (2007b). A set of two-dimensional plane strain finite element models of simple geometry permitted the use of refined meshes to estimate the stresses and strains of the waste package outer container in the vicinity of the contact region (Figure 9-3). Three-dimensional finite element models were used to estimate the contact length between the drip shield bulkhead and the waste package outer container and to validate the boundary conditions used in the plane strain models. The use of two different sets of numerical models and sensitivity studies to evaluate the consistency of the results provides model support to the abstractions.

The following assumptions were made to develop the drip shield–waste package mechanical interaction abstractions:

- The MECHFAIL abstractions derived from mechanical analyses of the 21-pressurized water reactor waste package are used for all the types of waste packages proposed for the potential repository.
- The vertical pressure demand on top of the collapsed drip shield is the same pressure transferred to the waste package outer container.
- Weld residual stresses, hydrogen embrittlement, and galvanic coupling (Chapter 8) do not contribute to waste package mechanical failure.
- The shell of a collapsed drip shield is able to transfer loads to the waste package outer container through the stiffeners and bulkheads until the drip shield shell completely corrodes due to general corrosion. Partial loss of drip shield shell structural capacity due to general corrosion is not considered.
- The bulkhead and longitudinal stiffeners are the only drip shield components that cause stress concentrations on the waste package outer container sufficient for breaching.

The waste package failure mode definition (Section 9.2.1) is based on several assumptions that need to be satisfied before the stresses can reach the ultimate tensile strength (Ibarra, et al., 2007b):

- Stress corrosion cracking does not occur in Alloy 22 in the Yucca Mountain environmental conditions.
- Localized corrosion has no effect on the mechanical stresses.
- The waste package outer container reaches the ultimate tensile strength without cracking.
- General corrosion is only partially coupled to mechanical stresses.

9.3 Implementation of Conceptual Model in TPA Version 5.1

9.3.1 Drip Shield Structural Performance

To assess the drip shield structural performance, the capacity of the drip shield is first evaluated as a function of the lateral-to-vertical load ratio parameter and is later modified to account for the effects of creep, temperature, general corrosion, and seismic loading.

9.3.1.1 Lateral Pressure Applied to the Drip Shield

DRIFTFAIL provides vertical static loads for lithophysal and nonlithophysal rocks in *mechfail_ds.inp*. Because the drip shield vertical-load-carrying capacity under static loading also depends on the lateral pressure acting on the drip shield (Ibarra, et al., 2007a), the horizontal-to-vertical load ratio parameter is implemented to estimate the lateral load for each

type of rock and subarea. The horizontal-to-vertical load ratio parameter is provided in *tpa.inp* (Section 9.4) and is identified as DripShieldHorizToVertLoadRatioRock1Subarea_#[] and DripShieldHorizToVertLoadRatioRock2Subarea_#[].⁷

9.3.1.2 Drip Shield Capacity Based on Vertical and Horizontal Loading

The drip shield vertical-load-carrying capacity, $P_{v,DScap}$, is first estimated in MECHFAIL as a function of the lateral load because variation of this parameter largely modifies the vertical loads that the drip shield can withstand (Ibarra, et al., 2007a). The first estimation of $P_{v,DScap}$ is based on a tenth-order polynomial equation that provides the drip shield capacity as a function of the horizontal-to-vertical load ratio. The coefficients for this polynomial equation are stored in *mechfail_ds.def*.

9.3.1.3 Effect of Temperature on Drip Shield Capacity

The abstraction discussed in Section 9.3.1.2 is based on structural evaluations (Ibarra, et al., 2007a,b) at a drip shield temperature of 150 °C [302 °F]. MECHFAIL includes a temperature multiplier, F_{temp} , to alter the drip shield vertical-load-carrying capacity, $P_{v,DScap}$, when the drip shield temperature exceeds 150 °C [302 °F]. The drip shield capacity is not altered if the temperature drops below 150 °C [302 °F].

The temperature multiplier, F_{temp} , is a function of the drip shield side temperature, which is computed in NFENV and passed to MECHFAIL. MECHFAIL linearly interpolates between the values provided in *mechfail_ds.def* to obtain the multiplier F_{temp} .

9.3.1.4 Effect of Creep on Drip Shield Capacity

Creep failure for the drip shield titanium alloys is defined in MECHFAIL as creep deformation leading to plastic strains associated with the ultimate tensile strength of the material and is reached when the stress levels are close to the yield stress (Ankem and Wilt, 2006). Thus, MECHFAIL further adjusts the drip shield vertical-load-carrying capacity, $P_{v,DScap}$, via the creep multiplier.

The creep multiplier, F_{creep} , is a combination of two parameters. Because creep failure is related to the drip shield capacity at which yield of drip shield components begins, the first parameter, C_{yield} , alters the drip shield vertical-load-carrying capacity to the drip shield yielding capacity. This parameter is located in *mechfail_ds.def*. The second parameter, C_{thresh} , is the creep threshold (with respect to the yield stress) for creep failure and is defined in *tpa.inp* as DripShieldCreepThreshold[].

$$F_{creep} = C_{yield} C_{thresh} \quad (9-1)$$

⁷ Where # refers to the TPA Version 5.1 subareas for the potential repository, and Rock1 and Rock2 refer to lithophysal and nonlithophysal rocks, respectively.

9.3.1.5 Effect of General Corrosion on Drip Shield Capacity

Drip shield shell thickness variation due to general corrosion is computed in DSFAIL and passed to MECHFAIL. Then the drip shield capacity, $P_{v,DScap}$, is altered according to the drip shield corrosion multiplier, $F_{DS,t}$, which is a function of the drip shield shell thickness variation. The multiplier $F_{DS,t}$ is based on a polynomial equation (Table 9-2). The coefficients for this equation are stored in *mechfail_ds.def*.

9.3.1.6 Effect of Seismic Loading on Drip Shield Capacity

MECHFAIL assumes that seismic events with a mean annual frequency of exceedance lower than 10^{-5} lead to the collapse of the drip shields that are able to withstand the static vertical load (Ibarra, et al., 2007a). For seismic events associated with a mean annual frequency of exceedance between 10^{-5} and 10^{-4} , TPA Version 5.1 includes a simplified approach in which the applied load in the vertical direction due to the inertial forces is increased proportionally to the peak ground acceleration.

9.3.2 Drip Shield–Waste Package Mechanical Interaction

To estimate waste package breaching due to mechanical failure, MECHFAIL evaluates the conditions in which a collapsed drip shield interacts with a waste package leading to stress concentrations in the outer container. MECHFAIL compares these static and seismic loading demands to the waste package vertical-load-carrying capacity, which is associated with the ultimate tensile strength of the waste package outer container material. The waste package capacity is modeled as a function of the contact angle and contact length between the drip shield and the waste package, the static and seismic demands, and thinning of the waste package outer container due to general corrosion.

9.3.2.1 Effect of Contact Angle on Waste Package Capacity

The *tpa.inp* parameter ContactAngleSubarea_#[degrees]⁸ refers to the angle (α) formed between the bulkhead or longitudinal stiffener of a collapsed drip shield and the waste package outer container (Figure 9-3). MECHFAIL utilizes a cubic piecewise Hermite polynomial to evaluate the static loading that the waste package can withstand for different contact angles as a force per unit length, F_{unit} (Table 9-2). Coefficients for the polynomial are stored in the auxiliary input data file *mechfail_wp.def*.

9.3.2.2 Effect of Contact Length on Waste Package Capacity

The contact length (continuous or a sum of intermittent contact lengths) between the drip shield component and the waste package outer container is required to convert the load-per-unit length obtained from the plane strain models to pressure. This parameter is provided in *tpa.inp* as ContactLengthSubarea_#[m].⁹ Once the contact length is estimated, MECHFAIL applies the

⁸ Where # refers to the TPA Version 5.1 subareas for the potential repository.

⁹ Ibid.

following equation to convert the force-per-unit length to the waste package vertical pressure capacity

$$P_{v,WPcap} = \frac{F_{unit}}{A_{trib}} \frac{L_{cont}}{L_{unit}} \quad (9-2)$$

where

- F_{unit} — force per unit length [kN/m]
- A_{trib} — tributary area of the drip shield bulkhead or stiffener (i.e., the area of drip shield crown that transfers loads throughout the evaluated drip shield component), as specified by the *tpa.inp* parameter DripShieldBulkheadTributaryArea[m^2]
- L_{cont} / L_{unit} — nondimensional term where the numerator is the contact length, as specified by the *tpa.inp* parameter ContactLengthSubarea_#[], and the denominator is unity

9.3.2.3 Effect of General Corrosion on Waste Package Capacity

General corrosion on the Alloy 22 and titanium plates is assumed to cause thinning of the drip shield shell and waste package outer container, which may be in contact for long periods of time. EBSFAIL provides the waste package outer container thickness.

The potential for mechanical breaching of the waste package outer container increases as its thickness reduces. A polynomial equation defines the relationship between the capacity and plate thickness of the waste package outer container in *mechfail_wp.def* (Section 9.5). This variation is represented as the thickness multiplier F_{tp} , which alters the vertical-load-carrying capacity of the waste package outer container, $P_{v,WPcap}$.

9.3.2.4 Vertical Pressure Due to Seismic Loading

The MECHFAIL abstraction for seismic loading is based on a simplified approach where a quasi-static vertical load represents the effect of potential seismic events as a function of the peak ground acceleration. Equation (9-3) approximates the effect that a seismic event may have on the applied static load

$$P_{v,dyn} = (1 + PGA_i) P_{v,stat} F_{dyn} \quad (9-3)$$

where

- $P_{v,dyn}$ — applied dynamic (seismic) pressure [kPa]
- PGA_i — peak ground acceleration of the evaluated seismic event [g]
- $P_{v,stat}$ — static pressure [kPa] provided by DRIFTFAIL
- F_{dyn} — dynamic amplification factor with respect to the inertial forces, as specified by *tpa.inp* parameter DynamicAmplificationFactor[]

As a consequence of seismic events, the rubble accumulated around the drip shield would compact after vibratory ground motions. The compaction will decrease the rubble bulking factor, increasing the static loading demands.

MECHFAIL receives as input parameters the number of seismic events, the time at which the events occur, and the remaining seismic parameters provided by the SAMPLER utility module (Chapter 3) through the array `Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_]` provided in *tpa.inp*. The first individual parameter in each line corresponds to the mean annual frequency of exceedance. The rest of the parameters in each line are associated with the mean annual frequency of exceedance and refer to the mean peak ground velocity in the horizontal direction, median peak ground acceleration along the vertical direction, standard deviation of the natural logarithm of peak ground acceleration, lower boundary for compaction factor, and upper boundary for compaction factor, respectively. As mentioned in Section 9.3.1.6, Eq. (9-3) is also used to evaluate the drip shield structural performance under seismic events associated with a mean annual frequency of exceedance between 10^{-5} and 10^{-4} .

9.4 Input Parameters in *tpa.inp*

Table 9-1 summarizes key input parameters in the order in which they appear in *tpa.inp*. The parameter values correspond to the reference case.

9.5 Auxiliary Input Data and External Process Models

The MECHFAIL section of *tpa.inp* provides the user with the flexibility to evaluate the input demand parameters affecting the engineered barrier system mechanical performance. Additional parameters related to the engineered barrier system capacities are included in *mechfail_ds.inp*, *mechfail_ds.def* and *mechfail_wp.def* (Table 9-2). These parameters are tailored to design specifications and site data and results of process-level modeling. The user should exercise caution when modifying these data.

Table 9-1. Reference Data for Parameters of tpa.inp Used by MECHFALL (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MECHFALL	CalculateTemperatureMultiplierFlag(yes=1,no=0)	Flag to perform drip shield temperature adjustment	iflag 1	Drip shield temperature adjustments are performed as part of the reference case.
MECHFALL	CalculateCreepMultiplierFlag(yes=1,no=0)	Flag to evaluate drip shield creep processes	iflag 1	Drip shield creep processes are evaluated as part of the reference case.
MECHFALL	Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax [1/yr,m/s,m/s ² ,_,_,_]	Array of seismic parameters associated with discrete points of the selected hazard curve [1/hr, m/s, s ² , unitless, unitless, unitless]	hazardcurve 5 1.0e-4 0.47 0.38 0.64 0.10 0.20 1.0e-5 1.05 1.85 0.64 0.20 0.40 1.0e-6 2.44 4.13 0.53 0.30 0.60 1.0e-7 5.35 11.04 0.53 0.40 0.60 1.0e-8 5.35 11.04 0.53 0.40 0.60	The natural number of the first row is a table link controlling the number of entries in the array. The first value of each subsequent row is the mean annual frequency of exceedance. The rest of the values are associated with the corresponding mean annual frequency of exceedance and refer to the mean peak ground velocity in the horizontal direction, median peak ground acceleration in the vertical direction, standard deviation of the natural logarithm of the peak ground acceleration, lower boundary for compaction factor, and upper boundary for compaction factor. Values are consistent with Ibarra, et al. (2007b).
MECHFALL	SeedForRandomNumberForSEISMO	A random number seed for sampling the time and magnitude of seismic events [unitless]	constant 1456789101.0	The value must be an odd number between 2 ³⁰ and 2 ³¹ (Iman and Shortencarier, 1984; Wyss and Jorgensen, 1998).

Table 9-1. Reference Data for Parameters of tpa.inp Used by MECHFALL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Remarks	Distribution Type and Parameter Value(s)	Remarks
MECHFALL	ContactAngleSubarea_1 [degrees], ContactAngleSubarea_2 [degrees], ContactAngleSubarea_3 [degrees], ContactAngleSubarea_4 [degrees], ContactAngleSubarea_5 [degrees], ContactAngleSubarea_6 [degrees], ContactAngleSubarea_7 [degrees], ContactAngleSubarea_8 [degrees], ContactAngleSubarea_9 [degrees], ContactAngleSubarea_10 [degrees]	α The angle between the drip shield bulkhead or the longitudinal stiffener and the waste package outer container [degrees]	normal -30.8, 30.8	The contact angle is expected to have values smaller than 10–15° (Ibarra, et al., 2007b). A normal distribution is selected for this parameter with zero mean and standard deviation of 10. The probability density area for some intervals of interest are obtained: $P(-30 \leq \alpha \leq 30) \approx 99.7$ percent $P(-20 \leq \alpha \leq 20) \approx 95.5$ percent $P(-10 \leq \alpha \leq 10) \approx 68.3$ percent $P(-5 \leq \alpha \leq 5) \approx 38.3$ percent

Table 9-1. Reference Data for Parameters of tpa.inp Used by MECHFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Remarks	Distribution Type and Parameter Value(s)	Remarks
MECHFAIL	ContactLengthSubarea_1[m], ContactLengthSubarea_2[m], ContactLengthSubarea_3[m], ContactLengthSubarea_4[m], ContactLengthSubarea_5[m], ContactLengthSubarea_6[m], ContactLengthSubarea_7[m], ContactLengthSubarea_8[m], ContactLengthSubarea_9[m], ContactLengthSubarea_10[m]	L_{cont} The contact length between the drip shield component and the waste package outer container [m]	normal 0.192, 0.808	The contact length is based on results from three-dimensional finite element models (Ibarra, et al., 2007b). A normal distribution with a mean value of 500 mm [19.7 in] and a standard deviation of 100 mm [3.9 in] is used for this parameter.
MECHFAIL	DripShieldBulkheadTributary Area[m^2]	A_{trib} Area of the drip shield crown that transfers loads throughout the evaluated drip shield component [m ²]	constant 2.3	The tributary area is assumed to be constant and is set at 2.3 m ² [24.8 ft ²] (Ibarra, et al., 2007b). This tributary area assumes that the drip shield component interacting with the waste package is a bulkhead.

Table 9-1. Reference Data for Parameters of tpa.inp Used by MECHFAIL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Remarks	Distribution Type and Parameter Value(s)	Remarks
MECHFAIL	DripShieldHorizToVertLoad RatioRock1Subarea_1[], DripShieldHorizToVertLoad RatioRock1Subarea_2[], DripShieldHorizToVertLoad RatioRock1Subarea_3[], DripShieldHorizToVertLoad RatioRock1Subarea_4[], DripShieldHorizToVertLoad RatioRock1Subarea_5[], DripShieldHorizToVertLoad RatioRock1Subarea_6[], DripShieldHorizToVertLoad RatioRock1Subarea_7[], DripShieldHorizToVertLoad RatioRock1Subarea_8[], DripShieldHorizToVertLoad RatioRock1Subarea_9[], DripShieldHorizToVertLoad RatioRock1Subarea_10[]	Lateral-to-vertical load ratio applied to the drip shield for Rock Type 1 (lithophysal) [unitless]	beta 0.0, 1.0, 9.8306, 9.8306	The probabilistic distribution for the horizontal-to-vertical load ratio (P_h/P_v) is based on the theory of lateral earth pressure for fragmental media (Ibarra, et al., 2007b, Appendix A). The median value for Rock Type 1 is proposed at $P_h/P_v = 0.5$, the lower limit is slightly smaller than $P_h/P_v = 0.20$, and the upper limit is $P_h/P_v = 1.0$. A standard beta distribution is selected with a mean value of 0.5 and a standard deviation of 0.11. The probability density areas at several intervals of interest follow. $P(P_h/P_v < 0.20) \approx 0.17 \text{ percent}$ $P(P_h/P_v < 0.50) \approx 50.0 \text{ percent}$ $P(P_h/P_v < 0.80) \approx 99.8 \text{ percent}$ $P(P_h/P_v < 1.00) \approx 100.0 \text{ percent}$ The probabilistic distributions for rock types 1 and 2 are the same because spatial variability is not considered in TPA Version 5.1.

Table 9-1. Reference Data for Parameters of tpa.inp Used by MECHFALL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Remarks	Distribution Type and Parameter Value(s)	Remarks
MECHFALL	DripShieldHorizToVertLoad RatioRock2Subarea_1[], DripShieldHorizToVertLoad RatioRock2Subarea_2[], DripShieldHorizToVertLoad RatioRock2Subarea_3[], DripShieldHorizToVertLoad RatioRock2Subarea_4[], DripShieldHorizToVertLoad RatioRock2Subarea_5[], DripShieldHorizToVertLoad RatioRock2Subarea_6[], DripShieldHorizToVertLoad RatioRock2Subarea_7[], DripShieldHorizToVertLoad RatioRock2Subarea_8[], DripShieldHorizToVertLoad RatioRock2Subarea_9[], DripShieldHorizToVertLoad RatioRock2Subarea_10[]	Lateral-to-vertical load ratio applied to the drip shield for Rock Type 2 (nonithophysal) [unitless]	beta 0.0, 1.0, 9.8306, 9.8306	The probabilistic distribution for the horizontal-to-vertical load ratio (P_h/P_v) is based on the theory of lateral earth pressure for fragmental media (Ibarra, et al., 2007b, Appendix A). The median value for Rock Type 2 is proposed at P_h / P_v = 0.5, the lower limit is slightly smaller than P_h/P_v = 0.20, and the upper limit is P_h/P_v = 1.0 (Ibarra, et al., 2007b). A standard beta distribution is selected with a mean value of 0.5 and a standard deviation of 0.11. The probability density areas at several intervals of interest follow. $P(P_h/P_v < 0.20) \approx 0.17$ percent $P(P_h/P_v < 0.50) \approx 50.0$ percent $P(P_h/P_v < 0.80) \approx 99.8$ percent $P(P_h/P_v < 1.00) \approx 100.0$ percent The probabilistic distributions for rock types 1 and 2 are the same because spatial variability is not considered in TPA Version 5.1.
MECHFALL	DripShieldCreepThreshold[]	C^{thresh} Threshold for creep failure of drip shield materials with respect to yield stress [unitless]	uniform 0.9, 1.2	The lower boundary corresponds to stresses exceeding 90 percent of the yield strength and the upper boundary is 120 percent of the yield strength (Ibarra, et al., 2007b).

Table 9-1. Reference Data for Parameters of tpa.inp Used by MECHFALL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Remarks	Distribution Type and Parameter Value(s)	Remarks
MECHFALL	DynamicAmplificationFactor[]	F_{dyn} Increase in the dynamic loading with respect to the peak ground acceleration [unitless]	constant 1.0	The dynamic amplification factor is taken from Ibarra, et al. (2007b).

Table 9-2. Auxiliary Input Data Files Used by MECHFAIL	
File	Contents
<i>mechfail_ds.def</i>	This file includes parameters related to the drip shield capacity. Section 1 of this file, “Control Flags,” provides the debug flag to create <i>mechfail_ds.dbg</i> and a mechanical failure flag to indicate that this file provides input to the MECHFAIL subroutines addressing drip shield performance. Section 2 contains coefficients of tenth-order polynomial equations related to drip shield capacity abstractions. For abstractions that require less than tenth-order polynomials, some of the coefficients are zero. The first set of coefficients is used for the equation that computes the vertical-load-carrying capacity of the drip shield as a function of the horizontal-to-vertical load ratio (Ibarra, et al., 2007a, Appendix B, Section B.3). The second and third set of coefficients are used for the step function defining the thickness multiplier, $F_{DS,t}$ (Section 9.3.1.4 and Ibarra, et al., 2007a, Appendix B, Section B.6). The fourth set of coefficients is for the parameter C_{yield} (Ibarra, et al., 2007a, Appendix B, Section B.5). Section 3 is an interpolation table to obtain the temperature multiplier, F_{temp} (Section 9.3.1.2 and Ibarra, et al., 2007a, Appendix B, Section B.4). Sections 4 through 7 refer to data used only when MECHFAIL is executed separately from TPA Version 5.1.
<i>mechfail_wp.def</i>	This file includes parameters related to the waste package capacity. The first section, “Control Flags,” contains the debug flag that creates <i>mechfail_wp.dbg</i> . The mechanical failure flag of <i>mechfail_ds.def</i> indicates that MECHFAIL will evaluate waste package outer container mechanical performance. The first nine columns of coefficients in Section 2 correspond to the spline function used to describe the effect of the contact angle parameter on the waste package capacity expressed as a force per unit length, F_{unit} (Ibarra, et al., 2007b, Appendix C, Section C.1). The last column includes the coefficients of the polynomial equation used to compute the variation of waste package outer container thickness due to general corrosion (Ibarra, et al., 2007b, Appendix C, Section C3). Sections 3 through 6 include data used only when MECHFAIL is executed separately from TPA Version 5.1.

9.6 Intermediate Outputs and Information Passed to Other Modules

Table 9-3 presents the intermediate output files produced by MECHFAIL. Table 9-4 shows the optional intermediate output files that contain information of both drip shield and waste package mechanical performance. These intermediate output files are activated in the *tpa.inp* input block titled <<Output Print Options>> by setting the output mode parameter, OutputMode(0=None,1=All,2=UserDefined), to a value of 1 or 2. When set to 1, all optional intermediate output for MECHFAIL will be saved for all realizations. When set to 2, optional intermediate output selected will be saved for realizations starting from *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by *tpa.inp* parameter UserDefinedUpperRealizationAppended (Table 4-7).

Setting OutputMode(0=Name,1=All,2=UserDefined) to 1 or 2 causes intermediate output files to be written for other modules if the parameter SelectAppendFiles remains set at the default value of 0. If the user is interested only in the MECHFAL intermediate outputs, the SelectAppendFiles parameter in the <<Output Print Options>> input block should be set to a value of 4 for just *mechfail.ech* and *mechfail.rlt* (Table 4-7).

Table 9-3. Intermediate Output Files Created During Execution of MECHFAL	
File	Contents
<i>mechfail_ds.res</i>	This file contains, for each realization, the output parameters computed in MECHFAL for drip shield performance such as static and seismic demands, drip shield capacity, creep threshold, and type of failure (static or dynamic).
<i>mechfail_ds.inp</i>	This intermediate file contains the input parameters from <i>tpa.inp</i> and <i>mechfail_ds.def</i> needed when the standalone code MECHFAL executes for the drip shield. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.
<i>mechfail_wp.res</i>	This output file contains, for each realization, the output parameters computed in MECHFAL when waste package failure occurs. The information presented includes static and seismic demands, contact angle, contact length, waste package outer container thickness, and type of failure (static or dynamic).
<i>dsfail.res</i>	This file contains failure time and the number of drip shield mechanical failures for each realization and subarea. See Chapter 19 for additional details.
<i>wpsfail.res</i>	For each realization and subarea, this file presents the failure time and the number of waste package mechanical failures. See Chapter 19 for additional details.
<i>mechfail_ds.dat</i>	This intermediate file contains the timesteps for the subarea indicating whether drip shield failure occurs due to static loading, dynamic loading, or corrosion. A summary at the end of the file shows the drip shield failure times, static and seismic demands at the time of failure (e.g., vertical pressure), and drip shield capacity parameters. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.

Table 9-3. Intermediate Output Files Created During Execution of MECHFALL (continued)	
File	Contents
<i>mechfail_ds.dbg</i>	This output file is created by activating the debug flag in <i>mechfail_ds.def</i> . The file contains debug information for mechanical drip shield failure such as timestep, drip shield temperature, drip shield thickness, static and dynamic demands, drip shield capacity, creep multiplier, and corrosion multiplier for both rock types. This file contains error messages that occur during the execution of MECHFALL of the last realization.
<i>mechfail_wp.inp</i>	This intermediate file contains the input parameters from <i>tpa.inp</i> and <i>mechfail_wp.def</i> needed when the standalone code MECHFALL executes for the waste package. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information.
<i>mechfail_wp.dat</i>	This intermediate file computes information about the waste packages exhibiting mechanical failure in MECHFALL. The file contains the timesteps for the subarea indicating whether waste package failure occurs due to static or dynamic loading. A summary at the end of the file shows the waste package failure times, vertical pressure, waste package thickness, contact angle, contact length, and peak ground acceleration. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.
<i>mechfail_wp.dbg</i>	This output file can be created by activating the debug flag in <i>mechfail_wp.def</i> . The file contains debug information for waste package mechanical failure such as timestep, waste package outer container thickness, static and dynamic demands, waste package capacity, and corrosion multiplier. This file contains error messages that occur during the execution of MECHFALL of the last realization.
<i>mechfail.inp</i>	This output file builds either <i>mechfail_ds.inp</i> or <i>mechfail_wp.inp</i> , depending on whether the standalone code MECHFALL was last executed for the drip shield or the waste package, respectively. This file is overwritten each time the standalone code MECHFALL is executed; at the end of a simulation, this file contains the input information for the last execution of MECHFALL for the last subarea of the last realization.

Table 9-4. Optional Intermediate Output Files Created During Execution of MECHFAIL	
File	Contents
<i>mechfail.ech</i>	The input parameters sent to MECHFAIL for the drip shield and waste package for every realization and subarea are presented in this file. This file displays information such as static and seismic demands, and drip shield and waste package thickness.
<i>mechfail.rlt</i>	This file presents the output parameters of each subarea for all timesteps for both the drip shield and waste package performance. The information includes timestep, drip shield, and waste package failures due to static or dynamic loading and corrosion.

9.7 Techniques for Understanding Module Performance

Although there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of MECHFAIL-modeled processes. Mechanical degradation processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques may be useful to understand the effects of mechanical degradation on system-level performance.

In addition, “pinch-point” techniques, where output or intermediate results produced by MECHFAIL can be understood in combination with output or intermediate results from other modules (e.g., DRIFTFAIL), may help evaluate subsystem processes. Key files useful for these comparisons include *mechfail_ds.inp*, *mechfail_ds.dat*, *mechfail_wp.inp*, and *mechfail_wp.dat*, which contain the inputs and results for individual drip shield and waste package failure calculations. An examination of these files allows the user to compare starting conditions (rock properties, seismic events, etc.) with end results (rubble heights, pressures, etc.). However, these files show only the results for the last subarea calculation. For more detailed evaluation of drip shield and waste package mechanical failure for each subarea, the user may examine the optional output file *mechfail.ech*, which contains the demands and capacities evaluated, and *mechfail.rlt*, which contains the times at which drip shields and waste packages fail for each subarea evaluated in each realization.

The effects of individual parameters with respect to particular subsystem processes can be examined by varying an input parameter and analyzing results from relevant output and intermediate output files. TPA Version 5.1 supports input parameters for their provided ranges; the user should exercise care in interpreting results from simulations in which input data are altered beyond their intended ranges.

Key input parameters that may significantly influence MECHFAIL results include the parameter representing the effect of lateral loading on the drip shield vertical load capacity, which is evaluated by varying the *tpa.inp* parameters `DripShieldHorizToVertLoadRatioRock1Subarea_#[]` and `DripShieldHorizToVertLoadRatioRock2Subarea_#[]`. Note that the vertical load applied to the drip shield is modified in the DRIFTFAIL section of *tpa.inp*.

The reference case includes several loading sources that may lead to drip shield structural instability. Some of these effects may be evaluated separately by adjusting explicit flags or by modifying some key parameter values. For instance, if the user is not interested in evaluating the effect of creep on the drip shield performance (Section 9.3.1.4), the flag CalculateCreepMultiplierFlag(yes=1,no=0) can be inactivated. This permits estimation of the drip shield performance in the inelastic range because creep deformation is associated with stress levels that are close to the yield stress.

Also, if the user is interested in evaluating the effect of temperature on the drip shield performance (Section 9.3.1.3), the flag CalculateTemperatureMultiplierFlag(yes=1,no=0) may be inactivated.

Variations of the seismic parameters clustered in the array Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s²,_,_,_] would provide insight into the parameters with the largest effect on waste package performance. The best alternative to manipulate waste package performance under degrading drifts is by means of the F_{dyn} parameter. This parameter linearly modifies the seismic demands on the waste package (Eq. 9-3).

9.8 References

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10 ENGINEERED BARRIER SYSTEM RADIONUCLIDE RELEASE (EBSREL)

The Engineered Barrier System Radionuclide Release module (EBSREL)¹ calculates the time-dependent release rate of radionuclides from the engineered barrier system. EBSREL computes water flow rates to waste forms inside breached waste packages, waste form dissolution, dissolved and colloid-facilitated radionuclide release from waste packages, and transport to the unsaturated zone. EBSREL receives as input the time-dependent seepage water flow rate and waste package temperature from the Near-Field Environment module (NFENV),² the drip shield corrosion breach time from the Drip Shield Corrosion Failure module (DSFAIL),³ waste package corrosion breach times from the Waste Package Corrosion Failure module (EBSFAIL),⁴ the time and number of mechanical drip shield and waste package breaches from the Drip Shield and Waste Package Mechanical Failure module (MECHFAIL),⁵ the time and number of waste packages breached by faulting from the Direct Faulting Disruptive Event module (FAULTO)⁶ (when activated), and the time and number of waste packages breached by igneous intrusion from the Igneous Disruptive Event Involving Magma module (VOLCANO)⁷ (when activated). EBSREL delivers subarea radionuclide release rates as a function of time to the Unsaturated Zone Flow and Transport module (UZFT).⁸ EBSREL is executed for each potential repository subarea specified in any TPA Version 5.1 realization for the reference case.

10.1 Conceptual Model

The purpose of EBSREL is to compute time-dependent radionuclide releases, in units of Ci/yr, to be used as boundary conditions for UZFT. EBSREL computes the release rate by taking into account (i) estimates of the amount of water flowing into and out of the waste package, (ii) waste form dissolution and radionuclide release, (iii) upscaling of radionuclide release rates from a representative waste package to a subarea for each of several failure modes, and (iv) a

¹The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

²The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

³The Drip Shield Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation DSFAIL will be used.

⁴The Waste Package Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

⁵The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAIL will be used.

⁶The Direct Faulting Disruptive Event module is referenced frequently throughout this chapter. The abbreviation FAULTO will be used.

⁷The Igneous Disruptive Event Involving Magma module is referenced frequently throughout this chapter. The abbreviation VOLCANO will be used.

⁸The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

source term for colloidal releases. Radionuclides released from the waste package in dissolved and colloidal form are transported directly to the unsaturated zone.

10.1.1 Flow Rate Per Waste Package to Mobilize Waste Forms

As percolating water moves toward the drift and waste package, flow is focused or diverted by several processes, and the flow rate of water contacting the waste package changes. Flow into waste packages is not possible when the drift temperature is greater than a threshold value. Deep percolation can be modified in the natural system by structural features such as fractures and faults—hydrogeological characteristics that determine the convergence or divergence of flow in the host rock. Degraded components of the engineered barrier system (e.g., drift, drip shield, and waste package) may partially divert seepage water. Water seepage into any failed waste packages will be affected by the physical nature of the waste package breach. Thus, waste forms in waste packages with different breach mechanisms, such as localized corrosion, mechanical breaching from rock load transfers due to drip shield collapse, and general corrosion, may be subject to different water flow conditions.

Specifically, flow in EBSREL is modified to account for the following features and processes. In each case, flow into waste packages also is affected by general corrosion of the waste package when this process occurs. In TPA Version 5.1, a waste package breached by general corrosion does not divert water. (Note that, in this chapter, the terms “fail” and “breach” suggest only that an opening has formed on a waste package—not that it is necessarily releasing radionuclides.)

10.1.1.1 Convergence/Divergence of Flow

In TPA Version 5.1, fractures are the primary sources of drips on waste packages, and water flowing in fractures is focused from an area proportional to the spacing between drips. The greater the spacing between seep points, the higher the flow rate in the wet fractures and, thus, the flow is more focused. Large-scale (greater than drift-scale) features can create convergence or divergence of deep percolation flow toward or away from the drift.

10.1.1.2 Near- and In-Drift Flow Diversion

Deep percolation that approaches a drift wall has the potential to contact waste packages as seepage. Processes causing flow to be altered include capillary diversion around the drift opening and water diversion in the form of film flow along drift walls. In addition, flow into the drift is not possible under elevated thermal conditions. Capillary diversion around drift openings will occur if fractures are small enough and the fracture network has adequate connectivity. Water flow crossing the capillary barrier into the drift can drip from the ceiling or from protuberances along the drift. Some of the water, however, may be diverted as film or rivulet flow along the drift walls.

10.1.1.3 Rubble

As drift degradation proceeds and rubble begins accumulating on the top of the drip shield (Chapter 6), water flow may converge or be diverted by the rubble pile.

10.1.1.4 Drip Shield

In TPA Version 5.1, the drip shield may fail by mechanical buckling (Chapter 9) or by general corrosion (Chapter 8). Mechanically collapsed drip shields may partially protect the waste package against seepage or water flow through rubble. Also, after the drip shield is breached by general corrosion, no credit is taken for flow diversion and the flow of unaltered seepage water is passed to the waste package surface.

10.1.1.5 Breached Waste Packages

In TPA Version 5.1, waste packages may be breached by initial defects, mechanical loading (Chapter 9), localized and general corrosion (Chapter 8), faulting (Chapter 13), and igneous activity (Chapter 14). The mode of breaching can affect the flow of water into the failed waste packages. Flow into the failed waste packages may be partially diverted when the breaching results from initial defects, mechanical loading, or localized corrosion. When breaching results from general corrosion, faulting, or igneous activity, no credit is taken for flow diversion and unaltered flow through the drip shield is passed directly into the failed waste package.

10.1.2 Waste Form Dissolution and Radionuclide Release

Water flow rates are used in mass conservation computations to estimate concentrations of radionuclides in water accumulated inside breached waste packages. Radionuclide concentration computations account for (i) inventories inside the waste package including waste forms, radionuclides in solution, and radionuclides in precipitated phases; (ii) decay and ingrowth of inventories; (iii) solubilities of radionuclide-bearing solid phases; (iv) different waste form dissolution rates for spent nuclear fuel and high-level waste glass; and (v) radionuclides carried by flowing water away from the waste package (i.e., advective release).

For release computations, two water contact modes are considered, referred to as “bathtub” and “flowthrough.” In the bathtub mode, water enters the waste package at a breached location, which gradually fills with water until an exit point is reached. At that time, the flow rate into the waste package is in balance with the outlet flow, and the volume of the water pool inside the waste package remains constant. Radionuclides carried by flowing water are not released until after the waste package overflows. The flowthrough mode is modeled as a particular case of the bathtub mode, with an instantaneous fill time immediately after water enters the waste package.

In EBSREL, a waste package contains only one of two waste form types: spent nuclear fuel or high-level waste glass. Both waste forms are treated in the same mathematical manner and are differentiated only by initial inventories and the adoption of different waste form dissolution rates. Four alternative models are available for spent nuclear fuel dissolution. 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 nuclear fuel dissolution rate, derived from tests in groundwater containing calcium and silicon. Model 3 allows direct user input of a constant rate, and Model 4 invokes dissolution control by the solubility of schoepite, a potential spent nuclear fuel alteration phase. For glass waste, the dissolution rate depends on temperature and pH.

An exploratory model to account for cladding protection of spent nuclear fuel is available in EBSREL. This model simulates gradual exposure of spent nuclear fuel as cladding degrades along the fuel rod longitudinal axis.

As the waste form degrades, radionuclides are released congruently to water in proportion to their inventories in the waste form. The dissolved concentration of an element (i.e., the combined mass of released isotopes) is subject to an equilibrium solubility limit. In addition, for all spent nuclear fuel dissolution models, a fraction of certain radionuclides in the spent nuclear fuel waste form inventory is released instantaneously when the waste form is exposed to water. This gap fraction represents rapid release from grain boundaries and the pellet-cladding gap.

EBSREL includes an exploratory model to simulate diffusive radionuclide release. The diffusive release model is a simplified representation of diffusion through a diffusive pathway composed of two segments: a water film inside the waste package and a narrow aperture across the waste package thickness.

10.1.3 Release Upscaling

The radionuclide source term for the groundwater pathway in TPA Version 5.1 depends on the definition of waste package failure classes. The waste package failure 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 failure classes are needed to quantify the number of waste packages contributing to radionuclide release and to define radionuclide releases of the representative waste package in a class. Waste packages in a class can undergo more than one degradation process (e.g., mechanically breached waste packages can also experience breaching due to localized and general corrosion). Water flow rates are adjusted as a function of time to model multiple degradation processes potentially affecting a waste package (Section 10.1.1).

Total subarea releases from a waste package failure class are computed by multiplying the release from a representative waste package by the total number of waste packages in the class that contribute to release. Within a class, the number of packages contributing to release may be a subset of the number of breached packages. Not all breached waste packages may be contacted by water, and not all breached waste packages contacted by water may allow water to enter the package.

10.1.4 Colloidal Release

Advective radionuclide releases are adjusted to simulate the release of colloids with irreversibly adsorbed plutonium, americium, thorium, and curium. The source term colloidal model is based on the concept of competitive sorption, under which radionuclides compete for available sorption sites on colloids according to element-dependent affinity factors (i.e., elements with higher affinities more readily occupy sorption sites in colloids). In the presence of colloids, equilibrium is maintained between waste form and solution for purposes of solubility control; (i.e., association with colloids can allow a radionuclide to be released at a total concentration that exceeds its solubility limit).

10.2 Model Support and Assumptions

10.2.1 Flow Rate Per Waste Package To Mobilize Waste Forms

A simple approach is adopted to abstract water flow rates per breached waste package. Deep percolation fluxes computed by NFENV (Chapter 7) are modified by multiplication factors representing convergence and divergence above the drift and flow-limiting characteristics of various breached engineered barrier system components (Section 10.1.1). The approach is computationally efficient and is easily and transparently factored into sensitivity analyses. It allows incorporation of alternative conceptual flow models, such as structural control of wetting along faults or fracture zones, without requiring code changes. Convergence and divergence of percolating flow above the drift is affected by fracture spacing (Basagaoglu, et al., 2007) (e.g., more widely spaced fractures drain water from larger volumes of rock). Water flow entering the drift can be diverted if the drift wall acts as capillary barrier or if the water travels as film flow along the drift walls; these processes are affected by the flow rate, the location of the flow along the sloping walls, and the physical characteristics of the drift walls (Phillips, 1996; Wood, et al., 2002; Basagaoglu, et al., 2007). Components of the engineered barrier system—rubble from drift degradation, the drip shield, and the waste package—will affect flow to the waste package to differing degrees, depending on its physical condition.

This model approach provides flexibility to evaluate the water flow models considered in the DOE performance assessment model accounting for partial diversion of water by structures of the engineered barrier system, such as the drift wall, drip shield, and waste package.

10.2.2 Waste Form Dissolution and Radionuclide Release

Radionuclide release rates of waste forms are based on expressions and parameters that reasonably summarize waste form dissolution rates reported in the literature (Ahn and Mohanty, 2004; Mohanty, et al., 2002, 2000). Four different alternatives are considered to compute the rate of spent fuel dissolution. In one alternative, the dissolution rate is computed as a function of temperature, pH, and carbonate concentration of solutions in contact with the spent fuel and is based directly on laboratory dissolution studies (Gray and Wilson, 1995). In the second alternative, the release rate is computed as an Arrhenius function of the temperature (Ahn and Mohanty, 2004). The expression incorporates various potential conditions of the in-package physical and chemical environment. The third alternative is a user-defined constant dissolution rate. This option provides a means for the user to apply an independently derived constant rate. In the fourth alternative, it is assumed that radionuclides are contained in schoepite and are released at a rate proportional to the flow rate through the waste package and the equilibrium concentration of uranium in contact with schoepite (Murphy and Codell, 1999). The fourth option is based on observations of schoepite as an important alteration phase after analog and laboratory spent nuclear fuel.

In the case of high-level waste glass, experimental results indicate that the dissolution rate dependence on pH and temperature is independent of the glass composition within the range of the glass compositions tested. Estimates of high-level waste glass dissolution rates are based on forward rate measurements on a five-component glass (Knauss, et al., 1990). The dissolution rate of glass waste forms tends to decrease in the presence of various dissolved ions; this effect was not included in the model because it is not easily quantified and would lead to lower radionuclide release rates. Radionuclide release from waste forms (spent fuel and

glass) is assumed to be congruent (i.e., radionuclide release rates are proportional to radionuclide mass fractions in the waste form, subject to solubility limits) (Bechtel SAIC Company, LLC, 2004a). Spent nuclear fuel packages and codisposal packages containing high-level waste glass waste differ in dimensions, but in TPA Version 5.1, for the sake of simplicity, the packages are assumed to have identical dimensions (i.e., diameter and length). The number of waste packages in the system is a function of the dimensions. TPA Version 5.1 properly tracks the total radionuclide inventory and releases; the number of waste packages is of secondary importance.

TPA Version 5.1 offers the flexibility to simulate either instantaneous or gradual degradation of spent nuclear fuel cladding. In the instantaneous case, cladding protection causes a decrease in the spent nuclear fuel dissolution rate equal to a constant factor throughout the simulation (the lower the extent of cladding degradation, the lower the adjusted dissolution rate). The slowing of the dissolution rate can be interpreted as due to the partial exposure of spent fuel to the environment due to degradation, while the complementary fraction of the spent fuel is protected by cladding. The gradual cladding degradation model is considered exploratory, to test alternative concepts, and is not subject to the same level of support as other models in TPA Version 5.1. The model for gradual cladding degradation, referred to as unzipping, is based on the concept that unzipping may occur at pinholes and hairline cracks as a result of spent nuclear fuel matrix alteration to secondary phases with higher molar volumes. As cladding degrades, more spent fuel is exposed, causing a gradual, effective increase in the total spent nuclear fuel dissolution rate.

The specific surface area used to compute effective release rates is assumed constant in time for both spent nuclear fuel and high-level waste glass. Processes potentially causing specific surface areas to change with time (e.g., gradual dissolution of spent nuclear fuel grains and development of fractures in glass) are not considered. This assumption of a constant specific surface is adopted for the sake of mathematical simplicity. Experimental analyses indicate that although grain boundary penetration and development of “wormy” textures in grains are noted in spent fuel, the overall fractional release generally tends to decrease with time (Bechtel SAIC Company, LLC, 2004a, pp. 6-38, 6-39). It is therefore assumed that uncertainty in the waste form dissolution rate is mainly controlled by corrosion rates, rather than by secondary processes such as changes in the specific surface area.

Waste forms corrode and dissolve in the presence of liquid water (Bechtel SAIC Company, LLC, 2004a,b). Corrosion of the waste form is assumed to start as soon as liquid water (seepage) contacts the waste form. Waste form dissolution in water films formed by humidity in air, which are likely to be ineffective at mobilizing radionuclides, is disregarded. For radionuclide solubility computations, for the sake of simplicity, and to enhance stability of integration routines, the water volume is considered to be constant at all times for both bathtub and flowthrough water contact modes (Mohanty, et al., 2003).

Radionuclide release into the unsaturated zone is constrained by solubility limits on aqueous concentration (Mohanty, et al., 2003; Murphy and Codell, 1999). A solubility limit is an appropriate maximum concentration because it is a thermodynamically-derived value that is unlikely to be exceeded in solution.

A fraction of the spent nuclear fuel inventory of fission products and low-atomic-mass radionuclides tends to migrate during in-reactor operations and accumulate at regions such as

grain boundaries, the interface between pellets and cladding, the rod plenum regions, and pellet fracture surfaces (Bechtel SAIC Company, LLC, 2004a). This inventory is referred to as the “gap inventory” and is specified via gap fraction parameters. The gap inventory may be loosely attached to the spent fuel matrix (Bechtel SAIC Company, LLC, 2004a). Accordingly, it is assumed that the gap inventory dissolves instantaneously as liquid water contacts spent nuclear fuel.

Based on laboratory and field studies, radionuclides such as thorium, plutonium, americium, and curium are known to sorb significantly—perhaps largely irreversibly—to iron oxyhydroxide minerals that result from aqueous corrosion of the stainless steel inner container and other in-package steel components (Bechtel SAIC Company, LLC, 2005b; Lu, et al., 2000, 1998). These corrosion products, if present and immobile in a breached waste package, could delay the release of radionuclides from the waste package to the invert and unsaturated zone. This retardation process is not simulated in EBSREL.

In EBSREL, the dominant mechanism of radionuclide release from the waste package is water advection because, in general, advective transport is much faster than diffusion. However, an exploratory model to simulate diffusive transport in water films connecting waste forms with the exterior of the waste package is available. The diffusive release model is a simplified representation of diffusion through a pathway composed of two segments: a water film inside the waste package and a narrow aperture across the waste package thickness. The cross section aperture on the waste package is assumed to increase linearly with time, and the concentration at the terminus of the diffusive pathway is assumed zero. In the diffusion model, processes such as retardation, decay, and ingrowth are ignored. The exploratory diffusion model allows assessment of diffusive releases DOE considered in its performance assessment model (Bechtel SAIC Company, LLC, 2005c) by appropriate selection of input parameters. Because the diffusion model is exploratory, it is not subject to the same level of support as other models in TPA Version 5.1.

A simplified advective-diffusive transport model is available to simulate radionuclide transport through the invert. However, the model is considered legacy code and it is not supported as part of TPA Version 5.1.

10.2.3 Release Upscaling

For computing radionuclide release rates, waste package failure classes are used to group waste packages exhibiting similar evolution of degradation based on a plausible set of mechanisms. The waste packages in a class in a subarea are assumed identical (e.g., same breach time, water flow rates, water volumes, water chemistry, temperature). Therefore, total releases of a class are derived by multiplying the release of a representative waste package by the total number of waste packages in the class.

To determine the number of waste packages in a class, probability factors are used to recognize that (i) not all of the breached waste packages may contribute to release (it is assumed that liquid water is a requirement to mobilize radionuclides in waste forms; not all of the waste packages may be contacted by liquid water) and (ii) a series of requirements must be fulfilled for waste packages to be breached by complex processes such as localized corrosion. The probability factors are assumed constant in time, but can account for variability in

phenomena such as the extent of drip shield damage, conditions favoring localized corrosion of the waste package, and the sizes of waste package ruptures.

10.2.4 Colloidal Release

Radionuclide release via irreversible attachment to colloids is included in EBSREL. Mobilization of radionuclides by colloid association is expected to be more effective if the radionuclide is permanently associated with the colloid (Bechtel SAIC Company, LLC, 2005b). Colloidal release is applied to release of those actinides—thorium, plutonium, americium, and curium—that tend to be strongly sorbed to engineered and natural materials (e.g., McMurry and Bertetti, 2005; Lu, et al., 2000, 1998). Release and transport of less sorptive elements are not appreciably enhanced by colloid association and, thus, are not included in the irreversible colloid release abstraction. The abstraction simulates colloidal mobilization by way of a model of irreversible sorption to the surfaces of iron oxyhydroxide colloids formed by corrosion of steel internal waste package components and the stainless steel inner container. (Note: In TPA Version 5.1, corrosion resistance of the stainless steel inner container is not considered; the stainless steel inner container is included here only as a source of corrosion product colloids.) This model assumes a single layer of sorption sites available on the colloid surface. Colloidal mobilization could also include the effects of waste form, groundwater, and true radionuclide colloids (Bechtel SAIC Company, LLC, 2005b); however, iron oxyhydroxide colloids were chosen for the abstraction because (i) laboratory data show the particular effectiveness of iron corrosion products in essentially irreversibly sorbing these actinides (Lu, et al., 2000, 1998), (ii) the combination of iron corrosion product colloid sorptive properties and potential concentration in in-package waters suggests that they dominate the colloidal actinide budget (Pickett, 2007a), (iii) the abundance and stability of waste form colloids in spent nuclear fuel waste packages is still in question (Buck, et al., 2004), and (iv) true colloids may dissolve during transport away from the engineered barrier system. The model for partitioning of radionuclides to the iron oxyhydroxide colloids considers limits to attachment arising from sorptive capacity and competition for sorption sites among actinides. Waste form, solution, and colloids interact directly, such that equilibrium is maintained between solution and waste form. This approach is valid from an equilibrium standpoint, because ions associated irreversibly with colloids do not affect solubility reactions controlling the dissolved concentration.

10.3 Implementation of Conceptual Model in TPA Version 5.1

EBSREL includes two standalone programs: RELEASET and EBSFILT. For a representative waste package, RELEASET computes radionuclide release from the waste package. EBSFILT computes transport through the invert when activated, although it is considered legacy code and it is not supported as part of TPA Version 5.1. EBSREL applies flow factors and enhanced solubility limits and computes colloid species release rates. Information flow within EBSREL is summarized as follows and is depicted in Figure 10-1.

NFENV passes the time-dependent water flow rate, and EBSREL modifies it by flow factors that account for processes that can adjust some of the flow before it enters the waste package (Section 10.3.1). This flow modification uses drip shield and waste package breach times from EBSFAIL and DSFAIL, as well as waste package breach times from the scenario-appropriate module (MECHFAIL, FAULTO, or VOLCANO). The resulting waste package water flow rate is passed, along with waste package temperature data (from NFENV) and enhanced solubility limits for the colloid model, to RELEASET to compute waste form dissolution and radionuclide

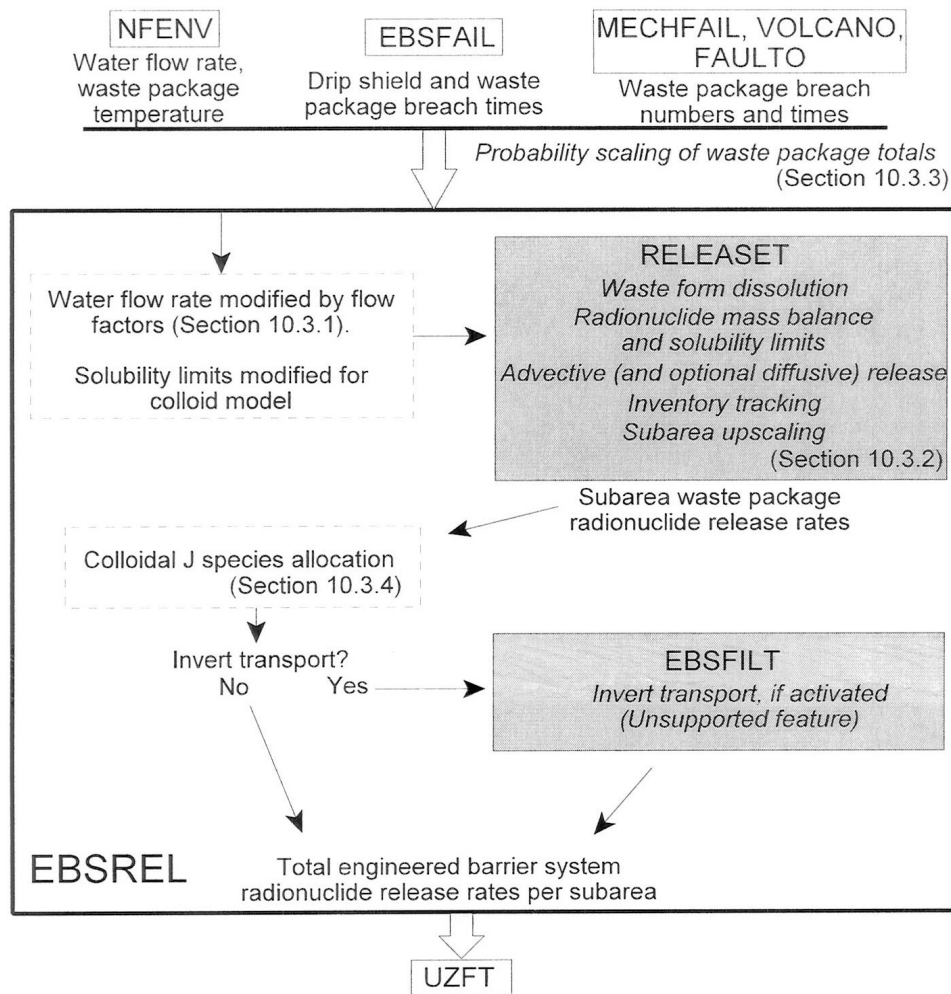


Figure 10-1. Information Flow Diagram for EBSREL

release rates for the representative waste package for each class (Section 10.3.2). RELEASET scales radionuclide release rates up from the representative waste packages to total releases for each subarea, using information on breach times and the number of breached waste packages from EBSFAIL, MECHFAL, FAULTO, and VOLCANO. The number of breached waste packages is adjusted in TPA Version 5.1 prior to calling EBSREL using probability factors that account for the number of waste packages with waste forms that are actually contacted and mobilized by water. Application of the probability factors is implemented in the utility module CUMFAIL2 (Chapter 4), but is described in detail in this chapter (Section 10.3.3). The RELEASET radionuclide release rates are used in EBSREL for allocation of radionuclide mass among dissolved and colloidal species (Section 10.3.4). The subarea release rate for each radionuclide species (including distinct colloidal species) in Ci/yr is then passed to UZFT.

10.3.1 Flow Rate Per Waste Package To Mobilize Waste Forms

This section describes the algorithm to estimate water flow rates per waste package (in units of m^3/yr) with the potential to mobilize waste forms. In the postthermal period, meteoric water at the site flows through fractured unsaturated rock and approaches the engineered barrier system at the volumetric flow rate Q_R [see the Climate and Infiltration module (UZFLOW)⁹ (Chapter 5) for a description of the estimation of ambient deep percolation]. In the thermal period, the volumetric flow rate Q_R is determined by the reflux rate breaching the vaporization barrier (Chapter 7). In EBSREL, flow factors related to components of the natural and engineered barrier system are used to modify Q_R to estimate water flow rates per waste package. The flow factors for the natural system account for structural features that determine the convergence or divergence of flow in the host rock. The engineered barrier system flow factors are defined as functions of breach times of different engineered features.

EBSREL computes the amount of water available for release according to

$$q_{in} = Q_R F_{FMF} F_{ow} F_{mult} F_r F_d F_{WP} \quad (10-1)$$

where

q_{in}	—	water flow rate into the waste package [m^3/yr]
Q_R	—	percolation flow per waste package [m^3/yr], from NFENV (Chapter 7)
F_{FMF}	—	factor to account for flow convergence and divergence [unitless] as specified by the <i>tpa.inp</i> parameter WastePackageFlowMultiplicationFactor (Section 10.3.1.1)
F_{ow}	—	temporal flow focusing factor interpolated from data in <i>wflow.def</i> (Section 10.3.1.1) [unitless]
F_{mult}	—	near- and in-drift flow diversion factor (Section 10.3.1.2) [unitless]
F_r	—	rubble flow factor (Section 10.3.1.3) [unitless]
F_d	—	drip shield flow factor (Section 10.3.1.4) [unitless]
F_{WP}	—	waste package flow factor (Sections 10.3.1.5 to 10.3.1.7) [unitless]

The flow factors F_{FMF} , F_{ow} , F_{mult} , F_r , F_d , and F_{WP} are used in EBSREL to modify flow rates to simulate the effect of components of the engineered barrier system (e.g., drift wall, drip shield, waste package). Figure 10-2 illustrates flow factors, each of which is used to compute flow rates at particular locations inside the drift. After all of the flow factors are applied, the final result is the flow rate available to mobilize waste forms, q_{in} .

In EBSREL, damaged drip shields and waste packages may partially divert water, depending on the type of failure experienced by the drip shield or waste package. The waste package factor, F_{WP} , is selected based on the waste package failure class. For waste packages in the general

⁹The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

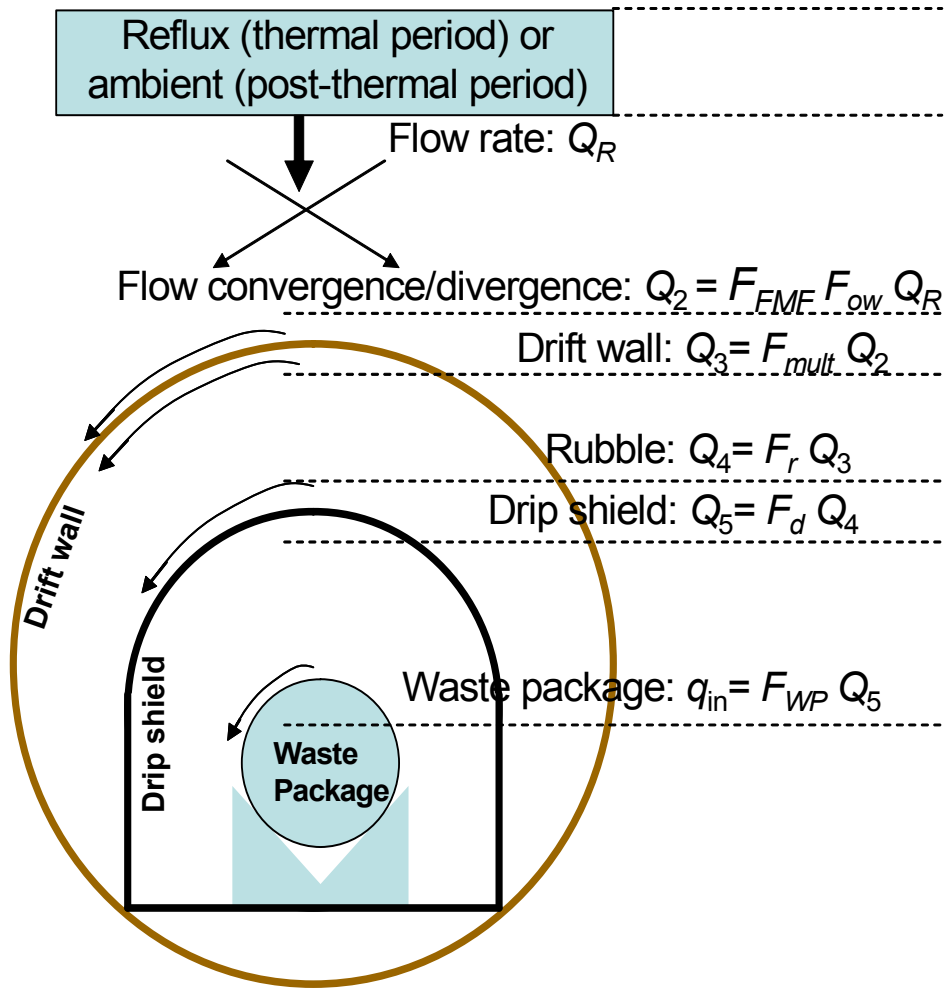


Figure 10-2. Graphical Definition of Flow Factors

corrosion class, $F_{WP} = 1$. Special constructs of the factor F_{WP} are implemented for (i) initially defective; (ii) mechanical; and (iii) faulting, intrusive igneous, and localized corrosion waste package classes. The symbols adopted for flow factors in these waste package classes are F_{id} , F_{wm} , and F_{wc} , respectively (Sections 10.3.1.5 to 10.3.1.7). When MECHFAIL provides two mechanical breach times, there are two separate values for F_{wm} , denoted F_{wm1} and F_{wm2} .

Time-dependent values for F_{mult} , F_{ow} , F_{wet} (Section 10.3.3.3), F_r , F_d , F_{wc} , F_{wm1} , F_{wm2} , and F_{id} are listed in the auxiliary input file *wflow.def* (Section 10.5), which serves as a template for the computed or adopted values written into *wflow.dat* and *ebsflo.dat*. For flexibility in testing alternative conceptual models, there is an optional procedure for imposing user-defined values for the flow factors that can be written in *wflow.def* and used by EBSREL.

10.3.1.1 Convergence/Divergence of Flow (F_{FMF} and F_{ow})

Convergence or divergence of deep percolation flow toward or away from the drift is implemented using two parameters— F_{FMF} and F_{ow} . The *tpa.inp* parameter WastePackageFlowMultiplicationFactor [F_{FMF} in Eq. (10-1)] is used as a scaling factor for flow rates (Q_R , Chapter 7) to estimate maximum flow rates potentially impinging on waste packages. The values of WastePackageFlowMultiplicationFactor are selected proportional to the spacing between drips. Average drip spacing greater than waste package lengths implies that some waste packages are not contacted by seepage. This is simulated by choosing a value of less than 1 for the *tpa.inp* parameter SubAreaWetFraction (see Section 10.3.3.3). In that instance, water is diverted onto neighboring waste packages (flow enhancement simulated by selecting WastePackageFlowMultiplicationFactor >1). Water mass balance requires that the product of SubAreaWetFraction and WastePackageFlowMultiplicationFactor is equal to one. This water balance constraint is approximately implemented by sampling these two parameters with a rank correlation coefficient of -0.9999 from mutually inverse distributions.

For flexibility in testing alternative conceptual models, temporal variability in convergence or divergence of flow is introduced via the column titled F_{ow} in the auxiliary file *wpflow.def*. At any timestep, flow rates are scaled by the product of WastePackageFlowMultiplicationFactor and F_{ow} (with the F_{ow} value interpolated from data in *wpflow.def*) to estimate maximum flow rates potentially contacting waste packages.

10.3.1.2 Near- and In-Drift Flow Diversion Factor, F_{mult}

Seepage reduction at the drift wall is quantified by the parameter F_{mult} , which accounts for reductions due to capillary diversion at the drift wall and film flows on inner surfaces of the drift wall. F_{mult} is defined as a function of the time-variant rate during the thermal period or the deep percolation rate above the drift in the postthermal period. This parameter is computed by the following empirical sigmoidal expression (Basagaoglu, et al., 2007), which represents results of a mechanistic model for the capillary barrier (Or, et al., 2005) and a bounded representation of along-wall flow.

$$F_{mult} = \begin{cases} \frac{a}{1 + e^{\ln \left(\frac{M^{yr} Q_R F_{ow}}{L_{WP} D_{WP}} \right) - x_o}} & \text{if } t < t_B \\ 1 & \text{if } t \geq t_B \end{cases} \quad (10-2)$$

where

- a — shape parameter [unitless], as specified by the *tpa.inp* parameter AFmultCoefficient
- b — scale parameter [unitless], as specified by the *tpa.inp* parameter BfmultCoefficient
- x_o — shift parameter [unitless], as specified by the *tpa.inp* parameter X0FmultCoefficient

M	—	unit conversion factor, 1,000 yr/m
L_{WP}	—	waste package length [m], as specified by the <i>tpa.inp</i> parameter WPLength[m]
D_{WP}	—	waste package diameter [m], as specified by the <i>tpa.inp</i> parameter WPDiameter[m]
t_B	—	time at which rubble starts accumulating on top of the drip shield [yr]

The parameters a , b , and x_0 determine the shape of the F_{mult} curve plotted against the flow rate Q_R . The shape parameter a determines the maximum value of F_{mult} , the scale parameter b controls the slope of the middle portion of the curve, and the shift parameter x_0 controls the lateral position of the curve.

As a result of drift degradation, rubble first fills a volume next to the drip shield base before accumulating on top of the drip shield (Chapter 6). As conceptualized in TPA Version 5.1, diversion of deep percolation near and in the drift is limited by the extent of drift degradation. The time at which rubble starts accumulating on the top of the drip shield, t_B , is equated with the time that (i) the rubble pile inhibits capillary diversion and (ii) the drift wall is so degraded and irregular that the drift wall is unable to divert flow. Therefore, after time t_B there is no flow diversion and, as shown by Eq. 10-2, F_{mult} is equal to 1. The values of F_{mult} calculated for each timestep are written in *ebsflo.dat* and *wpflow.dat* for computing radionuclide release. When any of the *tpa.inp* parameters *AfmultCoefficient*, *BfmultCoefficient*, and *X0FmultCoefficient* are set to a negative value, then values for F_{mult} defined in the auxiliary input file *wpflow.def* are adopted. In this way, a user-defined time history for F_{mult} may be imposed using *wpflow.def*.

The shift parameter x_0 (specified in *tpa.inp* as *X0FmultCoefficient*) is correlated to deep percolation parameters defined for UZFLOW (Table 5-1). Because a complete correlation matrix must be specified for correct sampling of input parameters and because the deep percolation parameters are correlated to *SubareaWetFraction* (Section 10.3.3.3), correlations among *X0FmultCoefficient*, *SubareaWetFraction*, and *WastePackageFlowMultiplicationFactor* must also be specified in *tpa.inp* (Section 10.4).

10.3.1.3 Rubble Flow Factor, F_r

The factor F_r , used to simulate the effect of rubble on flow rates, is defined as depicted in Figure 10-3. Initially, F_r is equal to one. As soon as rubble starts accumulating on top of the drip shield at time t_B , F_r is defined by the *tpa.inp* parameter *SeepageRubbleFactor*. When the user selects a negative value for *SeepageRubbleFactor*, then values for F_r defined in the auxiliary input file *wpflow.def* are adopted. In this way, a user-defined time history for F_r may be imposed using the input file *wpflow.def*.

10.3.1.4 Drip Shield Flow Factor, F_d

The factor to simulate decrease in flow rates impinging on the waste package due to partial protection by the drip shield is F_d and is depicted in Figure 10-4. The drip shield flow factor is equal to the value of *tpa.inp* parameter *InitialSeepageReductionFractionByMechFailedDS* at the earliest time of mechanical breaching of the drip shield, t_{df} , computed by MECHFAIL.

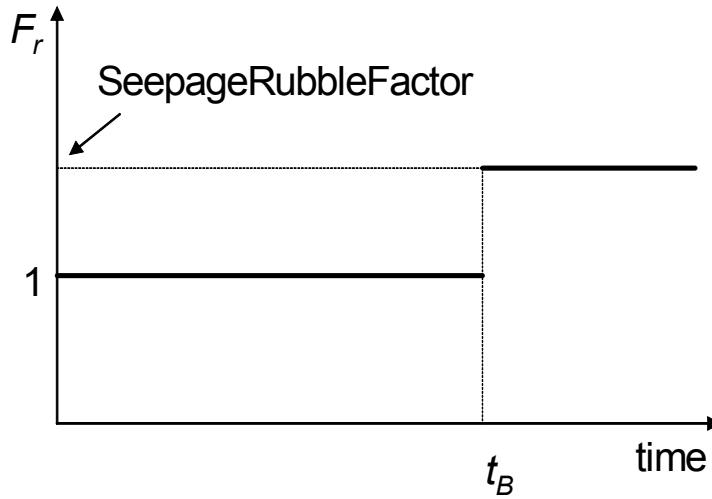


Figure 10-3. Definition of the Rubble Flow Factor, F_r , as a Function of Time

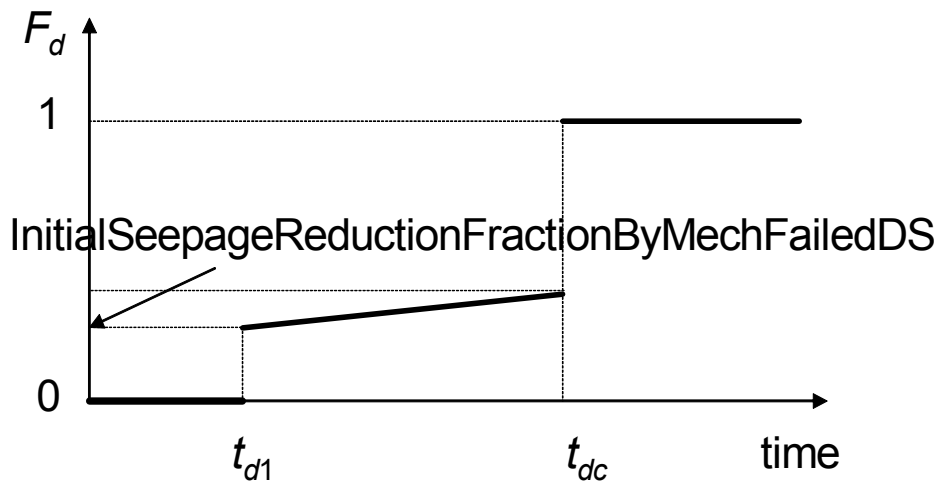


Figure 10-4. Definition of the Drip Shield Flow Factor, F_d , as a Function of Time, With $DSseepageProtectionDegradationRate[1/yr] > 0$

(two values per subarea, one for each rock type, are computed by MECHFALL). At the time the drip shield is breached by general corrosion, t_{dc} , $F_d = 1$. A gradual linear increase in the flow factor can be defined by specifying a nonzero value for the *tpa.inp* parameter $DSseepageProtectionDegradationRate[1/yr]$ (see sloped line segment in Figure 10-4). When a negative value is set for $InitialSeepageReductionFractionByMechFailedDS$, then values of F_d defined in the auxiliary input file *wflow.def* are adopted. In this way, a user-defined time history for F_d may be imposed using the input file *wflow.def*.

In the case of the faulting and igneous disruptive scenarios, $F_d = 1$ after the time of the event. This factor is used to compute water flow rates to mobilize waste forms only for waste packages

damaged by the event. For the other waste packages, or at times previous to the disruptive event, F_d is computed following the standard approach described in the previous paragraph.

10.3.1.5 Initially Defective Flow Factor, F_{id}

In TPA Version 5.1, waste packages in the initially defective failure class also undergo localized corrosion and general corrosion when these occur in the subarea. Because initial defects on the waste package outer container are assumed to be small, in TPA Version 5.1, initially defective waste packages partially protect waste forms against seepage. In TPA Version 5.1, after waste packages are breached by general corrosion, they offer no further protection against seepage. The flow factor F_{WP} for waste packages in the initially defective class is equal to F_{id} , which is depicted in Figure 10-5.

The sizes of the steps of the flow factor F_{id} in Figure 10-5 are defined by the *tpa.inp* parameters InitialSeepageReductionFractionInitiallyDefWP, InitialSeepageReductionFractionWeldLC, and InitialSeepageReductionFractionLC. The latter two are applied only when localized corrosion occurs in the subarea. At the time the waste package outer container is breached by general corrosion, t_{GC} , the flow factor is equal to 1.0. In Figure 10-5, t_{id} is the time defined by the *tpa.inp* parameter InitialFailureTime[yr]. The symbols t_{LC1} and t_{LC2} are the times of localized corrosion breach on welded and mill-annealed areas of the waste package computed by EBSFAIL.

A slope is available, specified by *tpa.inp* parameter WPSeepageProtectionDegradationRateInitiallyDefWP[1/yr], to allow for defining a linear increase in time in the flow factor (i.e., a gradual increase in water flow rate into the

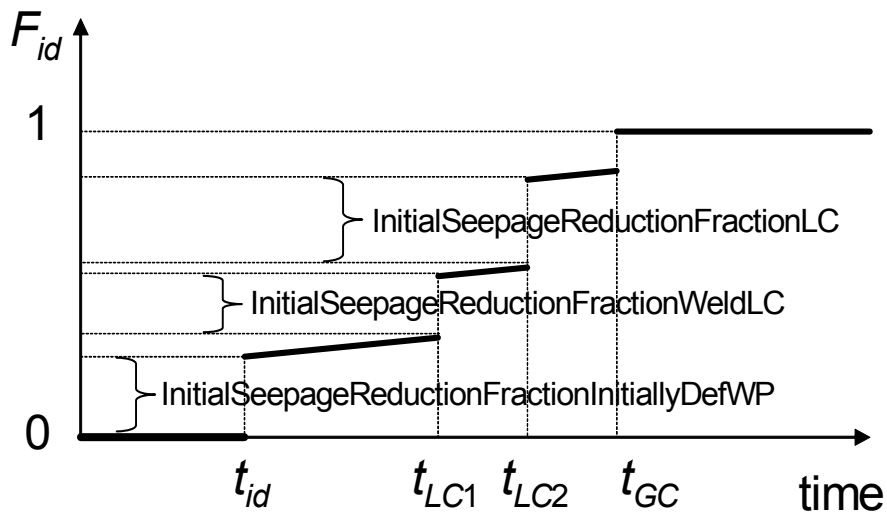


Figure 10-5. Definition of the Initially Defective Flow Factor, F_{id} , as a Function of Time, With WPSeepageProtectionDegradationRateInitiallyDefWP[1/yr] > 0

waste package). The slope is applied for any time greater than $t_{id} = \text{InitialFailureTime[yr]}$ and is illustrated by the sloping line segments in Figure 10-5. When a negative value is set for $\text{InitialSeepageReductionFractionInitiallyDefWP}$, values of F_{id} defined in the auxiliary input file *wpflow.def* are adopted. In this way, a user-defined time history for F_{id} may be imposed using *wpflow.def*.

In EBSREL, initially defective waste packages release radionuclides only at times beyond $\text{InitialFailureTime[yr]}$. The user may opt to define a nonzero time for $\text{InitialFailureTime[yr]}$ for stylized computations. When a value for $\text{InitialFailureTime[yr]}$ greater than t_{LC1} and t_{LC2} is selected, then F_{id} includes contributions from $\text{InitialSeepageReductionFractionWeldLC}$ and $\text{InitialSeepageReductionFractionLC}$. Therefore, the user can account for localized corrosion and general corrosion contributions to the flow factor in stylized analyses. Alternatively, localized corrosion can be disabled in stylized computations based on initially defective waste packages (see Chapter 8 for instructions on how to disable localized corrosion).

10.3.1.6 Mechanical Flow Factor, F_{wm}

The flow factor F_{WP} for waste packages in the mechanical failure class is denoted as F_{wm} . Waste packages in the mechanical class also undergo localized corrosion and general corrosion breaches when these occur in the subarea. In TPA Version 5.1, mechanically breached waste packages may partially protect waste forms against seepage; after waste packages are breached by general corrosion, they offer no further protection against seepage. The factor to simulate reduction in flow rates contacting waste forms in mechanically damaged packages is depicted in Figure 10-6.

The sizes of the steps in Figure 10-6 are defined by the *tpa.inp* parameters $\text{InitialSeepageReductionFractionWeldLC}$, $\text{InitialSeepageReductionFractionLC}$ (when localized corrosion occurs in the subarea), and $\text{InitialSeepageReductionFractionByMechFailedWP}$.

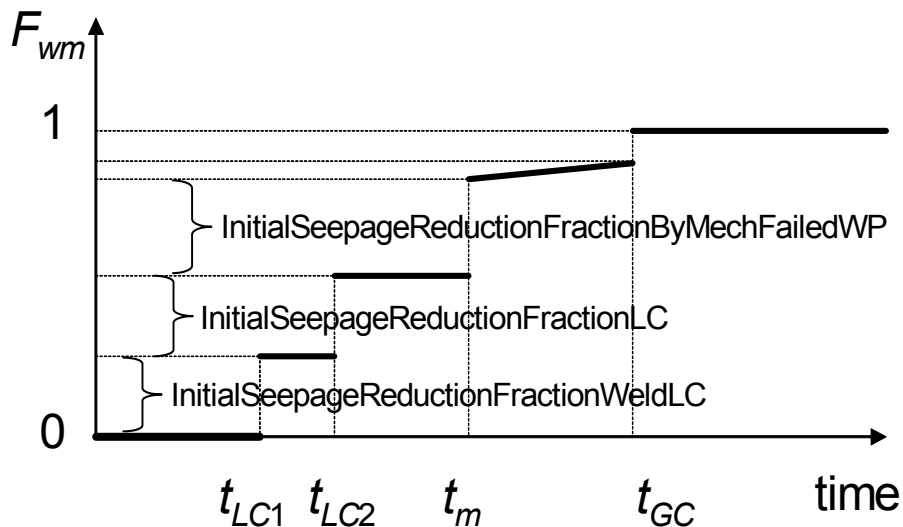


Figure 10-6. Definition of the Mechanical Flow Factor, F_{wm} , as a Function of Time, With $\text{WPSeepageProtectionDegradationRate[1/yr]} > 0$

At the time the waste package outer container is breached by general corrosion, the flow factor is equal to 1.0.

A slope is available, as specified by the *tpa.inp* parameter

WPSeepageProtectionDegradationRate[1/yr], to allow for linear increase in the flow factor with time. The slope is applied for times later than t_m (time of mechanical breach computed by MECHFAIL) and is illustrated by the sloped line segment in Figure 10-6. Because two rock types (lithophysal and nonlithophysal) are present in the model for a given subarea, MECHFAIL can provide two breach times per subarea. When two breach times are provided, the corresponding flow factors F_{wm1} and F_{wm2} are constructed for different breach time values. The two breach times, t_{m1} and t_{m2} , are used in place of t_m in Figure 10-6. The same slope, as specified by the *tpa.inp* parameter WPSeepageProtectionDegradationRate[1/yr], would be applied in each case. When a negative value is set for InitialSeepageReductionFractionByMechFailedWP, values of F_{wm} defined in the auxiliary input file *wflow.def*, under the columns labeled F_{wm1} and F_{wm2} , are used. In this way, user-defined time histories for F_{wm1} and F_{wm2} may be imposed using *wflow.def*; the previously discussed slope is not applied to the history defined by *wflow.def*. In TPA Version 5.1, waste packages in the mechanical failure class start releasing radionuclides as soon as waste package breach by localized corrosion occurs (in either the body or welded areas on the waste package) if this time preceeds the time of mechanical breach.

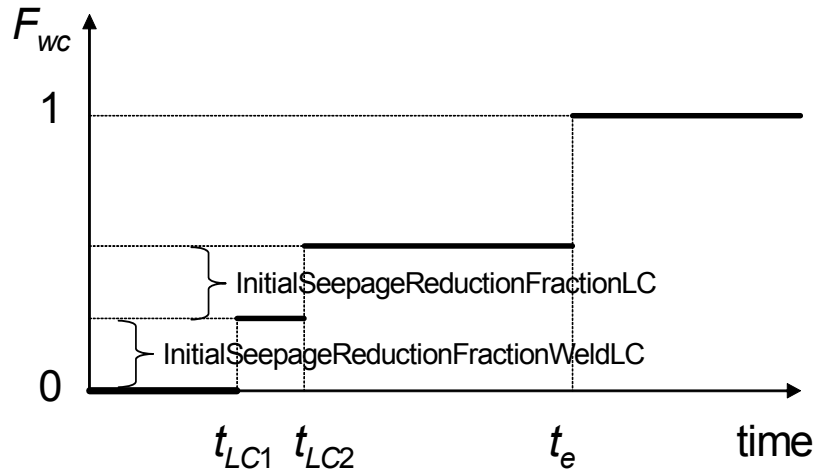
10.3.1.7 Faulting, Intrusive Igneous, and Localized Corrosion Flow Factor, F_{wc}

The flow factor F_{WP} for waste packages in the faulting, intrusive igneous, and localized corrosion failure classes is denoted as F_{wc} . In EBSREL, waste packages in the faulting and intrusive igneous classes also undergo localized corrosion when the conditions for localized corrosion are established before the disruptive event in the subarea. The factor to simulate reduction in flow rates contacting waste forms in packages from these classes is depicted in Figure 10-7.

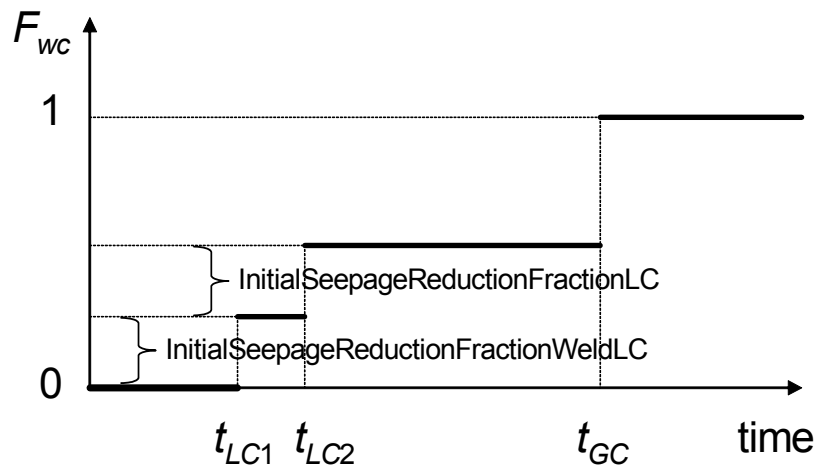
In TPA Version 5.1, for waste packages in the faulting and intrusive igneous classes, radionuclide release rates are activated at either the time of localized corrosion breach or the time of the event, t_e , whichever occurs first (Figure 10-7a). In the abstraction, waste packages breached by localized corrosion partially protect waste forms from water contact. After the time of the faulting or igneous event, t_e , the waste package no longer protects against flow, and F_{wc} is 1.0. The flow factor for waste packages in the localized corrosion class is similarly constructed. In this case, there is no further protection against flow at times later than the general corrosion breach, t_{GC} (Figure 10-7b). If a negative value is set in *tpa.inp* for either InitialSeepageReductionFractionLC or InitialSeepageReductionFractionWeldLC, values of F_{wc} defined in the auxiliary input file *wflow.def* are adopted. In this way, a user-defined time history for F_{wc} can be entered into *wflow.def*.

10.3.2 Waste Form Dissolution and Radionuclide Release (RELEASET)

EBSREL provides the time-dependent volumetric water flow rate into the package and the waste package temperature to the RELEASET standalone code. Computations performed for the representative waste package include dissolution rates for each waste form type, advective radionuclide release rates (including the effects of a gap fraction), and tracking of waste package radionuclide inventory. An alternative model employing diffusive release is also available.



(a)



(b)

Figure 10-7. Definition of Flow Factor, F_{wc} , as a Function of Time for (a) Faulting and Intrusive Igneous and (b) Localized Corrosion Waste Packages

The fraction of waste exposed to water is controlled by the height of the pool of water in the container (Mohanty, et al., 2002, Figure 8-1). The waste package gradually fills with water until water finds an exit point in the bathtub mode or instantaneously in the flowthrough mode. Radionuclide releases via advective pathways are activated after this time. The extent of the waste form exposed to water in both the bathtub and flowthrough modes is computed as a function of sampled parameters independently assigned to the different waste package failure classes.

10.3.2.1 Spent Nuclear Fuel Dissolution

Dissolution rates of the spent nuclear fuel matrix when in contact with liquid water are computed in RELEASET. Four alternative models for spent nuclear fuel dissolution rates are available in RELEASET (Mohanty, et al., 2002). These models are described in Sections 10.1.2 and 10.2.2. The spent nuclear fuel dissolution model is specified by the value of the *tpa.inp* parameter IModel. The spent nuclear fuel specific surface area is also a term calculated in RELEASET.

Model 1, which invokes a groundwater solution containing carbonate anions, describes the dissolution rate with the following equation (Gray and Wilson, 1995)

$$\log r = 9.310 + 0.142 \log [CO_3^{2-}] - 16.7 \log (p_{o_2}) + 0.140 \log [H^+] - \frac{2130}{T} + 6.81 \log [T] \log (p_{o_2}) \quad (10-3)$$

where

- r — spent nuclear fuel dissolution rate [mg/m²/day]
- $[CO_3^{2-}]$ — total carbonate concentration [mol/L], as specified by and converted from the *tpa.inp* parameter NegativeLog10CarbonateConcentration[mol/L]
- p_{o_2} — oxygen partial pressure [atm], as specified by the *tpa.inp* parameter OxygenPartialPressure[atm]
- $[H^+]$ — aqueous concentration of hydrogen ions [mol/L], as specified and converted from the *tpa.inp* parameter ReferencepH
- T — waste package temperature, obtained from NFENV [K]

In Model 2, dissolution rates are determined by considering various potential conditions of the in-package physical and chemical environment. Factors affecting dissolution rate that were considered include chemical effects (such as silicon and calcium water concentrations, pH, and oxygen concentration), temperature effects, spent nuclear fuel preoxidation/hydration and grain boundary effects, and immersion and water flow rates. An Arrhenius equation with a preexponential term and activation energy is selected with effective values to summarize these factors (Ahn and Mohanty, 2004; Mohanty, et al., 2002, 2000). The Model 2 equation for dissolution rate is

$$r = r_o \exp\left(\frac{-34300 \text{ J/mol}}{R T}\right) \quad (10-4)$$

where

- r_o — reference dissolution rate, as specified by the *tpa.inp* parameter Preexponential_SFDDissolutionModel2 [mg/m²/ day]
- R — ideal gas constant [8.314 J/(mol K)]

Spent nuclear fuel dissolution rate Model 3 allows the user to specify the dissolution rate as a fixed value for each simulation. This option is used for simulating release rates based on other models not considered explicitly, such as models based on natural analog data (Murphy and Codell, 1999). The rate is specified by the *tpa.inp* parameter UserLeachRate[kg/yr/m²].

For Models 1, 2, and 3, RELEASET computes the fractional waste form release rate in units of 1/yr by multiplying the spent nuclear fuel dissolution rate, after converting to units of kg/m²/yr, when necessary, by an effective specific surface area in units of m²/kg. The specific surface area is computed based on waste fragmentation into particles. The effective specific surface area is

$$a_{SF} = \frac{3f_w}{r_{part} \rho_{SF}} \quad (10-5)$$

where

- a_{SF} — effective specific surface area of spent nuclear fuel [m²/kg]
- r_{part} — spent nuclear fuel particle radius [m], as specified by the *tpa.inp* parameter InitialRadiusOfSFParticle[m]
- ρ_{SF} — spent nuclear fuel density [kg/m³], as specified by the *tpa.inp* parameter SFDensity[kg/m3]
- f_w — volume fraction of the waste form contacted by water [unitless]

The term f_w is computed as

$$f_w = \begin{cases} \left[\cos^{-1}(1 - 2 f_{sfwf}) + 2\sqrt{f_{sfwf}(1 - f_{sfwf})} (2 f_{sfwf} - 1) \right] \frac{1}{\pi} & \text{when } f_{sfwf} < 0.5 \\ \left[\pi - \cos^{-1}(2 f_{sfwf} - 1) + 2\sqrt{f_{sfwf}(1 - f_{sfwf})} (2 f_{sfwf} - 1) \right] \frac{1}{\pi} & \text{when } f_{sfwf} \geq 0.5 \end{cases} \quad (10-6)$$

where

- f_{sfwf} — spent fuel wetted fraction [unitless], as specified by *tpa.inp* parameters as described in the next paragraph

The parameter f_{sfwf} is the ratio of the in-package water pool height to the waste package internal diameter. This parameter is independently sampled per waste package failure class to allow for the possibility of different breaching mechanisms leading to different water volumes and extent of waste form contacted by water. The parameter f_{sfwf} is defined in *tpa.inp* via SFWettedFraction_Initial, SFWettedFraction_FAULTO, SFWettedFraction_VOLCANO, SFWettedFraction_MECH1, SFWettedFraction_MECH2, SFWettedFraction_LC, or SFWettedFraction_Corrosion. The last characters in the parameter name refer to the waste package class.

Spent nuclear fuel dissolution rate Model 4 accounts for the formation of a secondary uranium mineral that controls dissolution (Murphy and Codell, 1999). All radionuclides (except those in the gap fraction; Section 10.3.2.4) are contained in schoepite and are released at a rate proportional to the flow rate through the waste package and the equilibrium concentration of

uranium in contact with schoepite. The concentration of uranium is calculated by a model for aqueous uranium species in the waste package under oxidizing conditions in the presence of carbonate and as a function of pH and temperature. Total uranium concentration in solution is the sum of the concentrations of five aqueous species

$$[U(Total)] = [UO_2^{2-}] + [UO_2CO_3] + [UO_2(OH_2)] + [UO_2(CO_3)_2^{2-}] + [UO_2(CO_3)_3^{4-}] \quad (10-7)$$

where brackets denote molal concentration. Each of the five aqueous species can be related chemically to schoepite (nominally $UO_3 \cdot 2H_2O$) through coupled reactions with H^+ , HCO_3^- , and H_2O according to the reactions and corresponding mass action relations given in Murphy and Codell (1999, Table 1). The temperature dependence of the equilibrium constants for the five reactions controlling uranium species is given by the Van't Hoff equation

$$\ln K_i = \ln K_i^0 + \frac{\Delta H_i^0}{R} \left[\frac{1}{T_0} - \frac{1}{T} \right] \quad (10-8)$$

where

- K_i — equilibrium constant for reaction i [unitless]
- K_i^0 — equilibrium constant at the reference temperature T_0 [unitless]
- ΔH_i^0 — standard molar enthalpy of reaction i [kJ/mol]
- R — ideal gas constant [0.008314 kJ/mol/K]
- T_0 — reference temperature [298.15 K]

Values for thermodynamic parameters in this equation were given by Murphy and Codell (1999, Table 2) and were derived from data in Grenthe, et al. (1992); these data are not specified in *tpa.inp*. For calculation of the total uranium concentration in RELEASET Model 4 according to Eq. (10-7), the mass-action relations (Murphy and Codell, 1999, Table 1) are solved using aqueous H^+ and HCO_3^- concentrations and calculated values of the equilibrium constants at the waste package temperature (from NFENV). The H^+ and HCO_3^- concentrations are computed from the *tpa.inp* parameters NegativeLog10CarbonateConcentration[mol/L] and ReferencepH, respectively. The activities of schoepite and H_2O are set to 1.0, as are the activity coefficients in the mass action relations. The release rate of uranium from the waste form is given by the product of the water flow rate q_{out} and the calculated total uranium concentration. Release rates of other radioelements contained in schoepite are assumed to be released according to their proportion relative to uranium in spent nuclear fuel.

10.3.2.2 Glass Dissolution

The glass dissolution rate dependence on pH and temperature for a five-component glass composition is defined in the following equation for the glass dissolution rate (Knauss, et al., 1990; Bechtel SAIC Company, LLC, 2001).

$$r_g = k_o 10^{\eta pH} \exp\left(-\frac{E_{ag}}{RT}\right) \quad (10-9)$$

where

r_g	—	glass waste form dissolution rate [g/m ² /day]
k_o	—	intrinsic dissolution rate [g/m ² /day]
η	—	pH dependence coefficient [unitless], as specified by the <i>tpa.inp</i> parameter pHParameterLowRange[] or pHParameterHighRange[]
pH	—	pH of the in-package water [unitless], as specified by the <i>tpa.inp</i> parameter pHForGlassModel[]
E_{ag}	—	effective activation energy [kJ/mol/K], as specified by the <i>tpa.inp</i> parameter GlassActivationEnergyLowRange[kJ/mol-K] or GlassActivationEnergyHighRange[kJ/mol-K]
R	—	ideal gas constant [8.314 J/(mol K)]

The parameter k_o is specified in *tpa.inp* as $\log_{10}(k_o)$ via the parameters LogOfGlassDissolutionConstantHighRange[] and LogOfGlassDissolutionConstantLowRange[], with k_o in units g/m²/day. The “LowRange” and “HighRange” parameters, identified above, are selected when the value of the *tpa.inp* parameter pHForGlassModel[] is less than or greater than six, respectively (Bechtel SAIC Company, LLC, 2001).

RELEASET computes the fractional release rate in units of 1/yr by multiplying the glass dissolution rate [Eq.(10-9)] after converting to units of kg/m²/yr by an effective specific surface area in units of m²/kg. The effective specific surface area is computed as

$$a_{glass} = a_{glass}^o f_w \quad (10-10)$$

where

a_{glass}	—	glass waste form effective specific surface area [m ² /kg]
a_{glass}^o	—	reference specific surface area of glass waste form [m ² /kg], as specified by the <i>tpa.inp</i> parameter SurfaceAreaOfGlass[m ² /kg]

10.3.2.3 Cladding Degradation Abstraction

TPA Version 5.1 includes the ability to model either instantaneous or gradual degradation of spent nuclear fuel cladding. In the instantaneous case, cladding protection causes a decrease in the spent nuclear fuel dissolution rate that is implemented by multiplying the computed dissolution rate (Section 10.3.2.1) by a factor specified by the *tpa.inp* parameter CladdingCorrectionFactor. This factor, which is applied as a constant throughout the simulation period, represents the fractional extent of cladding failure in the instantaneous degradation model. For example, a value of 1 for CladdingCorrectionFactor invokes complete cladding

degradation, such that there is no cladding protection and the spent nuclear fuel dissolution rate is not decreased. Smaller values for CladdingCorrectionFactor will lead to slower adjusted dissolution rates.

The exploratory gradual degradation model is activated when a value other than zero is selected for the *tpa.inp* parameter FuelRodHalfLength[m]. The model computes a time-variant cladding exposure factor, F_c , which represents the fraction of spent nuclear fuel exposed to water due to cladding failure and is used to adjust the computed spent nuclear fuel dissolution rate. In the gradual degradation model, the maximum extent of fuel exposure is defined by the *tpa.inp* parameter CladdingCorrectionFactor, or C_{CF} . The fuel exposure at any time is computed by integrating the cladding degradation velocity. In RELEASET, there is no explicit treatment of cladding material other than Zircaloy (e.g., stainless steel).

In the exploratory gradual degradation model, the cladding degradation velocity is computed using the following equation

$$v_c = \frac{3f_w r(T)}{r_{part} \rho_{SF}} r_{rod} f_c \quad (10-11)$$

where

- v_c — cladding degradation velocity [m/yr]
- $r(T)$ — spent nuclear fuel dissolution rate as a function of waste package temperature, T [kg/m²/yr]
- r_{rod} — radius of spent nuclear fuel rod inside the cladding material [m], as specified by the *tpa.inp* parameter FuelRadiusInRod[m]
- f_c — velocity multiplication factor [unitless], as specified by the *tpa.inp* parameter CladdingVelocityEnhancementFactor[]

The velocity is integrated over time to define the extent of cladding degradation measured along the longitudinal axis, or $L_c(t)$. The cladding exposure factor as a function of time is computed using the following equation

$$F_c(t) = \frac{L_c(t)}{L_{rod}} C_{CF} \quad (10-12)$$

where

- F_c — cladding exposure factor [unitless]
- $L_c(t)$ — degraded cladding length at time t [m]
- L_{rod} — half length of the cladding rod [m], as specified by the *tpa.inp* parameter FuelRodHalfLength[m]
- C_{CF} — correction factor [unitless], as specified by the *tpa.inp* parameter CladdingCorrectionFactor

A minimum value of 0.01 for the cladding exposure factor is used in RELEASET. When the value of $F_c(t)$ from Eq. (10-12) is computed to be less than 0.01, RELEASET sets the cladding exposure factor to 0.01. After the time at which $L_c(t)$ is equal to L_{rod} , the exposure factor $F_c(t)$ is equal to C_{CF} , which is specified by the *tpa.inp* parameter CladdingCorrectionFactor.

10.3.2.4 Release of Radionuclides From Waste Packages

When liquid water enters a failed waste package in EBSREL, the overall mass balance model for the radionuclide inventory in liquid water contacting the waste form is represented by (after Mohanty, et al., 2002)

$$\frac{dm_i}{dt} = w_{ji}(t) - w_{ci}(t) - m_i \lambda_i + m_{i-1} \lambda_{i-1} + m_i^g \delta(t) \quad (10-13)$$

where

- m_i — amount of radionuclide i in the waste package water at time t [mol]
- w_{ji} — rate of transfer from the waste form by way of leaching into waste package water [mol/yr]
- w_{ci} — rate of advective transfer out of the waste package [mol/yr]
- λ_i — decay constant of radionuclide [1/yr]
- m_{i-1} — amount of the parent at time t [mol]
- λ_{i-1} — decay constant of the parent [1/yr]
- m_i^g — amount of radionuclide in the “gap region” [mol]
- $\delta(t)$ — Dirac’s delta function [1/yr] (Bracewell, 1999)

The rate of radionuclide transfer from the waste form by way of leaching (w_{ji}) is determined by congruent dissolution using the waste form dissolution algorithms described in Sections 10.3.2.1 and 10.3.2.2. For glass waste form and spent nuclear fuel Models 1, 2, and 3, RELEASET computes w_{ji} as the product of the fractional waste form release rate (1/yr) and the waste package inventory for radionuclide i . Spent nuclear fuel Model 4 directly computes the U-238 release rate in mol/yr using the product of the uranium concentration and the water flow rate through the waste package; as noted in Section 10.3.2.1, other radionuclides are released congruently with U-238. In addition, for all spent nuclear fuel models, a fraction of certain radionuclides in the spent nuclear fuel waste form inventory is released instantaneously when the waste form is exposed to water [represented by the term $m_i^g \delta(t)$ in Eq. (10-13)].

The gap fraction is defined by *tpa.inp* parameters such as GapFractionForTC99.

As part of the solution for the mass balance computation summarized by Eq. (10-13), concentrations of radionuclides in water are computed. Concentrations of isotopes of an element are combined into an element concentration that is compared to the solubility limit for that element {e.g., *tpa.inp* parameter SolubilityNp[kg/m3]}. In TPA Version 5.1, when the concentration exceeds the solubility limit, the mass of the element exceeding the solubility limit

is transferred from the water to a precipitate phase. This precipitate phase is available in later timesteps, should the element concentration from waste form dissolution be lower than the solubility limit, to be added to solution up to the solubility limit. The element mass remaining in solution is then split into its component radionuclides for the water mass balance computation.

Advective mass transfer out of the waste package is represented by the following equation (NRC, 1995)

$$w_{ci}(t) = C_i(t)q_{out}(t) \quad (10-14)$$

where

- C_i — concentration of radionuclide i in waste package water [mol/m³]
 q_{out} — rate water leaves the waste package at time t [m³/yr]

The concentration C_i is determined by dividing m_i by the volume of water in the waste package. For the bathtub mode, Mohanty, et al. (2002) describe how water volume is computed. For the reference case flowthrough mode, the water volume is the product of the waste package internal volume {WPInternalVolume[m3]} and the volume fraction of the waste form contacted by water [f_w in Eq. (10-6)]. For the flowthrough mode, the water flow rate out of the waste package q_{out} is equal to the water inflow rate q_{in} [Eq. (10-1)].

RELEASET includes an exploratory model to compute diffusive radionuclide release from the waste package. Diffusive releases are computed according to the equation

$$J_i = N \frac{f_t D_w f_2(T)}{\frac{L_{cr}}{A_{cr}^a + A_{cr}^b t} + \frac{L_{in}}{A_{in}}} f_i C_i(t) \quad (10-15)$$

where

- J_i — diffusive release rate of radionuclide i [Ci/yr]
 N — unit conversion factor, 3.1536×10^7 sec/yr
 f_t — adjustment factor [unitless], as specified by the *tpa.inp* parameter FractionOfWPsWithDiffusionTilt[]
 D_w — self-diffusion coefficient of water at 20 °C [58 °F], as specified by the *tpa.inp* parameter SelfDiffusionCoefficientOfWaterAt20C[m²/s]
 $f_2(T)$ — temperature correction [unitless]
 L_{cr} — diffusive pathway length [m], as specified by the *tpa.inp* parameter WeldCrackLength[m]
 A_{cr}^a — diffusive pathway initial cross section [m²], as specified by the *tpa.inp* parameter TotalAreaOfCracksPerWPAtEmplacement[m²]
 A_{cr}^b — cross section growth rate [m²/yr], as specified by the *tpa.inp* parameter SlopeOfCrackAreaCurve[m²/yr]

L_{in}	—	internal diffusive pathway length [m], as specified by the <i>tpa.inp</i> parameter LengthOfFilmPathInsideWP[m]
A_{in}	—	internal diffusive pathway cross section [m ²], as specified by the <i>tpa.inp</i> parameter InternalFilmCrossSectionalArea[m^2]
f_i	—	correction factor to account for radioelement-dependent diffusivity [unitless], as specified by the <i>tpa.inp</i> element-specific parameter DiffusionCorrectionFactorX[], where X is specific to each element noted in <i>tpa.inp</i>
$C_i(t)$	—	concentration of radionuclide <i>i</i> at time <i>t</i> in the in-package water [Ci/m ³]

The temperature correction factor, $f_2(T)$, is a function of the waste package temperature, varying almost linearly from 1 to 4.5 when the temperature changes from 20 to 100 °C [60 to 212 °F]. The diffusive release equation is a simplified representation of diffusion through a diffusive pathway composed of two segments: a water film inside the waste package and a narrow aperture across the waste package thickness. The cross section aperture on the waste package increases linearly with time, and the concentration at the terminus of the diffusive pathway is zero. The exploratory diffusive release model is activated by setting the correction factor FractionOfWPsWithDiffusionTilt[] to a value other than zero.

RELEASET computes the failed waste package inventory by a material balance expression [Eq. (10-13)] accounting for depletion caused by decay, generation of radioactive progeny, and mass depletion from diffusive and advective releases. For the case in which no mass leaves the waste package, Eq. (10-13) reduces to

$$\frac{dm_i}{dt} = -m_i \lambda_i + m_{i-1} \lambda_{i-1} \quad (10-16)$$

$$m_i|_{t=0} = m_{i0} \quad (10-17)$$

These differential equations are solved to determine the remaining solid mass of the radionuclides in a chain at a given time *t* using the Bateman equation (Bateman, 1910) as discussed in Mohanty, et al. (2002).

10.3.2.5 Invert Radionuclide Transport (EBSFILT)

An approximated advective-diffusive transport model is available to simulate radionuclide transport through the invert. However, the model is considered legacy code, and it is not supported as part of TPA Code Version 5.1. In the reference case, retardation and dispersion effects of the invert are neglected (the invert transport model is disabled) by transferring waste package releases directly to the unsaturated zone. Invert transport computations in EBSREL, if activated, are performed in the EBSFILT program using J-species and other radionuclide species release rates provided by EBSREL (Figure 10-1). Bypass of the invert in the reference case is accomplished by setting the *tpa.inp* control switch parameter InvertBypass(0=ebisfilt,1=bypass-ebisfilt) equal to one. The EBSFILT invert transport is an

approximated solution in the limit when the residence time of radionuclides in the invert is short. If the residence time is long, EBSFILT computations could be in error due to the disregard of decay chains and ingrowth. Any outputs from the invert transport portion of EBSFILT, if activated, are passed back to EBSREL as subarea release rates for transfer to UZFT. Details on the invert transport model in EBSFILT are available in Mohanty, et al. (2002).

10.3.3 Release Upscaling

Within RELEASET, representative waste package radionuclide release rates (Section 10.3.2) for each waste package class are combined and upscaled to produce time-dependent total subarea release rates in Ci/yr. This upscaling accounts for the subarea fraction with rock fractures carrying water and for the number of breached waste packages in a given subarea with waste forms contacted by liquid water. The number of waste packages contributing to release, as described in this section, is computed in TPA Version 5.1 before EBSREL is called and is provided as input to EBSREL (Figure 10-1). These computations are discussed in the EBSREL chapter for convenience.

10.3.3.1 Waste Package Failure Classes

In EBSREL, the effects of the various breaching processes on water flow to the waste form are implemented by use of the flow factors according to the waste package failure class (Section 10.3.1). How the flow factors are applied in EBSREL depends, in most cases, on the relative timing of breach events computed in TPA Version 5.1. The possible sequences of breaching events, described in the following paragraphs, also affect how waste package numbers are computed by TPA Version 5.1 for EBSREL release upscaling (Section 10.3.3.2).

In TPA Version 5.1, initially defective waste packages undergo localized and general corrosion when the time of these latter breaching processes (provided by EBSFAIL) is later than the value specified by the *tpa.inp* parameter InitialFailureTime[yr].

Waste packages in the mechanical class can also experience localized corrosion and general corrosion. Localized corrosion can occur before or after the time of mechanical breaching (provided by MECHFAIL). Because two rock types are considered in MECHFAIL (lithophysal and nonlithophysal), this failure class is treated as two sets with a split fraction defined by MECHFAIL. In the mechanical class, general corrosion occurs only at a later time than the mechanical breaching event.

Waste packages in the localized corrosion class are initially breached by localized corrosion in either the body or welded regions (Chapter 8). These waste packages can also be affected by general corrosion at later times when the latter process occurs in a simulation.

Faulting and intrusive igneous waste packages experience localized corrosion only when localized corrosion occurs before the faulting or igneous event, at a time defined by FAULTO or VOLCANO. Otherwise, localized corrosion makes no difference in the release computations.

Waste packages in the general corrosion failure class are breached only by general corrosion at a time provided by EBSFAIL. There are no multiple breaching processes for waste packages in this category.

10.3.3.2 Waste Package Counting Per Subarea

The algorithm to select the number of waste packages in a class contains the following steps.

1. Determine the degradation process causing the earliest waste package breaching (disregarding localized corrosion).
2. Assign the number of waste packages for the earliest breaching process.
 - Initially defective waste packages are defined by the fraction DefectiveFractionOfWPs/cell.
 - The fraction of mechanically breached waste packages is defined by MECHFAIL.
 - FAULTO and VOLCANO determine the number of waste packages affected in a subarea.
 - In the case of general corrosion provided by EBSFAIL, all waste packages in a subarea are breached.
3. If unclassified waste packages remain, repeat Step 2 for the next breaching process, and so on.
4. If unclassified waste packages remain, assign those waste packages to the localized corrosion failure class, provided that localized corrosion occurred in the subarea.

Only an integer number of waste packages is considered for release computations. Therefore, rounding is applied in the counting process.

In TPA Version 5.1, an additional step implements probability factors that account for the possibility that not all of the breached waste packages contribute to radionuclide release. These probability factors are applied to the number of packages in the waste package classes, and the scaled number represents the packages with waste forms contacted and mobilized by water. For waste forms to be mobilized by water, two processes must occur: water must contact waste packages, and water must infiltrate breached packages to contact waste forms. Two factors, $P_{contact}$ and $P_{allowance}$, quantify conditional probabilities that these requirements are met. Use of these probability factors, which are specific to each waste package failure class, recognizes that waste package breaching may not be sufficient to cause radionuclide release. The following paragraphs describe implementation of $P_{contact}$ and $P_{allowance}$.

10.3.3.2.1 $P_{contact}$

For waste packages in any failure class but the localized corrosion class, $P_{contact}$ is the probability of packages to be contacted by water capable of mobilizing radionuclides from waste forms. For waste packages not in the localized corrosion class, $P_{contact}$ is a function only of the capability of damaged drip shields to divert water. In the model, if drip shields are not damaged, waste forms cannot be contacted by liquid water (water vapor and condensation are ignored as sources of water to transport radionuclides, as stated in Section 10.2).

For waste packages in the localized corrosion failure class, the interpretation of $P_{contact}$ is different. In addition to accounting for diversion by damaged drip shields, $P_{contact}$ abstracts additional requirements for localized corrosion of waste packages. In defining the localized corrosion class, TPA Version 5.1 tracks the maximum number of waste packages that could be contacted by water with the potential to support localized corrosion. If additional requirements for localized corrosion are not fulfilled, then localized corrosion cannot initiate. At moderate temperatures {i.e., less than 110°C [230°F]}, localized corrosion of Alloy 22 is initiated as crevice corrosion when the corrosion potential exceeds a critical potential, computed as a function of in-drift water compositions and waste package temperature (Chapter 8; Dunn, et al., 2005). Initiation and propagation of crevice corrosion requires the presence of tight crevices and water of sufficient ionic strength and appropriate composition to support electrochemical processes. When neither of these requirements is met, crevice corrosion does not initiate. Recent experiments suggest varying degrees of susceptibility to localized corrosion depending on crevice quality (He and Dunn, 2007). Susceptibility is also a function of metallurgical state; for example, welded areas are more susceptible than mill-annealed parts (Pensado, et al., 2006; Dunn, et al., 2005); however, welds are only a small percentage of the waste package surface.

In summary, in the initially defective, mechanical, faulting, intrusive igneous, and general corrosion waste package classes, only a fraction ($P_{contact}$) of the total number of breached waste packages is contacted by water. For the localized corrosion class, when additional requirements are not met, then crevice corrosion cannot initiate; $P_{contact}$ is used to define the actual number of waste packages exhibiting localized corrosion.

The $P_{contact}$ factor is specified in *tpa.inp* as follows:

Probability_WPWaterContact_InitialDefects	—	initially defective waste package class
Probability_WPWaterContact_MechFail	—	mechanical class
Probability_WPWaterContact_LC	—	localized corrosion class
Probability_WPWaterContact_GC-Flt-Ig	—	general corrosion, faulting, and igneous classes

10.3.3.2.2 $P_{allowance}$

Use of the factor $P_{allowance}$ for the waste package failure classes acknowledges that contact of all breached waste packages in a class by liquid water is not sufficient to mobilize radionuclides in waste forms—water must also enter the package. $P_{allowance}$ is used to quantify the probability that breached regions on a waste package surface coincide with water contact regions and that water enters the waste package. $P_{allowance}$ is a function of dimensions of breached and water catchment regions on the waste package. As stated in Section 10.2, it is assumed that $P_{allowance}$ is constant in time, which is clearly an approximation as water flow may be redistributed, and breached and water catchment regions may change with time. The $P_{allowance}$ factor is specified in *tpa.inp* as follows:

Probability_WPWaterAllowance_InitialDefects	—	initially defective waste package class
Probability_WPWaterAllowance_MechFail	—	mechanical class

Probability_WPWaterAllowance_LC	—	localized corrosion class
Probability_WPWaterAllowance_GC-Flt-Ig	—	general corrosion, faulting, and igneous classes

To compute the number of waste packages contributing to radionuclide release, TPA Version 5.1 applies the product of $P_{contact}$ and $P_{allowance}$ to the number of waste packages determined according to the algorithm described at the start of this section. Each waste package class is assigned a value of the product of $P_{contact}$ and $P_{allowance}$ according to the *tpa.inp* parameters described in the previous paragraphs. The total number of waste packages across all classes is rounded to an integer number for radionuclide release computations (i.e., the “scaled down” number of waste packages). An additional step is applied to identify the number of waste packages that is breached by general corrosion only. When general corrosion is computed to occur in a subarea, the number of waste packages affected is identified as the total number in a subarea minus the “scaled” number of waste packages. In other words, the general corrosion class is composed of waste packages that do not belong to another waste package class.

10.3.3.3 Subarea Wet Fraction

In EBSREL, only a fraction of the waste packages in a subarea are contacted by seepage. The fraction is defined as SubareaWetFraction in *tpa.inp* and is used to account for the potential that water does not necessarily flow in all fractures that intersect the drift wall above any given waste package (Basagaoglu, et al., 2007). The factor SubareaWetFraction is correlated to *tpa.inp* parameters representing deep percolation (Table 5-1).

The factor F_{wet} , presented in the auxiliary input file *wpflow.def* (Section 10.5), allows definition of temporal variability in the number of waste packages contacted by seepage. For any timestep, the value of F_{wet} is interpolated from data in *wpflow.def*, and releases are scaled by the product of F_{wet} and SubareaWetFraction. Such an approximate approach to implementing temporal dependency is appropriate in relatively short timeframes (during which the unexposed inventory is not expected to change greatly). For long timeframes, this approximation can result in gross errors with respect to more detailed computations independently tracking the inventory in each waste package. User-defined values can be entered into *wpflow.def*.

In EBSREL, the term SubareaWetFraction is a factor directly scaling radionuclide release computations. The scaling is applied as a last step to define total radionuclide releases from waste packages in a subarea. The same scaling factor SubareaWetFraction is applied to all subareas.

10.3.4 Colloidal Release

The irreversible colloid release model is implemented by setting the *tpa.inp* parameter IrreversibleColloidModel[0=no,1=yes]. The solubility enhancement described in this section, which allows colloid attachment to enhance release at concentrations above the solubility limit, is actually performed before RELEASET is executed when the irreversible model is activated (Figure 10-1). After RELEASET completes computation of subarea radionuclide release rates, EBSREL then allocates a portion of mass from some radionuclides to a category of

radionuclides called J-species, which represent radionuclides irreversibly attached to colloids. For both spent nuclear fuel and glass waste forms, J-species release rates are computed, and corresponding dissolved species are accordingly reduced. For example, the released Pu-239 mass from RELEASET is apportioned between the dissolved Pu-239 species and the colloidal Pu-239 designated as Jp-239 species; these species are treated separately in subsequent transport computations.

The radionuclides that are assigned a J-species for purposes of irreversible attachment to colloids are Th-230, Pu-239, Pu-240, Am-241, Am-243, Cm-245, and Cm-246. In EBSREL, the colloid sorption capacity, which limits the extent of colloid mass loading, is based on colloid concentration in water, specific surface area, and sorption site density. In this model, thorium, plutonium, americium, and curium compete for these sites along with uranium, with relative affinities estimated based on consideration of sorption rates. Uranium is included in the competition model because of its high abundance and relatively high solubility in the waste package environment. Because colloids can allow a radioelement to be released at a total (dissolved plus colloidal) concentration exceeding the solubility limit, the EBSREL abstraction includes an enhancement of the sampled solubility limit. This estimated enhancement ensures that, when the radioelement was released at its sampled solubility limit, and after J-species are created, the remaining dissolved radionuclides are in solution in accordance with their sampled solubility limit.

Release of the colloidal J-species is implemented as follows. Before RELEASET is called, the *tpa.inp* input parameter SorptionCapacity[moles/m³] is sampled; this parameter controls the mass of actinides allowed to sorb to iron oxyhydroxide colloids and is based on single-layer sorption site densities. Affinity factors relative to plutonium for thorium, uranium, americium, and curium (e.g., the *tpa.inp* parameter AffinityFactorCm), which quantify sorption competition among these actinides, are then sampled from *tpa.inp*. Solubility limits are then sampled for all elements, and effective solubility limits are calculated for uranium, plutonium, and americium, but not thorium and curium. As discussed in the previous paragraph, implementation of release via irreversible attachment to colloids requires this solubility limit enhancement. The thorium solubility limit is not enhanced, because it has a very low mass concentration, and the curium value is not enhanced, because curium release is not consistently solubility limited. The equation for the effective solubility limit for plutonium is

$$C_{Seff,Pu} = C_{S,Pu} + S_X \frac{Y_{Pu} C_{S,Pu}}{Y_{Pu} C_{S,Pu} + Y_{Am} C_{S,Am} + Y_U C_{S,U}} \quad (10-18)$$

where

- $C_{Seff,Pu}$ — effective plutonium solubility limit for colloid model [kg/m³]
- $C_{S,Pu}$ — plutonium solubility limit [kg/m³], as specified by the *tpa.inp* parameter SolubilityPu[kg/m³]
- $C_{S,Am}$ — americium solubility limit [kg/m³], as specified by the *tpa.inp* parameter SolubilityAm[kg/m³]
- $C_{S,U}$ — uranium solubility limit [kg/m³], as specified by the *tpa.inp* parameter Solubility_U[kg/m³]

S_X	—	colloid sorption capacity [kg/m ³], as specified by the <i>tpa.inp</i> parameter SorptionCapacity[moles/m ³] (converted to kg/m ³ , using a generic atomic mass of 240)
Y_{Pu}	—	plutonium affinity factor [unitless], always equal to 1
Y_{Am}	—	americium affinity factor [unitless], as specified by the <i>tpa.inp</i> parameter AffinityFactorAm
Y_U	—	uranium affinity factor [unitless], as specified by the <i>tpa.inp</i> parameter AffinityFactor_U

Analogous equations apply for $C_{Seff,Am}$ and $C_{Seff,U}$, with the same denominator in the second term on the right-hand side. RELEASET is then executed with the effective solubility limits used for uranium, plutonium, and americium. The resulting radionuclide release rates are passed to EBSREL, where the following operations are performed for Th-230, U-238, Pu-239, Pu-240, Am-241, Am-243, Cm-245, and Cm-246. For these eight species, dissolved concentrations are converted by

$$C_i = \frac{Release_i t_{1/2,i} A_i Z}{q_{out}} \quad (10-19)$$

where

C_i	—	mass concentration of radionuclide <i>i</i> in water [kg/m ³]
$Release_i$	—	subarea RELEASET output release rate for radionuclide <i>i</i> [Ci/yr]
q_{out}	—	aggregate subarea RELEASET water flow rate out of waste packages [m ³ /yr]
$t_{1/2,i}$	—	radionuclide <i>i</i> half-life [yr]
A_i	—	radionuclide <i>i</i> atomic mass [g/mol]
Z	—	factor to convert, along with half-life and atomic mass, curies to kg; 2.796×10^{-9}

For plutonium, americium, and curium, masses for the two isotopes are combined to give an elemental concentration C_i (kg/m³). For uranium, U-238 is the most mass-abundant isotope, so it is reasonable to set $C_U = C_{U-238}$; likewise, $C_{Th} = C_{Th-230}$. For thorium, plutonium, americium, and curium, a total J-species element concentration is then calculated by an equation accounting for sorption capacity and competitive sorption. The equation for plutonium is shown here as an example

$$C_{JPu} = S_X \frac{Y_{Pu} Min(C_{Pu}, C_{S,Pu})}{\sum Y_i Min(C_i, C_{S,i})} \quad (10-20)$$

where

C_{JPu}	—	total plutonium J-species (i.e., colloidal) concentration [kg/m ³]

C_{Pu} — plutonium RELEASET elemental concentration [kg/m³], combining isotope concentrations from Eq. (10-19)

and the denominator is summed over thorium, uranium, plutonium, americium, and curium, using the affinities, concentrations, and sampled solubility limits for these elements. The minimum value selections ensure that the actual aqueous concentrations are used if the sampled solubility limit was not met and that the aqueous concentration does not exceed the sampled solubility limit.

The radionuclide J-species concentrations are then computed from the element values. For Th-230, the radionuclide value is equal to C_{JTh} . For plutonium, americium, and curium, the elemental concentration must be apportioned between the two isotopes according to the relative released masses. For example, for Pu-239, the J-species concentration is

$$C_{JPu-239} = C_{JPu} \frac{C_{Pu-239}}{C_{Pu-239} + C_{Pu-240}} \quad (10-21)$$

where

$C_{JPu-239}$ — Pu-239 J-species concentration [kg/m³]

C_{Pu-239} — concentration of total released Pu-239 from Eq. (10-19) [kg/m³]

C_{Pu-240} — concentration of total released Pu-240 from Eq. (10-19) [kg/m³]

A mass balance check is performed to ensure that the J-species concentration does not exceed the released radionuclide concentration; for example

$$C_{JFPu-239} = \text{Min}(C_{Pu-239}, C_{JPu-239}) \quad (10-22)$$

where

$C_{JFPu-239}$ — final Pu-239 J-species concentration [kg/m³]

Next, the dissolved released radionuclide concentration is calculated by mass balance; for example

$$C_{DissPu-239} = C_{Pu-239} - C_{JFPu-239} \quad (10-23)$$

where

$C_{DissPu-239}$ — Pu-239 dissolved concentration [kg/m³]

Note that it is possible for the entire mass of a radionuclide to be associated irreversibly with colloids. This is consistent with sorption experiments that show strong uptake and little desorption of plutonium and americium (Lu, et al., 2000, 1998).

In TPA Version 5.1, solubility enhancement [Eq. (10-18)] is estimated to simulate colloid attachment while ensuring that the dissolved concentration is maintained at the solubility limit if

the limit is reached in a given timestep. If solubility limits have not been reached in RELEASET for a given timestep, some solubility limits may be overly enhanced. It is possible, therefore, that the final dissolved concentration for a radionuclide will somewhat exceed what should have resulted from the sampled solubility limit.

Finally, the water concentration for each species—whether dissolved or colloidal—is converted to a subarea total release rate in Ci/yr using the inverse of the calculation performed in Eq. (10-19). These release rates for each dissolved species and J-species are transferred to UZFT as the source term for transport calculations.

10.4 Input Parameters in *tpa.inp*

Table 10-1 shows the input parameters needed for EBSREL in *tpa.inp*, along with remarks on the basis for the adopted values.

10.5 Auxiliary Input Data and External Process Models

Table 10-2 lists and describes the auxiliary input data files for EBSREL. EBSREL uses no external process models.

10.6 Intermediate Outputs and Information Passed to Other Modules

The intermediate output files from EBSREL are described in Table 10-3. Two results files showing key inputs to EBSREL are *wpsfail.res* and *dsfail.res*, which contain waste package and drip shield failure information.

In addition to the output files in Table 10-3, the user can specify that calculated information passed to and from EBSREL be saved as intermediate output for specific realizations. Table 10-4 lists and describes these optional intermediate output files. To specify the optional intermediate output files, the user must set *tpa.inp* parameter OutputMode(0=None,1=All,2=UserDefined) to a value of 1 or 2. When set to 1, all optional intermediate output for EBSREL is saved for all realizations. When set to 2, optional intermediate output selected is saved for realizations starting from *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by *tpa.inp* parameter UserDefinedUpperRealizationAppended. When the *tpa.inp* parameter OutputMode(0=None,1=All,2=UserDefined) is set to 1 or 2 and SelectAppendFiles is set to its reference case value of 0, the EBSREL optional output files (Table 10-4) are printed along with those from all other modules. Only the files *ebsrel.cum*, *ebsrel.ech*, and *ebsrel.rlt* are written if SelectAppendFiles is set to a value of 7. Only the file *releaset.cum* is written when SelectAppendFiles is set to a value of 17. Only the file *infilper.cum* is written when SelectAppendFiles is set to a value of 23. The most complete and comprehensive presentation of EBSREL results is in *ebsrel.rlt*, containing the complete time history of output radionuclide release rates, as well as waste package failure data, per subarea and realization.

10.7 Techniques for Understanding Module Performance

Radionuclide release is affected by several factors. Among these are water flow rate, waste package and drip shield integrity, waste form dissolution rate, radioelement solubility limits, and colloids. While there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of processes

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of the TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	WasteFormDissolution EnhancementFactor[]	Waste form dissolution enhancement factor (1.0 = no enhancement) [unitless]	constant 1.0	Factor to change spent fuel dissolution rate. There is no enhancement in the reference case. Legacy parameter from previous TPA code versions. The user should not change this value.
EBSREL	WaterContactMode_Initial(0=Bath Tub, 1=FlowThrough)	Water contact mode for initial waste package failure with iflag = 0 for bathtub and iflag = 1 for flowthrough	iflag 1	The assumed spent nuclear fuel water contact mode is flowthrough in the reference case. In general, bathtub and flowthrough modes produce comparable release rates from the engineered barrier system. However, the bathtub has a delay in release, which is nonexistent in the flowthrough mode.
EBSREL	WaterContactMode_Faulting(0=BathTub, 1=FlowThrough)	Water contact mode for waste package failure from faulting with iflag = 0 for bathtub and iflag = 1 for flowthrough	iflag 1	The assumed spent nuclear fuel water contact mode is flowthrough in the reference case. In general, bathtub and flowthrough modes produce comparable release rates from the engineered barrier system. However, the bathtub has a delay in release, which is nonexistent in the flowthrough mode.
EBSREL	WaterContactMode_Volcanic(0=BathTub, 1=FlowThrough)	Water contact mode for waste package failure from igneous activity with iflag = 0 for bathtub and iflag = 1 for flowthrough	iflag 1	The assumed spent nuclear fuel water contact mode is flowthrough in the reference case. In general, bathtub and flowthrough modes produce comparable release rates from the engineered barrier system. However, the bathtub has a delay in release, which is nonexistent in the flowthrough mode.
EBSREL	WaterContactMode_Mechanical1(0=BathTub, 1=FlowThrough)	Water contact mode for waste package mechanical failure, seismic event 1, with iflag = 0 for bathtub and iflag = 1 for flowthrough	iflag 1	The assumed spent nuclear fuel water contact mode is flowthrough in the reference case. In general, bathtub and flowthrough modes produce comparable release rates from the engineered barrier system. However, the bathtub has a delay in release, which is nonexistent in the flowthrough mode.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	WaterContactMode_Mechanical2 (0=BathTub,1=FlowThrough)	Water contact mode for waste package mechanical failure, seismic event 2, with iflag = 0 for bathtub and iflag = 1 for flowthrough	iflag 1	The assumed spent nuclear fuel water contact mode is flowthrough in the reference case. In general, bathtub and flowthrough modes produce comparable release rates from the engineered barrier system. However, the bathtub has a delay in release, which is nonexistent in the flowthrough mode.
EBSREL	WaterContactMode_LocCorr (0=BathTub,1=FlowThrough)	Water contact mode for waste package failure from localized corrosion with iflag = 0 for bathtub and iflag = 1 for flowthrough	iflag 1	The assumed spent nuclear fuel water contact mode is flowthrough in the reference case. In general, bathtub and flowthrough modes produce comparable release rates from the engineered barrier system. However, the bathtub has a delay in release, which is nonexistent in the flowthrough mode.
EBSREL	WaterContactMode_Corrosion (0=BathTub,1=FlowThrough)	Water contact mode for waste package failure from general corrosion with iflag = 0 for bathtub and iflag = 1 for flowthrough	iflag 1	The assumed spent nuclear fuel water contact mode is flowthrough in the reference case. In general, bathtub and flowthrough modes produce comparable release rates from the engineered barrier system. However, the bathtub has a delay in release, which is nonexistent in the flowthrough mode.
EBSREL	SubAreaWetFraction	Subarea fraction contacted by deep percolation [unitless]	loguniform 0.25, 1.0	The range of this parameter is based on fracture data collected in the Exploratory Studies Facility and Enhanced Characterization of the Repository Block Facility. A detailed description of this parameter is available in the Seepage Workshop Report (Basagaoglu, et al., 2007). Mass balance requires that the product of SubAreaWetFraction and WastePackageFlowMultiplicationFactor is equal to 1. This water balance constraint is implemented by sampling these two parameters with a rank correlation coefficient of -0.9999 from mutually inverse distributions.
EBSREL	InitialFailureTime[yr]	t_{fd} Failure time for initially defective waste packages [yr]	constant 0.0	Initially defective waste packages are assumed present at emplacement time.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	DefectiveFractionOfWPs/cell	Fraction of total waste packages in an subarea that fails at time specified for InitialFailureTime[yr] [unitless]	loguniform 1.0e-4, 1.0e-2	Reported range estimated from analogous data in NRC (1988, 1984a,b, 1979, 1973); SKI (1996); Timmins (1998); Tschoepe, et al. (1994); and Jain, et al. (2003). A log-uniform distribution was selected to reflect that low values of the fraction are believed more likely than upper bound values.
EBSREL	WPInternalVolume[m3]	Internal waste package volume in which water can reside [m ³]	constant 4.6	This value is based on available design data (CRWMS M&O, 2001a).
NFENV	WPLength[m]	L_{wp} Outer length of the waste package [m]	constant 5.165	Value is based on CNWRA estimate using the range of waste package lengths presented in DOE (2002).
NFENV	WPDiameter[m]	D_{wp} Outer diameter of the waste package [m]	constant 1.659	Value is based on CNWRA estimate using waste package diameters presented in DOE (2002).
EBSREL	FlowOnsetTemperature[C]	Threshold temperature to allow water flow inside the waste package [°C]	constant 96.0	It is assumed that water flow inside the waste package is only feasible after the waste package temperature drops below FlowOnsetTemperature[C]. In the reference case, FlowOnsetTemperature[C] is selected as the boiling point of water at the repository altitude.
EBSREL	SFDensity[kg/m3]	ρ_{SF} Spent nuclear fuel density [kg/m ³]	constant 10600.0	Value is based on UO ₂ density in Wilson (1990).
EBSREL	IModel	Selection of model for computing spent fuel dissolution. 1 = empirical function of the in-package water chemistry, 2 = Arrhenius equation, 3 = user specified, 4 = schoepite equilibrium, 5 = glass model	iconstant 2	Model 2 is the reference case model (Mohanty, et al., 2002).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	OxygenPartialPressure[atm]	Oxygen partial pressure [atm]	constant 0.21	This value is based on atmospheric composition (Lide, 1990).
EBSREL	NegativeLog10CarbonateConcentration[mol/L]	Negative log ₁₀ of carbonate concentration in water in contact with spent fuel [mol/L]	constant 2.7	Upper bound from equilibrium calculation at 25 °C [77 °F] [Bechtel SAIC Company, LLC, 2004c; Eq. (3-16)] using upper bound for f _{CO2} = 0.01 bar (Bechtel SAIC Company, LLC, 2005d) and pH = 7.0 (Bechtel SAIC Company, LLC, 2004c). Calculations documented in Pickett (2007b).
EBSREL	UserLeachRate[kg/yr/m2]	User-provided leaching rate used when IModel = 3 [kg/yr/m ²]	constant 0	The user enters a value for this parameter when spent nuclear fuel dissolution Model 3 is invoked. Model 3 requires a user-defined spent nuclear fuel dissolution rate.
EBSREL	ReferencepH	pH for spent fuel dissolution models 1 and 4 [unitless]	uniform 5.5, 8.0	Based on review of Bechtel SAIC Company, LLC (2005e), 5.5 to 8.0 is a reasonable range for pH variability over long time scales in commercial spent nuclear fuel packages.
EBSREL	Preexponential_SFDDissolutionModel2	r _o Preexponential factor for spent nuclear fuel dissolution rate for Model 2 [mg/m ² -day]	loguniform 1.022e4, 1.022e7	Based on environmental effects on spent nuclear fuel dissolution rate (Ahn and Mohanty, 2004; Mohanty et al., 2000). Release rates are assumed to range from 0.01 to 10 mg/(m ² -d) at 25 °C [77 °F]. The activation energy of the Arrhenius equation [Eq. (10-4)] is assumed to equal 34.3 kJ/mol (Ahn and Mohanty, 2004; Mohanty, et al., 2000).
EBSREL	RD_Invert_Cm	Retardation factor of curium in invert [unitless]	beta 2001, 20001, 9.039, 18.079	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Pu	Retardation factor of plutonium in invert [unitless]	uniform 101, 1401	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_U	Retardation factor of uranium in invert [unitless]	beta 1, 21, 4.091, 4.091	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Am	Retardation factor of americium in invert [unitless]	beta 2001, 20001, 9.039, 18.079	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	RD_Invert_Np	Retardation factor of neptunium in invert [unitless]	beta 1, 21, 4.091, 4.091	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Th	Retardation factor of thorium in invert [unitless]	beta 2001, 20001, 9.039, 18.079	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Ra	Retardation factor of radium in invert [unitless]	uniform 1001, 2001	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Pb	Retardation factor of lead in invert [unitless]	uniform 2001, 10001	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Cs	Retardation factor of cesium in invert [unitless]	uniform 201, 2001	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_I	Retardation factor of iodine in invert [unitless]	constant 1.0	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Tc	Retardation factor of technetium in invert [unitless]	constant 1.0	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Ni	Retardation factor of nickel in invert [unitless]	beta 1, 10001, 3.061, 2.041	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Cl	Retardation factor of chlorine in invert [unitless]	constant 1.0	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Se	Retardation factor of selenium in invert [unitless]	beta(exp) 1, 21, 4.091, 4.091	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).
EBSREL	RD_Invert_Nb	Retardation factor of niobium in invert [unitless]	beta 2001, 20001, 9.039, 18.079	This is a legacy parameter defined for the legacy EBSFILT standalone program. Based on tuff data in CRWMS M&O (2001b).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	GapFractionForCM246	Fraction of Cm-246 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForU238	Fraction of U-238 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForCM245	Fraction of Cm-245 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForAM241	Fraction of Am-241 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	GapFractionForNP237	Fraction of Np-237 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForAM243	Fraction of Am-243 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForPU239	Fraction of Pu-239 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForPU240	Fraction of Pu-240 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	GapFractionForU234	Fraction of U-234 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForTH230	Fraction of Th-230 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForRA226	Fraction of Ra-226 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForPB210	Fraction of Pb-210 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	GapFractionForU233	Fraction of U-233 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForTH229	Fraction of Th-229 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForCS135	Fraction of Cs-135 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	triangular 8.8e-3, 2.5e-2, 5.8e-2	Combination of gap and grain boundary release and fission gas release data was used to estimate instant release fraction. Review data provided in Jain, et al. (2004).
EBSREL	GapFractionForI129	Fraction of I-129 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	triangular 5.4e-3, 1.1e-1, 3.2e-1	Combination of gap and grain boundary release and fission gas release data was used to estimate instant release fraction. Review data provided in Jain, et al. (2004).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	GapFractionForTC99	Fraction of Tc-99 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	triangular 5.0e-4, 1.3e-3, 2.8e-3	Combination of gap and grain boundary release and fission gas release data was used to estimate instant release fraction. Review data provided in Jain, et al. (2004).
EBSREL	GapFractionForNI59	Fraction of Ni-59 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	GapFractionForCL36	Fraction of Cl-36 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	triangular 5.4e-3, 1.1e-1, 3.2e-1	Combination of gap and grain boundary release and fission gas release data was used to estimate instant release fraction. Review data provided in Jain, et al. (2004).
EBSREL	GapFractionForSE79	Fraction of Se-79 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	triangular 8.8e-3, 2.5e-2, 5.8e-2	Combination of gap and grain boundary release and fission gas release data was used to estimate instant release fraction. Review data provided in Jain, et al. (2004).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	GapFractionForNB94	Fraction of Nb-94 in exposed spent nuclear fuel that is instantaneously released from the grain and pellet cladding gap [unitless]	constant 0.0	Expected to be small because solid state diffusion coefficients are very small; see also Johnson and Tait (1997) and Johnson and McGinnes (2002). Review of data provided in Jain, et al. (2004).
EBSREL	InitialRadiusOfSFParticle[m]	r_{part} Initial radius of spent nuclear fuel particle used to compute the specific surface area [m]	constant 1.286e-3	Value based on an expected value of the specific surface area $SA = 2.2 \times 10^{-7} \text{ m}^2/\text{mg}$ (Bechtel SAIC Company, LLC, 2004a). The radius was computed as a function of the specific surface area using Eq. (10-5) with $f_w = 1$.
EBSREL	CladdingCorrectionFactor	C_{CF} Cladding correction factor [unitless]	constant 1.0	In the reference case, it is assumed that cladding offers no protection of spent nuclear fuel. This assumption is implemented by setting CladdingCorrectionFactor=1 and FuelRodHalfLength[m]=0.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	SolubilityAm[kg/m3]	$C_{S,Am}$ Solubility limit for americium [kg/m ³]	loguniform 1.6e-5, 2.7e-1	Range of abstraction in pH range of 6.0 to 8.0, and logf(CO ₂) of -2 to -3 (Bechtel SAIC Company, LLC, 2005a). Very high values modeled at pH 5.5 and 5.75 (Bechtel SAIC Company, LLC, 2005a) vastly exceeded any laboratory measurements of americium solubility limits and were not used in developing this distribution.
EBSREL	SolubilityNp[kg/m3]	Solubility limit for neptunium [kg/m ³]	loguniform 1.0e-4, 1.4e-1	Documented in Pickett (2007b). Based on data in Bechtel SAIC Company, LLC (2005a).
EBSREL	Solubility_I[kg/m3]	Solubility limit for iodine [kg/m ³]	constant 1.29e2	Based on assumption that there is no solubility-controlling phase for iodine (Gauthier, 1993). Assumed to be 1.0 mol/L.
EBSREL	SolubilityTc[kg/m3]	Solubility limit for technetium [kg/m ³]	constant 9.93e1	Based on assumption that there is no solubility-controlling phase for technetium (Gauthier, 1993). Assumed to be 1.0 mol/L.
EBSREL	SolubilityCl[kg/m3]	Solubility limit for chlorine [kg/m ³]	constant 3.6e1	Based on assumption that there is no solubility-controlling phase for chlorine (Gauthier, 1993). Assumed to be 1.0 mol/L.
EBSREL	Solubility_U[kg/m3]	$C_{S,U}$ Solubility limit for uranium [kg/m ³]	loguniform 5.1e-4, 1.1e0	Range of abstraction in pH range of 5.5 to 8.0, and logf(CO ₂) of -2 to -3 (Bechtel SAIC Company, LLC, 2005a). Additional 0.5 log units appended at max and min for uncertainty (based on uncertainty term with normal distribution and 1-sigma = 0.5 log).
EBSREL	SolubilityCm[kg/m3]	Solubility limit for curium [kg/m ³]	loguniform 1.6e-5, 2.7e-1	Assumed that curium behaves similarly to Am ³⁺ (see Fuger, 1992). Same as SolubilityAm[kg/m3]

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	SolubilityPu[kg/m3]	$C_{S,Pu}$ Solubility for plutonium [kg/m ³]	usersuppliedpwiscdf 23 7.11E-07, 0 3.79E-06, 0.05 6.27E-06, 0.1 8.41E-06, 0.15 1.07E-05, 0.2 1.37E-05, 0.25 1.68E-05, 0.3 2.02E-05, 0.35 2.42E-05, 0.4 2.86E-05, 0.45 3.36E-05, 0.5 4.01E-05, 0.55 4.61E-05, 0.6 5.53E-05, 0.65 6.73E-05, 0.7 8.22E-05, 0.75 1.00E-04, 0.8 1.25E-04, 0.85 1.68E-04, 0.9 2.55E-04, 0.95 3.23E-04, 0.97 5.15E-04, 0.99 1.32E-03, 1	Based on information in Bechtel SAIC Company, LLC (2005a). Calculations documented in Pickett (2007b).
EBSREL	SolubilityTh[kg/m3]	Solubility limit for thorium [kg/m ³]	loguniform 5.6e-7, 3.6e-3	Range of solubility in pH range of 5.5 to 8.0 and logf(CO ₂) of -2 to -3 (Bechtel SAIC Company, LLC, 2005a). Additional 0.5 log units appended at maximum and minimum for uncertainty.
EBSREL	SolubilityRa[kg/m3]	Solubility limit for radium [kg/m ³]	loguniform 2.0e-5, 1.2e-3	Maximum and minimum are two values adopted in Bechtel SAIC Company, LLC (2005a) for radium below and above pH 7.75, respectively. Values do not reflect likely solid solution with barium and strontium, which cannot be quantified in the absence of barium and strontium release simulations.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	SolubilityPb[kg/m3]	Solubility limit for lead [kg/m ³]	logtriangular 2.1e-6, 6.6e-5, 2.1e-3	Based on TRW Environmental Safety Systems, Inc. (1995, Table 6.3-1), based on expert elicitation described in Gauthier (1993), Andersson (1988), and Tien, et al. (1985).
EBSREL	SolubilityCs[kg/m3]	Solubility limit for cesium [kg/m ³]	constant 1.35e2	Based on assumption that there is no solubility controlling phase for cesium. Assumed a solubility limit of 1.0 mol/L.
EBSREL	SolubilityNi[kg/m3]	Solubility limit for nickel [kg/m ³]	logtriangular 5.9e-5, 1.1e-1, 5.9e0	Based on TRW Environmental Safety Systems, Inc. (1995, Table 6.3-1), based on expert elicitation described in Gauthier (1993), Andersson (1988), and Siegel, et al. (1993).
EBSREL	SolubilitySe[kg/m3]	Solubility limit for selenium [kg/m ³]	constant 7.9e1	Based on assumption that there is no solubility-controlling phase for selenium (Gauthier, 1993). Assumed to be 1.0 mol/L.
EBSREL	SolubilityNb[kg/m3]	Solubility limit for niobium [kg/m ³]	loguniform 9.3e-8, 9.3e-6	Based on TRW Environmental Safety Systems, Inc. (1995, Table 6.3-1), based on expert elicitation described in Gauthier (1993) and Andersson (1988).
EBSREL	SFWettedFraction_Initial	f_{sfrf} Ratio of the height of the in-package water line and the waste package internal diameter, waste packages in the initially defective class [unitless]	uniform 0.033, 1.0	Staff expert judgment based on the following rationale. This parameter controls the in-package water volume and the waste form dissolution rate. It is assumed that the volume fraction of the waste form contacted by water, f_w , ranges from 0.01 to 1.0. The parameter f_{sfrf} is selected to be consistent with this range in f_w . The term f_w [Eq. (10-6)] is a factor affecting the effective waste form dissolution rate. Small openings on the waste package may lead to a limited extent of contact of the waste form by water. However, it is difficult to support very small values of the parameter f_{sfrf} as hydration alone could cause an increase in the waste form exposed surface. It is considered that 0.01 is a reasonable low bound on the volume fraction f_w (smaller values of f_{sfrf} can lead to extremely long waste form depletion times).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	SFWettedFraction_FAULTO	f_{swf} Ratio of the height of the in-package water line and the waste package internal diameter, waste packages in the faulting class [unitless]	uniform 0.033, 1.0	Staff expert judgment based on the following rationale. This parameter controls the in-package water volume and the waste form dissolution rate. It is assumed that the volume fraction of the waste form contacted by water, f_w , ranges from 0.01 to 1.0. The parameter f_{swf} is selected to be consistent with this range in f_w . The term f_w [Eq. (10-6)] is a factor affecting the effective waste form dissolution rate. Small openings on the waste package may lead to a limited extent of contact of the waste form by water. However, it is difficult to support very small values of the parameter f_{swf} as hydration alone could cause an increase in the waste form exposed surface. It is considered that 0.01 is a reasonable low bound on the volume fraction f_w (smaller values of f_{swf} can lead to extremely long waste form depletion times).
EBSREL	SFWettedFraction_VOLCANO	f_{swf} Ratio of the height of the in-package water line and the waste package internal diameter, waste packages in the igneous class [unitless]	uniform 0.033, 1.0	Staff expert judgment based on the following rationale. This parameter controls the in-package water volume and the waste form dissolution rate. It is assumed that the volume fraction of the waste form contacted by water, f_w , ranges from 0.01 to 1.0. The parameter f_{swf} is selected to be consistent with this range in f_w . The term f_w [Eq. (10-6)] is a factor affecting the effective waste form dissolution rate. Small openings on the waste package may lead to a limited extent of contact of the waste form by water. However, it is difficult to support very small values of the parameter f_{swf} as hydration alone could cause an increase in the waste form exposed surface. It is considered that 0.01 is a reasonable low bound on the volume fraction f_w (smaller values of f_{swf} can lead to extremely long waste form depletion times).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	SFWettedFraction_MECH1	f_{swf} Ratio of the height of the in-package water line and the waste package internal diameter, waste packages in the mechanical class (rock type 1) [unitless]	uniform 0.033, 1.0	Staff expert judgment based on the following rationale. This parameter controls the in-package water volume and the waste form dissolution rate. It is assumed that the volume fraction of the waste form contacted by water, f_w , ranges from 0.01 to 1.0. The parameter f_{swf} is selected to be consistent with this range in f_w . The term f_w [Eq. (10-6)] is a factor affecting the effective waste form dissolution rate. Small openings on the waste package may lead to a limited extent of contact of the waste form by water. However, it is difficult to support very small values of the parameter f_{swf} as hydration alone could cause an increase in the waste form exposed surface. It is considered that 0.01 is a reasonable low bound on the volume fraction f_w (smaller values of f_{swf} can lead to extremely long waste form depletion times).
EBSREL	SFWettedFraction_MECH2	f_{swf} Ratio of the height of the in-package water line and the waste package internal diameter, waste packages in the mechanical class (rock type 2) [unitless]	uniform 0.033, 1.0	Staff expert judgment based on the following rationale. This parameter controls the in-package water volume and the waste form dissolution rate. It is assumed that the volume fraction of the waste form contacted by water, f_w , ranges from 0.01 to 1.0. The parameter f_{swf} is selected to be consistent with this range in f_w . The term f_w [Eq. (10-6)] is a factor affecting the effective waste form dissolution rate. Small openings on the waste package may lead to a limited extent of contact of the waste form by water. However, it is difficult to support very small values of the parameter f_{swf} as hydration alone could cause an increase in the waste form exposed surface. It is considered that 0.01 is a reasonable low bound on the volume fraction f_w (smaller values of f_{swf} can lead to extremely long waste form depletion times).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	SFWettedFraction_LC	f_{sfrf} Ratio of the height of the in-package water line and the waste package internal diameter, waste packages in the localized corrosion class [unitless]	uniform 0.033, 1.0	Staff expert judgment based on the following rationale. This parameter controls the in-package water volume and the waste form dissolution rate. It is assumed that the volume fraction of the waste form contacted by water, f_w , ranges from 0.01 to 1.0. The parameter f_{sfrf} is selected to be consistent with this range in f_w . The term f_w [Eq. (10-6)] is a factor affecting the effective waste form dissolution rate. Small openings on the waste package may lead to a limited extent of contact of the waste form by water. However, it is difficult to support very small values of the parameter f_{sfrf} as hydration alone could cause an increase in the waste form exposed surface. It is considered that 0.01 is a reasonable low bound on the volume fraction f_w (smaller values of f_{sfrf} can lead to extremely long waste form depletion times).
EBSREL	SFWettedFraction_Corrosion	f_{sfrf} Ratio of the height of the in-package water line and the waste package internal diameter, waste packages in the general corrosion class [unitless]	uniform 0.033, 1.0	Staff expert judgment based on the following rationale. This parameter controls the in-package water volume and the waste form dissolution rate. It is assumed that the volume fraction of the waste form contacted by water, f_w , ranges from 0.01 to 1.0. The parameter f_{sfrf} is selected to be consistent with this range in f_w . The term f_w [Eq. (10-6)] is a factor affecting the effective waste form dissolution rate. Small openings on the waste package may lead to a limited extent of contact of the waste form by water. However, it is difficult to support very small values of the parameter f_{sfrf} as hydration alone could cause an increase in the waste form exposed surface. It is considered that 0.01 is a reasonable low bound on the volume fraction f_w (smaller values of f_{sfrf} can lead to extremely long waste form depletion times).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	CladdingVelocityEnhancementFactor[]	f_c Multiplication factor to enhance clad splitting velocity [unitless]	triangular 1.0, 40.0, 240.0	In the reference case, it is assumed that cladding instantaneously unzips as soon as water contacts the spent fuel rods. This parameter is not used in the reference case. Values are legacy from previous TPA code versions.
EBSREL	FuelRodHalfLength[m]	L_{rod} Fuel rod half length [m]	constant 0.0	Set to zero to force instantaneous cladding degradation. This parameter needs to be set to a nonzero value to invoke the cladding protection abstraction.
EBSREL	FuelRadiusInRod[m]	r_{rod} Fuel radius in rod [m]	constant 0.005	Dimensions are consistent with typical light water reactor fuel, especially from pressurized water reactors (Bechtel SAIC Company, LLC, 2004a).
EBSREL	SurfaceAreaOfGlass[m^2/kg]	a_{glass}^0 Glass waste form reference-specific surface area [m^2/kg]	constant 2.77	Value selected consistent with literature values (Bechtel SAIC Company, LLC, 2001).
EBSREL	pHForGlassModel[]	pH of in-package water for glass waste form dissolution model [unitless]	uniform 4.0, 10.0	Based on simulations of water chemistry in codisposal packages (Pan, et al., 2003).
EBSREL	LogOfGlassDissolutionConstantHighRange[]	$\log_{10}$ of k_0 Intrinsic dissolution rate for the glass dissolution model for pH > 6, in g/[m^2day] [unitless]	uniform 4.708618, 5.708618	Value selected consistent with literature values (Bechtel SAIC Company, LLC, 2001).
EBSREL	pHParameterHighRange[]	n pH dependence coefficient for glass dissolution for pH > 6 [unitless]	constant 0.49	Value selected consistent with literature values (Bechtel SAIC Company, LLC, 2001).
EBSREL	GlassActivationEnergyHighRange[kJ/mol-K]	E_{ag} Effective activation energy for glass dissolution model for pH > 6 [kJ/mol-K]	constant 69.0	Value selected consistent with literature values (Bechtel SAIC Company, LLC, 2001).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	LogOfGlassDissolutionConstantLowRange[]	$\log_{10}$ of k_0 Intrinsic dissolution rate for the glass dissolution model for $\text{pH} < 6$, in $\text{g}/[\text{m}^2\text{day}]$ [unitless]	uniform 6.308618, 8.308618	Value selected consistent with literature values (Bechtel SAIC Company, LLC, 2001).
EBSREL	pHParameterLowRange[]	n pH dependence coefficient for glass dissolution for $\text{pH} < 6$ [unitless]	constant -0.49	Value selected consistent with literature values (Bechtel SAIC Company, LLC, 2001).
EBSREL	GlassActivationEnergyLowRange [kJ/mol-K]	E_{ag} Effective activation energy for glass dissolution model for $\text{pH} < 6$ [kJ/mol-K]	constant 31.0	Value selected consistent with literature values (Bechtel SAIC Company, LLC, 2001).
EBSREL	WeldCrackLength[m]	L_{cr} Diffusive pathway length [m]	constant 0.1	Parameter of exploratory diffusive release model. In the reference case, diffusive release is not simulated. A pathway length is highly uncertain. A value of 10 cm was selected as an order of magnitude estimate.
EBSREL	TotalAreaOfCracksPerWPAt Emplacement[m^2]	A_{cr}^a Diffusive pathway initial cross section [m^2]	constant 2.0e-5	Parameter of exploratory diffusive release model. In the reference case, diffusive release is not simulated. The cross section is highly uncertain. Assuming ellipsoidal cracks 15 mm in length and 0.2 mm in width, and that up to eight cracks develop on the waste package, results in a total cross section equal to 22 mm ² . The value of 2×10^{-5} m ² was selected for exploratory purposes.
EBSREL	SlopeOfCrackAreaCurve[m^2/yr]	A_{cr}^b Cross section growth rate [m^2/yr]	constant 2.0e-9	Parameter of exploratory diffusive release model. In the reference case, diffusive release is not simulated. Value selected for exploratory purposes to allow for the initial cross section to increase with time.
EBSREL	LengthOfFilmPathInsideWPI[m]	L_{in} Internal diffusive pathway length [m]	constant 0.2	Parameter of exploratory diffusive release model. In the reference case, diffusive release is not simulated. The pathway length is highly uncertain. A value of 20 cm was selected as an order of magnitude estimate.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	InternalFilmCrossSectionalArea [m^2]	A_{in} Internal diffusive pathway cross section [m ²]	constant 2.0e-5	Parameter of exploratory diffusive release model. In the reference case, diffusive release is not simulated. A value of 2×10^{-5} m ² was selected to be consistent with A_{cr} value.
EBSREL	SelfDiffusionCoefficientOfWaterAt 20C [m^2/s]	D_w Self diffusion coefficient of water at 20 °C [m ² /s]	constant 2.2e-9	Parameter of exploratory diffusive release model (Lide, 1990). In the reference case, diffusive release is not simulated. This is accomplished by setting $f_t = 0$, as f_t is a scaling factor for the diffusive release rate.
EBSREL	FractionOfWPsWithDiffusionTilt[]	f_t Diffusive release adjustment factor [unitless]	constant 0.0	Parameter of exploratory diffusive release model. In the reference case, diffusive release is not simulated. This is accomplished by setting $f_t = 0$, as f_t is a scaling factor for the diffusive release rate.
EBSREL	DiffusionCorrectionFactorCm[]	f_{Cm} Correction factor to account for curium diffusivity [unitless]	constant 0.25	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactor_U[]	f_U Correction factor to account for uranium diffusivity [unitless]	constant 0.29	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorAm[]	f_{Am} Correction factor to account for americium diffusivity [unitless]	constant 0.26	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorNp[]	f_{Np} Correction factor to account for neptunium diffusivity [unitless]	constant 0.33	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorPu[]	f_{Pu} Correction factor to account for plutonium diffusivity [unitless]	constant 0.25	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	DiffusionCorrectionFactorTh[]	f_{Th} Correction factor to account for thorium diffusivity [unitless]	constant 0.25	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorRa[]	f_{Ra} Correction factor to account for radium diffusivity [unitless]	constant 0.25	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorPb[]	f_{Pb} Correction factor to account for lead diffusivity [unitless]	constant 0.55	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorCs[]	f_{Cs} Correction factor to account for cesium diffusivity [unitless]	constant 1.0	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorI[]	f_I Correction factor to account for iodine diffusivity [unitless]	constant 0.96	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorTc[]	f_{Tc} Correction factor to account for technetium diffusivity [unitless]	constant 0.64	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorNi[]	f_{Ni} Correction factor to account for nickel diffusivity [unitless]	constant 0.55	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorSe[]	f_{Se} Correction factor to account for selenium diffusivity [unitless]	constant 0.32	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	DiffusionCorrectionFactorNb[]	f_{Nb} Correction factor to account for niobium diffusivity [unitless]	constant 0.55	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	DiffusionCorrectionFactorCl[]	f_{Cl} Correction factor to account for chlorine diffusivity [unitless]	constant 0.96	Correction factor to adjust diffusion coefficient of element with respect to the self-diffusion coefficient of water (Lide, 1990). In the reference case, diffusive release is not simulated.
EBSREL	SorptionCapacity[moles/m3]	S_x Maximum allowable moles of thorium, uranium, plutonium, americium, and curium attached irreversibly to steel corrosion product colloids [moles/m ³]	usersuppliedpwiseCDF 21 7.37E-06, 0 9.45E-05, 0.05 1.93E-04, 0.1 2.84E-04, 0.15 3.76E-04, 0.2 4.63E-04, 0.25 5.49E-04, 0.3 6.39E-04, 0.35 7.49E-04, 0.4 8.69E-04, 0.45 1.03E-03, 0.5 1.23E-03, 0.55 1.50E-03, 0.6 1.76E-03, 0.65 2.09E-03, 0.7 2.49E-03, 0.75 3.04E-03, 0.8 3.73E-03, 0.85 4.53E-03, 0.9 5.97E-03, 0.95 1.10E-02, 1	Calculated from distributions for corrosion product colloid concentration and specific surface area. Based on data from Bechtel SAIC Company, LLC (2005b), adjusted to account for elimination of carbon steel from commercial spent nuclear fuel waste canister design (DOE, 2006). Documented in Pickett (2007a).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	AffinityFactorAm	Y_{Am} Affinity of americium, relative to plutonium, for irreversible attachment to iron oxyhydroxide colloids [unitless]	uniform 5.0, 15.0	The affinity factors can be shown to be ratios of rate constants in a kinetically controlled sorption process. Sorption of americium was generally faster than plutonium in the Lu, et al. (2000, 1998) experiments, but rates are difficult to quantify; the values reflect a staff estimate. A higher affinity for americium with respect to plutonium is consistent with the significantly higher K_D values reported for americium on iron oxyhydroxides and other substrates (Bechtel SAIC Company, LLC, 2005b). This parameter is used in the numerator of an americium version of Eq. (10-18); in the denominator of the uranium, plutonium, and americium versions of Eq. (10-18); in the numerator of an americium version of Eq. (10-20); and in the denominator of all versions of Eq. (10-20).
EBSREL	AffinityFactorCm	Y_{Cm} Affinity of curium, relative to plutonium, for irreversible attachment to iron oxyhydroxide colloids [unitless]	uniform 5.0, 15.0	Set to AffinityFactorAm due to lack of data and similar chemical characteristics. This parameter is used in the numerator of a curium version of Eq. (10-20) and in the denominator of all versions of Eq. (10-20).
EBSREL	AffinityFactorTh	Y_{Th} Affinity of thorium, relative to plutonium, for irreversible attachment to iron oxyhydroxide colloids [unitless]	uniform 5.0, 15.0	Set to AffinityFactorAm due to lack of data. This parameter is used in the numerator of a thorium version of Eq. (10-20) and in the denominator of all versions of Eq. (10-20).
EBSREL	AffinityFactor_U	Y_U Affinity of uranium, relative to plutonium, for irreversible attachment to iron oxyhydroxide colloids [unitless]	loguniform 0.005, 0.05	The affinity factors are, effectively, proportional to rate constants in a kinetically controlled sorption process. In Lu, et al. (2000), uranium sorption was significantly slower than plutonium. This parameter is used in the numerator of a uranium version of Eq. (10-18), in the denominator of all versions of Eq. (10-18), and in the denominator of all versions of Eq. (10-20).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSFILT	PermanentLossColloidFilterFactor_Invert_Ja[]	The proportion of americium irreversibly attached to colloids that is permanently removed by filtration in the invert [unitless]	constant 0.0	This is a legacy parameter defined for the obsolete EBSFILT standalone program.
EBSFILT	PermanentLossColloidFilterFactor_Invert_Jc[]	The proportion of curium irreversibly attached to colloids that is permanently removed by filtration in the invert [unitless]	constant 0.0	This is a legacy parameter defined for the obsolete EBSFILT standalone program.
EBSFILT	PermanentLossColloidFilterFactor_Invert_Jp[]	The proportion of plutonium irreversibly attached to colloids that is permanently removed by filtration in the invert [unitless]	constant 0.0	This is a legacy parameter defined for the obsolete EBSFILT standalone program.
EBSFILT	PermanentLossColloidFilterFactor_Invert_Jt[]	The proportion of thorium irreversibly attached to colloids that is permanently removed by filtration in the invert [unitless]	constant 0.0	This is a legacy parameter defined for the obsolete EBSFILT standalone program.
EBSFILT	InvertBypass(0=ebsfilt, 1=bypass-ebsfilt)	Flag for selecting whether to perform calculations for transport through the invert. A value of 1 indicates that the transport through invert is skipped	iflag 1	Program control switch to investigate effects of the invert. Invert transport is bypassed in the reference case. The EBSFILT invert transport model is legacy code and unsupported in TPA Version 5.1.
EBSFILT	InvertRockPorosity	Porosity of the invert [unitless]	constant 0.13	This is a parameter defined for the legacy EBSFILT standalone program.
EBSFILT	InvertThickness[m]	Invert thickness [m]	constant 0.806	This is a parameter defined for the legacy EBSFILT standalone program.

Table 10-1. Reference Data for Parameters of <i>tpa.inp</i> Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type	Remarks
EBSFILT	InvertDiffusionCoefficient[m ² /yr]	Diffusion coefficient for the invert [m ² /yr]	constant 3.0e-3	This is a parameter defined for the legacy EBSFILT standalone program.
EBSFILT	InvertMatrixPermeability[m ²]	Matrix permeability of the invert [m ²]	constant 7.0e-18	This is a parameter defined for the legacy EBSFILT standalone program.
EBSFILT	IrreversibleColloidModel [0=no, 1=yes]	Program switch to control the introduction of irreversible radionuclides into the groundwater transport models (0 = no colloids are introduced; 1 = colloids are introduced)	iconstant 1	Reference case value enables the irreversible colloid release model, which is the preferred approach (Bechtel SAIC Company, LLC, 2005b).
EBSREL	WastePackageFlowMultiplication Factor	F_{FMF} Scaling factor for deep percolation flow rates to estimate maximum flow rates potentially impinging on waste packages [unitless]	loguniform 1.0, 4.0	Values are selected proportional to the spacing between drips. Average drip spacing greater than waste package lengths implies that some waste packages are not contacted by water, with water diverted onto neighboring waste packages. Mass balance requires that the product of SubAreaWetFraction and WastePackageFlowMultiplicationFactor is equal to 1. This water balance constraint is implemented by sampling these two parameters with a rank correlation coefficient of -0.9999 from mutually inverse distributions. See Basagaoglu, et al. (2007).
EBSREL	SeepageRubbleFactor	Value of rubble flow factor F_r when rubble starts accumulating on top of the drip shield [unitless]	constant 1.0	In the reference case, it is assumed there is no water diversion/convergence caused by rubble accumulated on the drip shield top. This assumption is implemented by setting $F_r = 1$.
EBSREL	SeepageEngineeringBackfillFactor	Flow factor for engineering backfill [unitless]	constant 1.0	Flow factor to adjust seepage rates to estimate water flow rates to mobilize waste forms. This flow factor is only used when the value of the <i>tpa.inp</i> parameter <u>EmplacementBackfillThickness[m]</u> is greater than 0.
NFENV	EmplacementBackfillThickness[m]	Equivalent thickness of emplaced backfill [m]	constant 0.0	Value reflecting the current design, which includes no backfill.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	FlagPartialProtectionFromSeepageByMechFailedDS[1=yes, 0=no]	Flag for activating partial seepage reduction by mechanically breached drip shield	iflag 1	Reference case value activates partial seepage reduction by mechanically breached drip shield. When set to 0, F_d is equal to 1 at the earliest time of drip shield mechanical breaching.
EBSREL	InitialSeepageReductionFractionByMechFailedDS	Value for the drip shield flow factor F_d at the earliest time of mechanical breaching of the drip shield [unitless]	loguniform 0.01, 1.0	Staff expert judgment was used to define this distribution. If the damaged drip shield area is of the order of 0.5 m^2 [5.4 ft^2] and the projected drip shield surface (i.e., the size of the shadow) is of the order of 14 m^2 [150.7 ft^2], then the damage fraction is of the order of 0.03. If it is assumed that five water seeps impinge on the drip shield, then the probability that at least one is captured by the breached surface is $1 - (1 - 0.03)^5 = 0.16$. If a factor of 10 decrease is assumed, due for example to smaller damaged areas or fewer seeps, then 0.01 is a reasonable assumption for a low bound on the distribution. On the other hand, water catchment areas could be larger than damaged areas, and water could flow through rubble and the drip shield. Thus, an upper bound of one is proposed for the distribution. A log-uniform distribution was selected to reflect that low values of this parameter are thought to be more likely than higher values.
EBSREL	DSSeepageProtectionDegradationRate[1/yr]	Rate of linear increase in the drip shield flow factor F_d [1/yr]	constant 0.0	In the reference case, a constant value for F_d is assumed up to the time of drip shield breach by general corrosion.
EBSREL	FlagPartialProtectionFromSeepageByMechFailedWP[1=yes, 0=no]	Flag for activating partial seepage reduction by mechanically breached waste package	iflag 1	In the reference case, partial flow reduction by a mechanically breached waste package is assumed (flag equal to 1). When set to zero, $F_{wpm} = 1$ at the earliest time of waste package breaching by mechanical interaction with the drip shield.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	InitialSeepageReductionFractionByMechFailedWP	Change in the mechanical flow factor F_{wm} at the earliest time of mechanical breaching of the waste package [unitless]	uniform 0.01, 1.0	Staff expert judgment was used to define this distribution. As an extreme case, it is considered that all of the water contacting the waste package is available to mobilize radionuclides. A correlation could exist between the locations of damage on the drip shield, damage on the waste package, and the location water flow; thus, geometrical arguments to estimate this parameter appear of limited value. A uniform distribution is selected to reflect the extent of the uncertainty in this parameter. A low bound of 0.01 is selected to avoid extremely low estimates of water flow rates to mobilize waste forms.
EBSREL	WPSeepageProtectionDegradationRate[1/yr]	Rate of linear increase in the mechanical flow factor F_{wm} after the time of the waste package mechanical damage [1/yr]	constant 0.0	No linear increase in time in the factor F_{wm} is assumed in the reference case.
EBSREL	FlagPartialProtectionFromSeepageByInitialDefWP[1=yes, 0=no]	Flag for activating partial seepage reduction by initially defective waste package	iflag 1	In the reference case, partial flow reduction by initially defective waste packages is assumed (flag equal to 1). When set to zero, $F_{id} = 1$ at the time InitialFailureTime[yr].
EBSREL	InitialSeepageReductionFractionInitiallyDefWP	Value for the initially defective flow factor F_{id} at the initial failure time [unitless]	loguniform 0.001, 0.1	Staff expert judgement was used to define this distribution. Initially defective regions on the waste package are expected to be small. The same distribution as the parameter InitialSeepageReductionFractionLC is adopted.
EBSREL	WPSeepageProtectionDegradationRateInitiallyDefWP[1/yr]	Rate of linear increase in the initially defective flow factor F_{id} [1/yr]	constant 0.0	No linear increase in time in the factor F_{id} is assumed in the reference case.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	InitialSeepageReductionFractionWeldLC	Change in flow factors F_{id} , F_{wm} , and F_{wc} to account for enhanced water flow rates into waste packages after welded areas are compromised by corrosion [unitless]	loguniform 0.001, 0.1	Staff expert judgment was used to define this distribution. The same distribution as the parameter InitialSeepageReductionFractionLC is adopted.
EBSREL	InitialSeepageReductionFractionLC	Change in flow factors F_{id} , F_{wm} , and F_{wc} to account for enhanced water flow rates into waste packages after the waste package body is compromised by localized corrosion	loguniform 0.001, 0.1	Staff expert judgment was used to define this distribution. Values are likely small because of the following observations. Localized corrosion in Alloy 22 is in the form of crevice corrosion (Dunn, et al., 2005). Crevices must be tight for crevice corrosion to propagate (opening of crevices causes arrest of localized corrosion) (He and Dunn, 2007). If crevices are tight, water may not flow freely but rather diffuse into the crevice area. Pits in the crevice area are a few microns in diameter (He and Dunn, 2007) and full with corrosion products, further restricting the flow of water. Waste packages are heat sources that tend to move water away. Therefore, it is reasonable to assume that the infiltrated seepage is a small fraction (1/1000 or greater) of the seepage impinging on the waste package. Using smaller factors than 0.001 may cause TPA Version 5.1 to deal with flow rates inside and outside the waste package of few drops per year; thus, caution should be exercised in using too small values. For the reasons previously described, flow infiltrating the waste package is expected to be a fraction of the total flow contacting the waste package. As an order of magnitude estimate, at least a reduction of 0.1 is assumed. A log distribution is selected to reflect that lower values of the parameter are more likely.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	Probability_WPWaterContact_GC-Flt-Ig	Probability $P_{contact}$ that seepage contacts waste packages breached by general corrosion, faulting, or intrusive igneous event [unitless]	constant 1.0	This parameter is related to scaling the number of waste packages in a particular class. In the reference case, it is assumed that all of the waste packages breached by faulting and igneous events and by general corrosion are contacted by seepage.
EBSREL	Probability_WPWaterAllowance_GC-Flt-Ig	Probability $P_{allowance}$ that seepage infiltrates a breached waste package (general corrosion, faulting, intrusive igneous event), conditional on seepage contact [unitless]	constant 1.0	This parameter is related to scaling the number of waste packages in a particular class. In the reference case, it is assumed that water infiltrates all of the waste packages breached by faulting and igneous events and by general corrosion if contacted by seepage.
EBSREL	Probability_WPWaterContact_InitialDefects	Probability $P_{contact}$ that seepage contacts initially defective waste packages [unitless]	constant 1.0	This parameter is related to scaling the number of waste packages in the initially defective class. Because drip shields are eventually compromised by general corrosion, there is a high probability that initially defective waste packages are eventually contacted by seepage.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	Probability_WPWWaterAllowance_InitialDefects	Probability $P_{allowance}$ that seepage infiltrates an initially defective waste package, conditional on seepage contact [unitless]	uniform 0.001, 0.1	This parameter is related to scaling the number of waste packages in the initially defective class. It is assumed that there is no correlation between the location of defective areas on the waste package and the location of seeps or flowing water on the waste package. It is assumed that liquid water contacts the waste forms only in a fraction of initially defective waste packages. Because the interest in the EBSREL computations is in order of magnitude estimates, a maximum probability of 0.1 is assumed. A low bound of 0.001 is selected as a reasonable value. Smaller probability values than 0.001 result in a waste package count rounded to 0 because the number of waste packages in a subarea ranges from few hundreds to few thousands (and only a small fraction is considered initially defective). The number of waste packages for the EBSREL computations is always rounded to integers.
EBSREL	Probability_WPWWaterContact_MechFail	Probability $P_{contact}$ that seepage contacts a mechanically breached waste package [unitless]	constant 1.0	This parameter is related to scaling the number of waste packages in the mechanical class. Because drip shields are eventually compromised by general corrosion, there is a high probability that mechanically breached waste packages are eventually contacted by seepage.
EBSREL	Probability_WPWWaterAllowance_MechFail	Probability $P_{allowance}$ that seepage infiltrates a mechanically breached waste package, conditional on seepage contact [unitless]	uniform 0.01, 1.0	This parameter is related to scaling the number of waste packages in the mechanical class. Staff expert judgment was used to define this distribution. As an upper bound case, it is considered that water infiltrates all of the mechanically breached waste packages that are contacted by seepage. A low bound of 0.01 is selected to ensure that some waste packages in this damage class in a subarea contribute to radionuclide release.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	Probability_WPWWaterContact_LC	Probability $P_{contact}$ that seepage contacts appropriate regions on the waste package (e.g., crevice areas) to cause the formation of brines and induce localized corrosion [unitless]	uniform 0.001, 0.1	This parameter is used for scaling the number of waste packages in the localized corrosion class. The parameter $P_{contact}$ is also used to recognize the existence of additional requirements for waste packages to exhibit localized corrosion. For Alloy 22, localized corrosion is in the form of crevice corrosion (Dunn, et al., 2005). Initiation and propagation of crevice corrosion requires the presence of tight crevices and water of sufficient ionic strength and appropriate composition to support electrochemical processes. Recent experiments suggest varying degrees of susceptibility to localized corrosion depending on crevice quality (He and Dunn, 2007). Crevices could arise due to drip shield collapse. Crevices will be present on the waste package support at the base. However, radionuclide release pathways are unclear if crevice corrosion was to occur at the waste package base. It is apparent that the probability for crevices to develop on welded areas is limited (given the small portion of the surface covered by welds—approximately 1 percent in order of magnitude). The probability for crevices to develop on nonwelded regions is higher; however, the likelihood for localized corrosion to be exhibited in mill-annealed areas is less than in welds (Pensado, et al. 2006; Dunn, et al., 2005). It also appears that the probability for brines to develop next to crevices is limited. Therefore, it is reasonable to assume that favorable conditions for localized corrosion are only established in a fraction of the waste packages contacted by liquid water. Because the interest in EBSREL is in order of magnitude estimates, a maximum probability value of 0.1 is assumed. The parameter $P_{contact}$ is assumed uniformly distributed to reflect the parameter uncertainty. A lower bound of 0.001 is selected to ensure that at least a few waste packages in this class in a subarea contribute to radionuclide release.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
EBSREL	Probability_WPWWaterAllowance_LC	Probability $P_{allowance}$ that seepage infiltrates a waste package breached by localized corrosion, conditional on seepage contact [unitless]	constant 1.0	In the reference case, it is assumed that liquid water infiltrates waste packages compromised by localized corrosion and contacts the waste forms. Localized corrosion can only initiate and propagate if liquid water is available to support electrochemical reactions of corrosion processes. Because water is available at the position where the breaching occurs, it is assumed that it infiltrates the waste package.
EBSREL	AFmultCoefficient	a Shape parameter for calculating near- and in-drift flow diversion seepage factor F_{mult} [unitless]	constant 0.9	Parameter value computed based on the approach described in Basagaoglu, et al. (2007).
EBSREL	BFmultCoefficient	b Scale parameter for calculating near- and in-drift flow diversion seepage factor F_{mult} [unitless]	constant 0.5	Parameter value computed based on the approach described in Basagaoglu, et al. (2007).
EBSREL	X0FmultCoefficient	X_0 Shift parameter for calculating near- and in-drift flow diversion seepage factor F_{mult} [unitless]	triangular 2.3, 3.4, 4.6	Parameter value computed based on the approach described in Basagaoglu, et al. (2007).
Correlated Parameters	Independent Variable InitialSeepageReductionFraction InitiallyDefWP Dependent Variable SFWettedFraction Initial	Correlation between F_{id} at the initial failure time and f_{swf} for the initially defective class	correlateinputs 0.9	It is assumed that high water flow rates (due, for example, to large water catchment areas on the waste package) correlate with high fractions of the waste form volume contacted by water.

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
Correlated Parameters	Independent Variable InitialSeepageReductionFraction ByMechFailedWP Dependent Variable SFWettedFraction_MECH1	Correlation between the increase in F_{wm} at the time of the first mechanical breaching event and f_{sfrf} for the first mechanical class	correlateinputs 0.9	It is assumed that high water flow rates (due, for example, to large water catchment areas on the waste package) correlate with high fractions of the waste form volume contacted by water.
Correlated Parameters	Independent Variable InitialSeepageReductionFraction ByMechFailedWP Dependent Variable SFWettedFraction_MECH2	Correlation between the increase in F_{wm} at the time of the second mechanical breaching event and f_{sfrf} for the second mechanical class	correlateinputs 0.9	It is assumed that high water flow rates (due, for example, to large water catchment areas on the waste package) correlate with high fractions of the waste form volume contacted by water.
Correlated Parameters	Independent Variable InitialSeepageReductionFraction LC Dependent Variable SFWettedFraction_LC	Correlation between the increase in F_{lch} , F_{wm} , and F_{wc} at the time of localized corrosion (mill-annealed) and f_{sfrf} for the localized corrosion class	correlateinputs 0.9	It is assumed that high water flow rates (due, for example, to large water catchment areas on the waste package) correlate with high fractions of the waste form volume contacted by water.
Correlated Parameters	Independent Variable SFWettedFraction_MECH1 Dependent Variable SFWettedFraction_MECH2	Correlation between f_{sfrf} values for the first and second mechanical events	correlateinputs 0.9999	The spent fuel wetted fraction is the same for both mechanical breach events.
Correlated Parameters	Independent Variable SubAreaWetFraction Dependent Variable WastePackageFlowMultiplicationFactor	Correlation between subarea wet fraction and F_{FMF}	correlateinputs -0.9999	Water mass balance requires that the product of SubAreaWetFraction and WastePackageFlowMultiplicationFactor be equal to 1 (Section 10.3.1.1).
Correlated Parameters	Independent Variable SubAreaWetFraction XOf Dependent Variable MultCoefficient	Correlation between subarea wet fraction and X_o	correlateinputs 0.9	Consistent with other correlations (Table 5-1).

Table 10-1. Reference Data for Parameters of tpa.inp Used by EBSREL (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type	Remarks
Correlated Parameters	Independent Variable WastePackageFlowMultiplication Factor	Correlation between X_0 and F_{FMF}	correlateinputs -0.9	Consistent with other correlations (Table 5-1).
	Dependent Variable XOfMultCoefficient			

modeled by EBSREL. Processes with significant uncertainties are assigned probabilistic parameter distributions in the *tpa.inp* file, and several types of parametric sensitivity analysis techniques (e.g., Mohanty, et al., 2004) may be useful to understand their effects on system-level performance.

Table 10-2. Auxiliary Input Data Files Used by EBSREL

File	Description
<i>ebsfilt.def</i>	This is a template file for <i>ebsfilt.inp</i> , the input file for the legacy EBSFILT program [activated by setting the <i>tpa.inp</i> parameter InvertBypass(0=ebsfilt,1=bypass-ebsfilt) to 0]. To write <i>ebsfilt.inp</i> , EBSREL updates the contents of <i>ebsfilt.def</i> with invert radionuclide transport parameters and the colloid filter factors for the invert.
<i>ebsrel.def</i>	This is a template file for <i>ebsrel.inp</i> , the input file for RELEASET. EBSREL copies the contents of <i>ebsrel.def</i> , replaces a part of this information with (i) parameters set in the EBSREL section of <i>tpa.inp</i> , (ii) results from other modules (e.g., waste package breach times), (iii) EBSREL flow factor data from <i>ebsflo.dat</i> , and (iv) other EBSREL data files such as <i>ebspac.nuc</i> . The file <i>ebsrel.def</i> contains some input parameters that are not specified in <i>tpa.inp</i> (e.g., values setting numerical control, rock parameters, and diffusion rates).
<i>wpflow.def</i>	This file provides EBSREL with a template for time histories of flow factors that determine the quantity of water entering the waste package. For all these factors except F_{ow} and F_{wet} , these time histories provide alternatives to the flow factor abstractions described in Section 10.3.1. The following defined flow factors are mapped from <i>wpflow.def</i> to timesteps in EBSREL: flow diversion (F_{mult}); flow contacting waste packages (F_{ow}); fraction of subarea wetted (F_{wet}); rubble diversion (F_r); failed drip shield diversion (F_d); diversion by waste package failure due to faulting, igneous intrusion, or corrosion (F_{wc}); diversion by mechanically breached waste packages for breach events 1 and 2 (F_{wm1} and F_{wm2}); and diversion by initially defective waste packages (F_{id}). EBSREL writes any new values computed or assigned for these factors to the files <i>wpflow.dat</i> and <i>ebsflo.dat</i> (Table 10-3) using <i>wpflow.def</i> as a template. In the unmodified <i>wpflow.def</i> file, all factors at all times are set to 1.0. Discussions of each factor in Section 10.3.1 show how the user can define the time histories by modifying <i>wpflow.def</i> . For most factors, the use of the <i>wpflow.def</i> values (whether 1.0 or modified) is triggered by assigning negative values to certain parameters in <i>tpa.inp</i> . The negative-value trigger <i>tpa.inp</i> parameters are as follows: AfmultCoefficient, BfmultCoefficient, or X0FmultCoefficient for F_{mult} ; SeepageRubbleFactor for F_r ; InitialSeepageReductionFractionByMechFailedDS for F_d ; InitialSeepageReductionFractionInitiallyDefWP for F_{id} ; InitialSeepageReductionFractionByMechFailedWP for F_{wm1} and F_{wm2} ; and InitialSeepageReductionFractionLC or InitialSeepageReductionFractionWeldLC for F_{wc} . No such triggers are necessary for F_{ow} and F_{wet} , which are assigned the <i>wpflow.def</i> values in all cases.

Table 10-3. Intermediate Output Files Created During Execution of EBSREL	
File Name	Description
<i>cumrel.res</i>	This results file contains cumulative radionuclide species releases (dissolved and colloidal) from the engineered barrier system for each realization and is summed over all subareas. This file is described in further detail in Chapter 19.
<i>cumrel_c.res</i>	This results file contains cumulative radionuclide species releases (dissolved and colloidal) from the engineered barrier system for each realization, summed over all subareas, for the time period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. This file is described in further detail in Chapter 19.
<i>infilper.res</i>	From EBSREL, this file contains the flow rate after modification by each of the flow factors F_{ow} , F_{mult} , F_r , and F_d , as well as the weighted average flow rates into and out of the waste package, for every tenth timestep and all subareas. Also contains data from UZFLOW (Chapter 5). This file is described in more detail in Chapter 19.
<i>pkreltim.res</i>	This results file contains engineered barrier system peak radionuclide release rates (dissolved and colloidal) and times of peak releases in each subarea for each realization.
<i>pkrltm_c.res</i>	This results file contains engineered barrier system peak radionuclide release rates (dissolved and colloidal) and times of peak releases for the time period specified by the <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr].
<i>ebsflo.dat</i>	The time-varying volumetric flow rates after reflux from NFENV, the WastePackageFlowMultiplicationFactor in <i>tpa.inp</i> , and the factors that account for flow contacting the waste package (e.g., F_{mult} and F_{ow}) are written by EBSREL to <i>ebsflo.dat</i> . This file is input to the RELEASET standalone code; values reflect the final subarea and realization.
<i>ebsglass.dat</i>	Written in EBSREL, this file contains release rates, affected flag, and q_{out} per timestep per radionuclide for glass waste form. Values in this file reflect the final subarea and realization.
<i>ebsnef.dat</i>	This file contains results of the waste package release rate calculations for all groundwater nuclides, including colloidal species, plus water flow rate. In EBSREL, the colloid J-species release information in <i>ebscld.out</i> is added to the end of <i>ebsnef.out</i> to create the file <i>ebsnef.dat</i> for input to EBSFILT. Values in this file reflect the final subarea and realization.

Table 10-3. Intermediate Output Files Created During Execution of EBSREL (continued)	
File Name	Description
<i>ebsnef2.dat</i>	Results of the engineered barrier system release rates per timestep for all groundwater nuclides computed in the standalone code EBSFILT are provided in <i>ebsnef2.dat</i> . EBSREL accesses the release rates in <i>ebsnef2.dat</i> , and the information is then used as input to UZFT. Also contains water flow data. Values in this file reflect the final subarea and realization. When EBSFILT is disabled, <i>ebsnef2.dat</i> is identical to <i>ebsnef.dat</i> .
<i>ebssf.dat</i>	Written in EBSREL, this file contains release rates, affected flag, and q_{out} per timestep per radionuclide for spent nuclear fuel. Values in this file reflect the final subarea and realization.
<i>maxrel.dat</i>	Written by the RELEASET standalone code, this file contains the maximum fractional release of all radionuclides (prior to colloid allocation) and the time of each maximum release. Values in this file reflect the final subarea and realization.
<i>wpflow.dat</i>	This file is written in EBSREL using <i>wpflow.def</i> as a template. It contains the time history of seepage factors for flow diversion (F_{mult}), flow contacting waste packages (F_{ow}), fraction of subarea wetted (F_{wet}), rubble diversion (F_r), failed drip shield diversion (F_d), and breached waste package diversion by corrosion (F_{wc}), mechanical events 1 and 2 (F_{wm1} and F_{wm2}), and initially defective waste package diversion (F_{id}) used in RELEASET. Values in this file reflect the final subarea and realization.
<i>ebsfilt.dbg</i>	This file contains the same information as <i>ebsnef2.dat</i> , with an additional header reporting parameters from the legacy EBSFILT program (number of nuclides, flow rate, porosity, permeability, invert length, and diffusion coefficient). Created only if the legacy EBSFILT program is activated.
<i>ebsfilt.inp</i>	Generated by setting InvertBypass(0=ebsfilt,1=bypass-ebsfilt) to 0 in <i>tpa.inp</i> , this is an EBSFILT input file. EBSREL uses the template file <i>ebsfilt.def</i> and invert transport parameters from <i>tpa.inp</i> to write <i>ebsfilt.inp</i> . Values in this file reflect the final subarea and realization.
<i>ebsrel.inp</i>	EBSREL uses template file <i>ebsrel.def</i> and the release- and flow-related parameters specified in the EBSREL section of <i>tpa.inp</i> to write <i>ebsrel.inp</i> as input to RELEASET. The file includes waste package breach numbers and times, wetted fraction of the subarea, waste package and waste form physical characteristics, temperature, flow factors from <i>ebsflo.dat</i> , leaching parameters, water contact mode data, inventory, cladding parameters, and diffusion parameters. This file corresponds to <i>ebsrelglass.inp</i> or <i>ebsrelsf.inp</i> , depending on the modeled waste form. Values in this file reflect the final subarea, realization, and waste form.
<i>ebsrelglass.inp</i>	This RELEASET input file for glass waste form corresponds to <i>ebsrel.inp</i> . Values in this file reflect the final subarea and realization.

Table 10-3. Intermediate Output Files Created During Execution of EBSREL (continued)	
File Name	Description
<i>ebsrelsf.inp</i>	This RELEASET input file for spent nuclear fuel corresponds to <i>ebsrel.inp</i> . Values in this file reflect the final subarea and realization.
<i>ebspac.nuc</i>	This RELEASET input file contains initial radionuclide inventory per waste package, molecular weights, half-lives, and decay chain data from INVENT (Chapter 4) and solubility limits, invert retardation factors, and gap fractions specified in the EBSREL section of <i>tpa.inp</i> . The file corresponds to <i>ebspacglass.nuc</i> or <i>ebspacsf.nuc</i> , depending on the modeled waste form. Values in this file reflect the final realization and waste form.
<i>ebspacglass.nuc</i>	This RELEASET input file for glass waste form corresponds to <i>ebspac.nuc</i> . Values in this file reflect the final realization.
<i>ebspacsf.nuc</i>	This RELEASET input file for spent nuclear fuel corresponds to <i>ebspac.nuc</i> . Values in this file reflect the final realization.
<i>cumrelse.out</i>	This RELEASET output file contains the quantity of a radionuclide outside the waste package as a function of time for a given subarea. These values are interpolated from the internal time scale as given in <i>trelease.out</i> onto the system time scale. Values in this file reflect the final subarea and realization.
<i>diagnose.out</i>	This RELEASET output file contains information for diagnostic purposes only.
<i>ebscld.out</i>	Written in EBSREL, this file contains colloidal J-species release rates. Reflects the final subarea and realization.
<i>ebsfilt.out</i>	Generated by setting InvertBypass(0=ebsfilt,1=bypass-ebsfilt) to 0 in <i>tpa.inp</i> , this file contains screen output from the last execution of EBSFILT. The file contains only debugging information and reflects the final subarea and realization.
<i>ebsnef.out</i>	This RELEASET output file contains time-dependent waste package radionuclide release rates, affected flag (indicating whether release was solubility limited), and water flow rate q_{out} . Values in this file reflect the final subarea and realization.
<i>frac_rel.out</i>	The <i>frac_rel.out</i> file is written by RELEASET and contains the same information as <i>ebsnef.dat</i> . Values in this file reflect the final subarea and realization.
<i>inv1000.out</i>	The <i>inv1000.out</i> file is written by RELEASET and contains the inventory of the groundwater nuclides at 1,000 years and the initial inventory per waste package from <i>ebspac.nuc</i> . Reflects the final subarea and realization.

Table 10-3. Intermediate Output Files Created During Execution of EBSREL (continued)	
File Name	Description
<i>rel_flow.out</i>	Written in RELEASET, this file contains the weld surface fraction, weld failure flag and time, waste package general corrosion flag and breach time, and waste package localized corrosion failure flag and time. Reflects the final subarea and realization.
<i>relcum.out</i>	This file contains output from RELEASET, including number of breached waste packages per class, the time at which liquid water contacts the waste form, waste package water fill times, and radionuclide inventory data. The inventory values represent quantities inside the waste package if release had not occurred, cumulative quantities released from waste form but not from the waste package, and cumulative quantities released from the engineered barrier system. The file corresponds to <i>relcumglass.out</i> or <i>relcumsf.out</i> , depending on the modeled waste form. Values in this file reflect the final subarea, realization, and waste form.
<i>relcumglass.out</i>	This RELEASET output file for glass waste form corresponds to <i>relcum.out</i> . Values in this file reflect the final subarea and realization.
<i>relcumsf.out</i>	This RELEASET output file for spent nuclear fuel corresponds to <i>relcum.out</i> . Values in this file reflect the final subarea and realization.
<i>releaset.out</i>	This file contains screen output from the last execution of EBSREL. It contains only debugging information and reflects the final subarea and realization.
<i>relfrac.out</i>	This RELEASET output file, used by EBSREL, contains the time of maximum release rate for each radionuclide, the maximum normalized release rate for each radionuclide (prior to colloidal species allocation), and waste package water fill times. Values in this file reflect the final subarea and realization.
<i>trelease.out</i>	This file is generated by RELEASET and contains the quantity of a radionuclide outside the waste package as a function of the internal RELEASET timesteps. Values in this file reflect the final subarea and realization.
<i>wpfillstats.out</i>	This file contains the number of waste packages into which water flows and waste package fill time data for each subarea and realization.

Table 10-4. Optional Intermediate Output Files Created During Execution of EBSREL	
File	Description
<i>ebsrel.cum</i>	This file contains waste package corrosion failure times for each subarea and realization from RELEASET.
<i>infilper.cum</i>	Contains the same data as <i>infilper.res</i> (Table 10-3), but for every timestep. This file is described in more detail in Chapter 19.
<i>releaset.cum</i>	This file reports contents of all <i>releaset.out</i> files by subarea and by realization.
<i>ebsrel.ech</i>	This file contains a summary of the input data received by EBSREL from other modules. It includes time of waste package failure, number of breached waste packages by class, repository and waste package temperatures, relative humidity, pH, chloride concentration, maximum flow rate of water per waste package, time of drift backfill, and the drip shield corrosion failure time from each subarea by realization.
<i>ebsrel.rlt</i>	This file contains EBSREL radionuclide release rates from the engineered barrier system for all radionuclide species (dissolved and colloidal), all timesteps, all subareas, and all realizations. It also indicates whether release was solubility controlled and includes information on waste package breaches, water contact times, and radionuclide inventories.

In addition, “pinch-point” techniques, wherein output or intermediate results produced from EBSREL can be understood in combination with output or intermediate results from other modules (e.g., EBSFAIL, NFENV, and UZFT), may help to better evaluate subsystem processes. Key output files and intermediate result files useful for these comparisons (Section 10.6) include *cumrel.res*, *pkreltim.res*, and *ebsrel.rlt*. For instance, cumulative engineered barrier system radionuclide releases in *cumrel.res* can be compared to cumulative unsaturated zone radionuclide releases in the same file (Chapter 11) to evaluate the relative contributions of the two modeled subsystems to waste isolation. The full time histories, by subarea, of radionuclide release rates from the engineered barrier system and the unsaturated zone will also provide such a comparative evaluation; these data are contained in *ebsrel.rlt* (Table 10-4) and *uzft.rlt* (Table 11-4).

Further, single parameter importance analyses can be performed by repetitively varying input parameters associated with particular subsystem processes modeled by EBSREL and analyzing output and intermediate results from various consequence modules, as mentioned previously. Single parameter importance analyses could be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, a single parameter importance analysis could be performed by repetitively specifying smaller ranges within the parameter’s original distribution in the *tpa.inp* file. TPA Version 5.1 supports input parameters for their provided ranges only. The user should exercise care in interpreting results from simulations in which input parameters are altered beyond their intended ranges.

Key input parameters and data that can influence EBSREL results are discussed next in the context of suggested calculations that can be performed to understand release-relevant processes.

10.7.1 Amount of Water Contacting Waste Forms

The amount and rate of water entering a waste package are provided in *infilper.res*. For the flow of water entering the waste package, key *tpa.inp* parameters that may be varied include SubAreaWetFraction, WastePackageFlowMultiplicationFactor, and failure mode-specific parameters for the InitialSeepageReductionFraction.

To explore the effect of the flow factors in more detail, specialized simulations could be implemented considering only initially defective waste packages (i.e., DefectiveFractionOfWPs/cell = 1.0) and setting the parameter InitialSeepageReductionFractionInitiallyDefWP to various constant values (e.g., 0.001, 0.01, and 0.1). Comparative releases of elements with contrasting solubility limits (e.g., uranium and technetium) provide insight on the effect of variable flow rate on radionuclide releases from the engineered barrier system. For example, if uranium release is solubility limited, its release rate responds linearly to changes in water flow rates. On the other hand, Tc-99 release, which is unlikely to be solubility limited, is less influenced by flow rate changes and more by waste form dissolution rates (controlled, for example, by the parameter Preexponential_SFDDissolutionModel2).

To explore alternative conceptual flow models, the user may also directly input time-dependent values for the flow factors into *wpflow.def* using the methods outlined in Section 10.3.1.

10.7.2 Waste Form Dissolution

Uncertainty in the waste form dissolution rate can significantly affect uncertainty in total-system performance (Mohanty, et al., 2004). Combinations of alternative spent nuclear fuel and glass dissolution conceptual models and the choice of the failure mode-specific water contact model (flowthrough versus bathtub) may be exercised by selecting the appropriate flags in *tpa.inp* (e.g., IModel and WaterContactMode_Initial(0=BathTub,1=FlowThrough)).

The waste form water contact area plays a key role in defining the radionuclide release rate in EBSREL. The surface area effects can be investigated for spent nuclear fuel by varying parameters such as the failure mode-specific SFWettedFraction parameters (e.g. SFWettedFraction_LC) to gain an understanding of the effective specific surface area appropriate for emulating the mass release rates observed in laboratory studies. Effects of the glass dissolution model can be understood by varying the intrinsic glass dissolution rate constant, LogOfGlassDissolutionConstantHighRange[] or LogOfGlassDissolutionConstantLowRange[] (Section 10.3.2.2).

10.7.3 Radionuclide Release

Releases of some radionuclides are controlled by their solubility limits (Mohanty, et al., 2003). The degree to which solubility limits restrict release of radionuclides from the engineered barrier system could be investigated by changing the solubility limit parameters in *tpa.inp* {e.g., SolubilityNp[kg/m3]}. Results contained in the *ebsrel.rtf* and *ebsnef2.dat* files indicate whether releases were solubility limited. Solubility limits for many elements (e.g., actinides) vary with chemical parameters such as pH and dissolved carbonate content (Bechtel SAIC Company, LLC, 2005a). The performance effects of correlations between solubility limits can be considered by carefully constructing and applying correlations in *tpa.inp* (Section 3.2.1.7).

The impact of irreversible radionuclide attachment to colloids can be understood by disabling colloids by setting IrreversibleColloidModel[0=no,1=yes] to 0 in *tpa.inp*. Some colloid-relevant parameters are highly uncertain. The impacts of these uncertainties can be observed by studying sensitivity of dose from the J-species radionuclides to colloid sorption capacity {SorptionCapacity[moles/m³]} and element-specific sorption affinity factors (e.g., AffinityFactorAm). For example, an alternative conceptual model that assumes multiple layers of actinide ions may sorb to the iron oxyhydroxide colloid surface may be evaluated by using values from the high end of the range for SorptionCapacity[moles/m³]. Also, model concentrations of J-species radionuclides may be compared to experimental data on glass waste form colloids (e.g., Bechtel SAIC Company, LLC, 2005b).

The release rate for a J-species (Section 10.3.4) depends on the solubility limit for the radioelement if its release is solubility limited (which is typically the case for the actinides included in the colloid model). Because some solubility limit distributions are wide, the user may wish to directly vary solubility limits {e.g., SolubilityPu[kg/m³]} to observe the effects on colloid species dose. Such an analysis could also address the potential correlations among solubility limits discussed earlier in this section. The user should recognize that, because of the competitive sorption model, release rates for thorium, uranium, plutonium, americium, and curium are interrelated. Removal of one of these elements from an analysis could affect release for the others, in both colloidal and dissolved forms.

10.8 References

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11 UNSATURATED ZONE FLOW AND TRANSPORT (UZFT)

The Unsaturated Zone Flow and Transport module (UZFT)¹ describes the transport of dissolved radionuclides and radionuclides attached to colloids through the matrix or fractures of the rock layers of the unsaturated flow zone. UZFT receives as input (i) time-varying release rates, computed by the Engineered Barrier System Release module (EBSREL)² (Chapter 10), for all groundwater pathway radionuclides and (ii) the time history of the volumetric flow rate, computed by the Climate and Infiltration module (UZFLOW)³ (Chapter 5). The main functions of UZFT are to (i) create input files for transport calculations executed by the Network Flow and Transport in Time-Dependent Velocity Fields code (NEFMKS),⁴ adapted from the code NEFTRAN II (Olague, et al., 1991) that numerically solves the advection-dispersion equation for aqueous transport of radionuclides and their decay chains and (ii) provide time-varying radionuclide release rates from the unsaturated zone that are passed to the Saturated Zone Flow and Transport module (SZFT)⁵ (Chapter 12). UZFT is run for each potential repository subarea specified in any TPA Version 5.1 realization for the reference case.

11.1 Conceptual Model

11.1.1 Hydrostratigraphic Layers

At Yucca Mountain, the potential repository is expected to be located in the unsaturated zone, approximately 350 m [1,150 ft] above the water table in layered siliceous volcanic tuffs that have varying degrees of welding and fracturing. The three main geologic units between the potential repository and the water table are, from top to bottom, (i) the Topopah Spring welded tuff, in which the potential repository is expected to be located; (ii) the Calico Hills nonwelded tuff; and (iii) various welded and moderately welded tuffs of the Crater Flat Group, which includes the Prow Pass and Bullfrog tuffs. In the abstracted conceptual model, these three geologic units are divided into six hydrostratigraphic units, or layers (Figure 11-1). A seventh hydrostratigraphic unit, the Unsaturated Fault Zone, is a hypothetical fault that extends from beneath the potential repository to the top of the water table throughout the specified subarea. The layers in UZFT are based on the mapped stratigraphy at Yucca Mountain, but characteristics and depositional sequences of the rocks have been generalized and in some cases rearranged to give each hydrostratigraphic unit a uniform (homogeneous) set of rock properties. Groundwater travel times through the unsaturated zone depend on the percolation

¹The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

²The Engineered Barrier System Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

³The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

⁴The Network Flow and Transport in Time-Dependent Velocity Fields code is referenced frequently throughout this chapter. The abbreviation NEFMKS will be used.

⁵The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

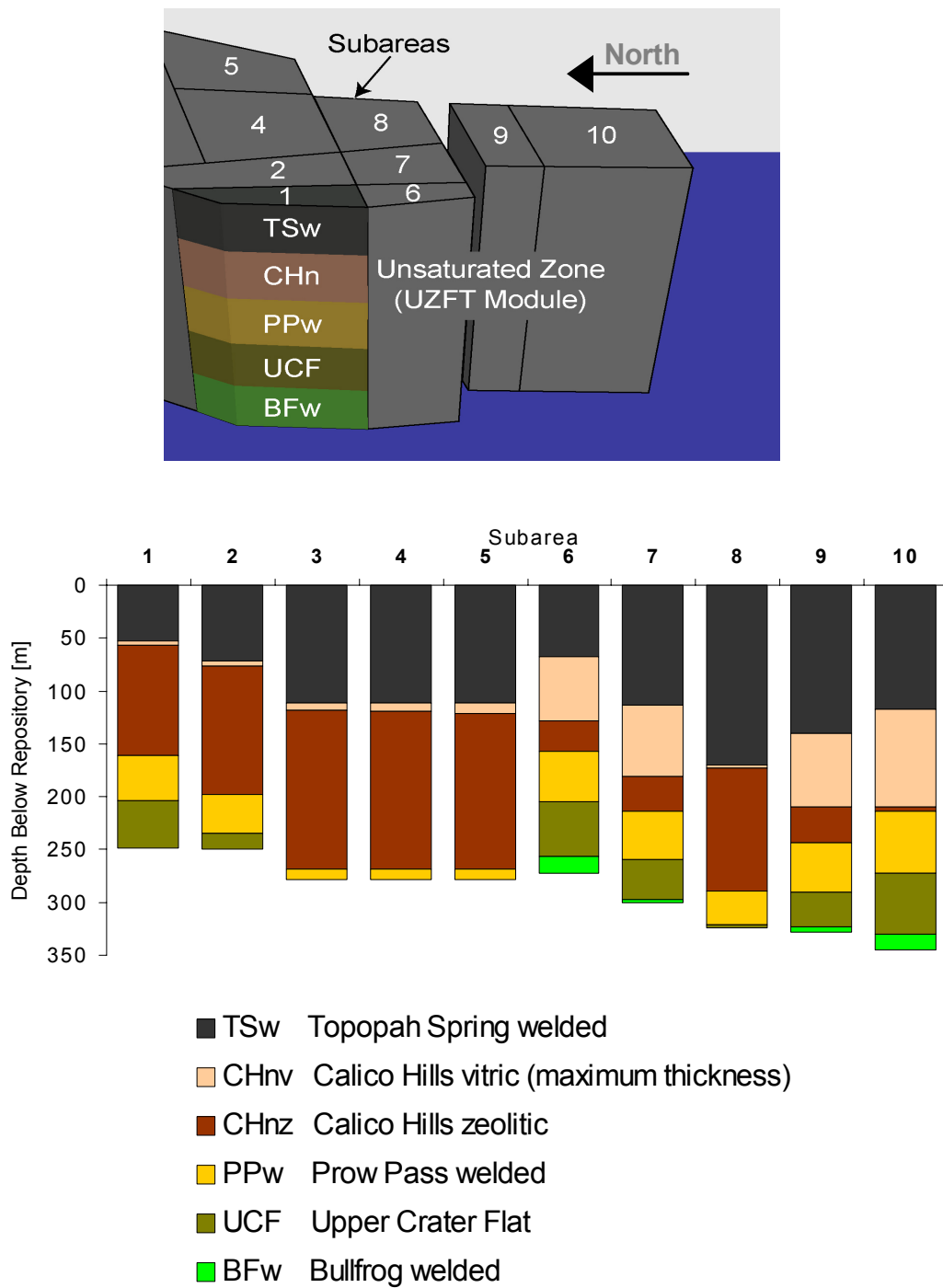


Figure 11-1. Subarea Outlines and Hydrostratigraphic Layer Thicknesses

rate and on the hydrologic properties and thickness of the hydrostratigraphic layers. The layer thicknesses differ from subarea to subarea to conform with regional variations in stratigraphy. In the model, radionuclides are transported through the unsaturated zone until they reach the water table, which marks the boundary between the unsaturated zone and the variably fractured, welded tuffs of the saturated zone.

The Calico Hills Formation is divided into two hydrostratigraphic layers to represent a transition in its flow and transport properties across the potential repository footprint. Much of the Calico Hills Formation is composed of porous, nonwelded vitric tuffs in which matrix flow conditions dominate. This may lead to slower groundwater travel times and more sorption than in units characterized by fracture flow conditions. In the model, the various interbedded nonwelded porous tuffs are represented hydrostratigraphically by the Calico Hills nonwelded vitric layer. The remaining Calico Hills tuffs are represented hydrostratigraphically by the Calico Hills nonwelded zeolitic layer, which correlates with an alteration zone in the northern part of the study area where permeability of the tuff is reduced due to secondary zeolite mineralization. The Calico Hills nonwelded zeolitic layer is characterized by fracture flow instead of matrix flow.

11.1.2 Groundwater Flow and Radionuclide Transport

In the UZFT conceptual model, water travels downward in each hydrostratigraphic layer either by fracture flow or matrix flow and there is no horizontal component of transport as a result of the dipping rock layers or permeability contrasts between rock units. The differentiation between fracture flow and matrix flow in UZFT depends on the conductivity of the rock matrix and the maximum rate at which water is supplied to the unsaturated zone.

In the conceptual model, radionuclides released from a potential repository at Yucca Mountain are transported through the unsaturated zone either as dissolved species or in association with colloids {small solid particles characteristically ranging in size from 10^{-9} to 10^{-6} m [1 m = 3.28 ft]}. The colloids considered in the UZFT conceptual model originate either in the natural environment (e.g., colloid-sized clay particles) or by degradation of the wasteform or engineered barriers (e.g., colloidal iron oxyhydroxide corrosion products). Radionuclide transport processes considered in UZFT include (i) advective transport with longitudinal dispersion, (ii) reversible sorption of dissolved radionuclides to host rock, (iii) migration of radionuclides attached to colloids, and (iv) radionuclide decay and ingrowth of progeny nuclides. The specific radionuclides considered in the transport abstraction are isotopes of 15 elements from the wasteform inventory that are expected to be present in sufficient amounts and be sufficiently mobile in groundwater to be of interest in postclosure performance assessment calculations (Chapter 4, Section 4.6).

Sorption of radionuclides to host rock minerals can delay the migration of some aqueous-phase species. Some elements such as iodine, chlorine, and technetium have little affinity for sorption to silicic rocks and are assumed to migrate freely as dissolved species in groundwater, with little or no retardation. Sorption is more important as a retarding mechanism for the other radionuclides, particularly in the rock matrix, which provides a large total surface area for sorption compared to that of fracture walls. Some of these other elements, including actinides (e.g., americium, neptunium, plutonium, thorium, uranium, and curium), have varying affinities for sorption, depending on geochemical conditions. Because of the relative importance of the actinides to performance and the influence of groundwater chemistry (particularly pH and

dissolved carbon dioxide concentration) on their sorption behavior, the sorption characteristics of actinides are represented in more detail in the transport model than those of the non-actinides.

The sorption capacity of the rock matrix is determined largely by its effective surface area and by the particular solid phases the rock contains. For example, many of the Yucca Mountain tuffs have abundant volcanic glass shards and pumice fragments that can provide a moderately attractive substrate for sorption (McMurry and Bertetti, 2005). Individual clay and zeolite minerals, such as in the devitrified and hydrothermally altered tuffs, typically have greater sorption capacity than the glass particles in the vitric tuffs. Sorption in the zeolitized tuffs is diminished because the permeability contrast between zeolitized matrix and fractures tends to result in fracture flow instead of matrix flow.

Radionuclides are associated with colloids either by attachment to a colloid surface (reversible or irreversible sorption) or as an intrinsic part of the colloid itself. Examples of intrinsic association include (i) colloid-sized pieces of vitrified waste or spent fuel spalled from a wasteform or (ii) a secondary precipitate of an oversaturated radionuclide-bearing phase such as thorium oxide (ThO_2). In the model, radionuclides that are strongly sorbed to a colloid (i.e., corrosion product colloids) and those that are an intrinsic part of a wasteform colloid are considered to be irreversibly bound to the colloid. Only four elements—curium, thorium, americium, and plutonium—are assumed to bind irreversibly to colloids, and all such colloids are assumed to originate in the waste package.

In contrast to irreversible attachment, reversible sorption onto colloids is conceptually equivalent to reversible sorption onto other solid phases (e.g., glass shards, clays, zeolites). Similarly, colloids themselves may be retarded by sorption to solid surfaces, depending on the composition, size, and surface charge of the colloid. Because of size restrictions in the matrix, the expected transport pathway for colloids is fracture flow. If a colloid is too large to fit through a narrow pore opening in the matrix, it may become permanently immobilized. In the conceptual model, the immobilization of colloids by filtration ultimately has little effect on migration for radionuclides that are reversibly sorbed to colloids, for the radionuclide eventually desorbs and continues to travel through the system. However, if a radionuclide is irreversibly attached to a colloid, removal of the colloid by filtration will also permanently immobilize the attached radionuclide at that location.

11.2 Model Support and Assumptions

The UZFT abstraction represents flow on a scale of tens or hundreds of meters, conforming to the overall scale of the potential repository system and corresponding to other modeling approaches for flow and transport in fractured, unsaturated rocks (National Research Council, 2001). Large-scale spatial heterogeneities are included in the model to the extent that each hydrostratigraphic unit has individual hydrogeological properties and the thickness of each unit differs according to subarea. Temporal variation is included by adapting and simplifying the time-varying deep percolation rates determined by UZFLOW. This approach assumes that (i) flow through the unsaturated zone is one dimensional and vertical; (ii) the unsaturated zone flow field is in equilibrium (i.e., time variations in the flow field occur rapidly in the unsaturated zone); and (iii) thermal perturbations do not affect unsaturated zone flow below the potential repository (i.e., at early times, when this assumption would be most in question, the waste containers are considered to be largely intact). If UZFT has attributed fracture flow properties to

a hydrostratigraphic layer, it is assumed that all water movement at all times in that layer is by fracture flow, regardless of any variations in flow rates.

The properties of the UZFT hydrostratigraphic layers are based on the documented geology and hydrogeology of the Yucca Mountain area (e.g., CRWMS M&O, 2001, 2000a, 1999). For each subarea, the UZFT conceptual model assumes that flow cannot switch back and forth over time between the fractures and the matrix of a particular hydrostratigraphic layer, nor can flow occur in both media simultaneously in that layer. This simplifying assumption is considered a reasonable representation for the bulk behavior of the flow system because the saturated hydraulic conductivity of the matrix in each hydrostratigraphic unit tends to be either much greater than the net flux, so that matrix flow will occur, or much less than the expected net flux, in which case fracture flow is likely. This assumption is supported by studies indicating that preferential flow along connected fractures or fault planes is an important large-scale feature of unsaturated rocks that have low matrix permeability (Davidson, et al., 1998; Nativ, et al., 1995; Yang, et al., 1996).

Sorption is represented in the model by a bulk linear (equilibrium) sorption isotherm, based on the assumption that the sorption process is rapid compared to the flow velocity. This K_D approach is a well documented and generally accepted modeling approach to approximate the effects of sorption on delaying radionuclide transport in groundwater (Chapman and McKinley, 1987).

Equations that are used to calculate retardation factors in saturated media typically are adjusted for unsaturated media to account for the differences in surface area available for sorption (i.e., wetted) in unsaturated conditions. However, the calculated retardation factors in UZFT are based on saturated properties, without adjustment for partially saturated (unsaturated) conditions, to facilitate transport calculations in NEFMKS. This assumption is most valid when the percolation rate and the saturated hydraulic conductivity of the media have similar values.

The following are other key assumptions in the TPA Version 5.1 abstraction of unsaturated zone flow and transport.

- Given uncertainties about the extent and effectiveness of matrix diffusion or other fracture–matrix interactions related to fracture flow in the unsaturated zone, the UZFT model abstraction assumes that there is no retardation of radionuclides by matrix diffusion during fracture flow.
- For reversible sorption of radionuclides to colloids and to stationary media (e.g., rock matrix), the time scale for attachment and detachment is small compared to the transport time (i.e., attachment kinetics are neglected).
- The reversible sorption of radionuclides involves equilibrium partitioning among three phases: aqueous (dissolved), colloid bound, and sorbed to the host rock.
- The elevation of the water table, which marks the contact between the unsaturated zone and the saturated zone, does not change over time.
- If no unsaturated zone hydrostratigraphic layer is capable of transmitting the maximum percolation rate as matrix flow, it is assumed that the fraction of flow that cannot be

accommodated by the most permeable matrix layer travels rapidly to the saturated zone in fractures; this fraction is referred to as the bypass fraction (Section 11.3.2.2).

- It is assumed that colloid filtration is not cumulative with each layer. Hence, filtration is applied only one time based on the unsaturated zone layer with the greatest filtration capacity. If a bypass fraction is present, the colloid filtration is applied to that portion of flow based on the filtration capacity of the Calico Hills nonwelded vitric layer. This layer is thin or absent in some unsaturated zone subareas (Figure 11-1), but the colloid filtration assumption for bypass flow is based on the observation that the Calico Hills nonwelded vitric layer also is present, due to faulting, in the saturated zone south of the potential repository location. Although its layer properties are not explicitly represented in the SZFT flow model (Chapter 12), transport through this unit is expected to occur along all anticipated saturated zone flow paths.

11.3 Implementation of Conceptual Model in TPA Version 5.1

In every realization of TPA Version 5.1, UZFT is called once for each subarea. The general flow of information in UZFT is illustrated in Figure 11-2. One of the main functions of UZFT is to provide information that NEFMKS needs to simulate flow and radionuclide transport in the unsaturated zone. To achieve this result, UZFT provides the following information to NEFMKS: (i) a time history of radionuclide mass entering the unsaturated zone, (ii) radionuclide and decay chain information, (iii) flow path characteristics and time-dependent flow velocity information, and (iv) radionuclide transport parameters for each radionuclide species.

11.3.1 Radionuclide Source Input

EBSREL calculates time-varying radionuclide source input for each subarea and passes it on to UZFT. UZFT formats this data and writes it to *sotnef.dat*, which NEFMKS uses as an input file. UZFT copies *sotnef.dat* to *nefiuz.src*, which is not used but has a file name that is more intuitive relative to the information contained within it. The *sotnef.dat* and *nefiuz.src* files are overwritten each time UZFT is called; in addition, *softnef.dat* subsequently is overwritten each time SZFT is called (Chapter 12). At the end of a TPA Version 5.1 run, *nefiuz.src* will reflect the source term provided to UZFT for the last subarea of the last realization.

Additional information pertaining to radionuclides, their half-lives, and decay chains is specified in *tpa.inp* and in *nuclides.dat*. See Chapter 4 for a description of radionuclide inventory specifications. UZFT formats and passes these data to the NEFMKS input file *nefiuz.inp* for transport calculations.

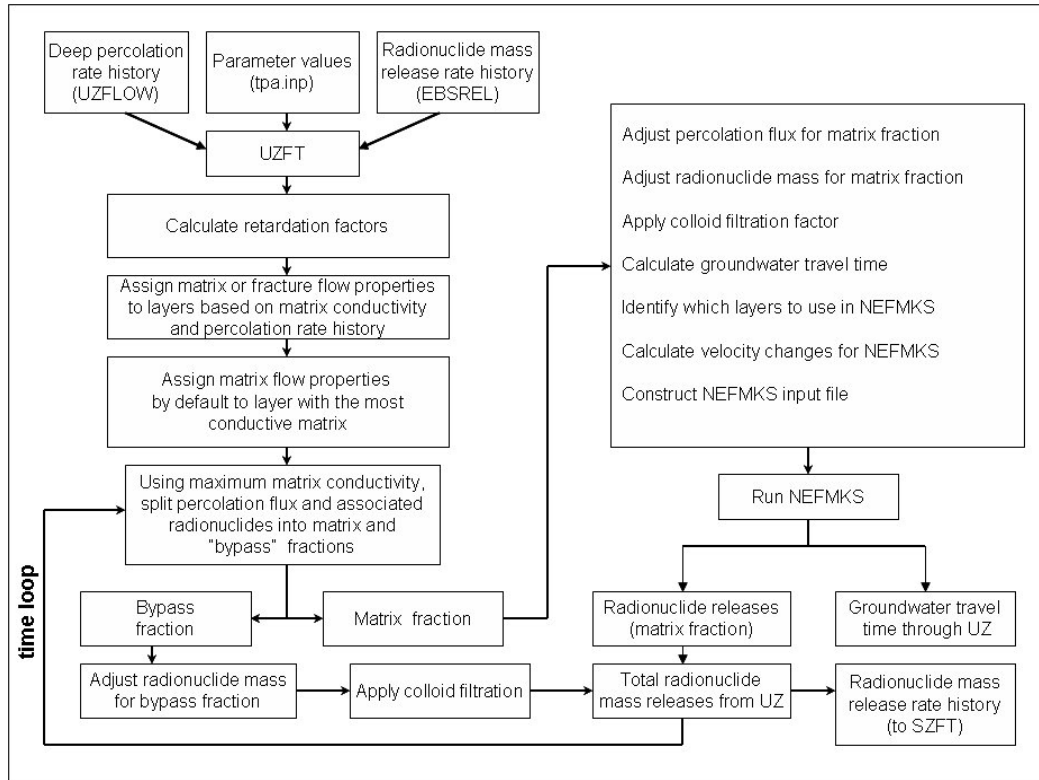


Figure 11-2. Information Flow Diagram for UZFT

11.3.2 Flow Model for NEFMKS

Water velocity in the fracture continuum tends to be large relative to velocity in the matrix because of differences in the structure of the porosity (i.e., the size of pores and their interconnectedness) between the two media types. In hydrostratigraphic layers where groundwater velocities are high and travel times are short, the computational effectiveness of NEFMKS is restricted by the need to use extremely small timesteps to simulate short travel times. This issue is addressed in TPA Version 5.1 by completely bypassing unsaturated zone transport calculations for layers where the average groundwater travel time is less than 20 years while ensuring that the model examines the effect of matrix properties on transport in at least one layer. The following discussion describes the process that UZFT implements to construct simplified flow model input files for the NEFMKS flow and transport calculations.

11.3.2.1 Hydrostratigraphic Layers and Layer Thicknesses

Hydrostratigraphic layer thicknesses are provided by the values for the parameters *UNIT_Thickness_#SubArea[m]*⁶ in *tpa.inp*, as indicated in Table 11-1 of Section 11.4. The transition between the Calico Hills vitric tuffs and the Calico Hills zeolitic tuffs and the thickness of the vitric unit are uncertain in many locations at Yucca Mountain. To account for this

⁶Where the term "UNIT" appears in a formal UZFT parameter name, it refers to the particular hydrostratigraphic unit specified by the abbreviation (see Figure 11-1 for abbreviation names). Where the symbol "#" is used in a formal *tpa.inp* parameter name in this chapter, it refers to the number for a particular subarea.

uncertainty in the model abstraction, a combined (vitric plus zeolitic) thickness for the Calico Hills nonwelded tuffs is specified in *tpa.inp* as CH_Total_Thickness_#SubArea[m] for each subarea. The thickness of the vitric layer itself, though bounded by this value, is then sampled from a range of values in *tpa.inp* as CHnvThickness_#SubArea[m]. UZFT then calculates the thickness of the Calico Hills nonwelded zeolitic layer by subtracting the sampled vitric layer thickness from the total thickness.

Due to the gently dipping structural orientation of the layered tuffs at Yucca Mountain, parts of the lower hydrostratigraphic units are below the water table (i.e., in the saturated zone) in some locations and above it (unsaturated) in others. Hydrostratigraphic units that are below the water table in a particular subarea are assigned a reference case value of zero for UNIT_Thickness_#SubArea[m], and UZFT uses only the layers with nonzero thicknesses in its calculations to construct the input file for NEFMKS.

11.3.2.2 Flow Properties and Flux Splitting

The model abstraction for UZFT assumes that in each hydrostratigraphic layer, water moves vertically downward either by fracture flow or by matrix flow. To determine which set of parameter values (matrix flow conditions or fracture flow conditions) will be assigned for the NEFMKS transport calculations for a particular layer, UZFT calculates the saturated hydraulic matrix conductivity of each layer according to the relationship

$$K_{sat} = \kappa \gamma / \mu \quad (11-1)$$

where

K_{sat}	—	saturated hydraulic conductivity of the matrix [m/yr]
κ	—	permeability of the matrix, as specified by the <i>tpa.inp</i> parameter MatrixPermeability_UNIT [m ²]
γ	—	specific weight of water [N/m ³]
μ	—	dynamic viscosity of water [N s/m ²]

In UZFT, values for γ and μ are assumed to be constant and apply to all layers. Thus, the matrix permeability in each case is multiplied by a factor of 3.087×10^{14} [m⁻¹ yr⁻¹] to obtain the matrix K_{sat} and convert units (s to yr) appropriately.

UZFT then divides the time-varying deep percolation volumetric flow rate, obtained from UZFLOW, by the area of the subarea, as specified by the *tpa.inp* parameter InletArea_#SubArea[m²], to obtain the time-varying percolation rate in meters per year and compares it with the calculated matrix K_{sat} of each layer. If the percolation rate is less than or equal to the matrix K_{sat} at all times, matrix flow properties are assigned to that layer. However, if UZFT determines that the percolation rate will exceed the matrix K_{sat} at any time, then fracture flow properties are assigned to that layer. The only exception to this classification is if all layers in a subarea have fracture flow properties. In this case, UZFT finds the layer with the largest matrix K_{sat} and assigns matrix flow properties to it. This step ensures that at least one layer in each subarea has matrix flow properties assigned to it. However, there will be times in the percolation rate history when the percolation rate exceeds the ability of the matrix in this layer to

transmit the flow. Should this occur, UZFT splits the percolation flux (and the radionuclides associated with it) into a matrix fraction, which passes through the matrix of the layer with the maximum K_{sat} , and a bypass fraction, which is immediately diverted to the bottom of the unsaturated zone.

UZFT performs the flux splitting by selecting the hydrostratigraphic layer with the largest calculated value of matrix K_{sat} and calculating the ratio of K_{sat} to percolation rate for this layer at each timestep in the percolation rate history. If the ratio is greater than or equal to one, it is assumed that the percolation will be accommodated by matrix flow, and the matrix fraction is set equal to one. If the ratio is less than one, the resulting fraction is the matrix fraction, which represents the proportion of the flux that will be transmitted by the matrix of this layer. Only the fraction of water and radionuclides that pass through the matrix of this layer are made available to any other layers in the model, because the bypass fraction, if any, is diverted past all the layers. Thus, for each timestep in the percolation rate history, UZFT multiplies the percolation rate by the matrix fraction and stores the result in an adjusted percolation array that is used for all subsequent flow and transport calculations. An adjusted array representing only the matrix fraction of radionuclide releases is prepared by the same approach. If the percolation rate never exceeds the matrix K_{sat} , then the matrix fraction equals one at every timestep, and the “adjusted” arrays have the same values as the original arrays. In cases where a bypass fraction is present, the radionuclide masses associated with the overflow are presumed to travel rapidly and without retardation (presumably through an undesignated set of fractures or a fault zone) to the bottom of the unsaturated zone. They are not included in the NEFMKS flow and transport calculations, but they are added back to the total radionuclide releases that are passed to SZFT (Figure 11-2).

To account for J-species radionuclides lost by permanent filtration of colloids in the unsaturated zone, UZFT also reduces the radionuclide mass in the matrix fraction adjusted array by a fractional amount associated with the hydrostratigraphic layer present in that subarea that has the largest colloid filtration factor, as specified by the *tpa.inp* parameter PermanentLossColloidFilterFactor_UNIT[]. If a bypass fraction is assigned by the flux splitting algorithm, the colloid filtration is applied to that portion of flow based on the value of PermanentLossColloidFilterFactor_CHnv[]. UZFT applies this reduction once per timestep, before NEFMKS flow and transport calculations commence. After the J-species are removed from transport by permanent filtration, it is assumed that they cannot be a secondary source for decay chain progeny.

11.3.2.3 Flow Velocity and Groundwater Travel Times

Next, UZFT determines the average groundwater travel time for each hydrostratigraphic layer. As a first step, a time-varying flow velocity is calculated for each layer using

$$v(t) = \frac{q(t)}{\phi S_w(t)} \quad (11-2)$$

where

- $v(t)$ — time-varying velocity for the hydrostratigraphic layer [m/yr] at time t
- $q(t)$ — time-varying adjusted percolation rate [m/yr] at time t

- ϕ — porosity of the hydrostratigraphic layer, corresponding to the matrix or fracture flow properties assigned to this layer as specified by the *tpa.inp* parameter MatrixPorosity_UNIT or FracturePorosity_UNIT [unitless]
- $S_w(t)$ — time-varying saturation of the hydrostratigraphic unit, corresponding to either the matrix saturation or the fracture saturation [unitless] at time t

The percolation rate is from the time-varying percolation rate history (as adjusted by the previous set of flux-splitting calculations). The saturation, S_w , varies with percolation rate and must be determined by UZFT at each timestep to complete the velocity calculation [Eq. (11-2)]. To estimate the saturation, UZFT uses the relation between relative hydraulic conductivity, water saturation, and layer-specific van Genuchten parameters according to the van Genuchten relation

$$K_{rel} = \sqrt{S_w} \left[1 - \left(1 - S_w^{1/\lambda} \right)^\lambda \right]^2 \quad (11-3)$$

where

- K_{rel} — relative hydraulic conductivity [unitless]
- S_w — water saturation [unitless]
- λ — $1-1/\beta$
- β — van Genuchten beta-fitting parameter, as specified by the *tpa.inp* parameter MatrixBeta_UNIT [unitless] or FractureBeta_UNIT [unitless]

To determine the water saturation at each timestep, UZFT first performs a set of many trial solutions of Eq. (11-3) by using the value of λ derived from the relevant matrix or fracture van Genuchten beta-fitting parameter for the hydrostratigraphic unit and varying the value of S_w in increments of 0.01 between zero and one. Figure 11-3 illustrates how a water saturation value is estimated from the percolation rate at one timestep for a particular hydrostratigraphic layer. The filled circles on the graph in Figure 11-3 are the example trial solutions that illustrate how the calculated relative hydraulic conductivity, K_{rel} , varies over nearly unsaturated ($S_w = 0.0000001$) to fully saturated ($S_w = 1.0$) conditions.

Next, for each calculated value of K_{rel} , UZFT calculates the effective hydraulic conductivity, K , by the relation

$$K = K_{rel} K_{sat} \quad (11-4)$$

where

- K — effective hydraulic conductivity [m/yr]
- K_{rel} — relative hydraulic conductivity [unitless]
- K_{sat} — saturated hydraulic conductivity [m/yr]

A single value of K_{sat} is calculated from Eq. (11-1) using the matrix or fracture permeability specified by the *tpa.inp* parameter MatrixPermeability_UNIT[m²] or

FracturePermeability_UNIT[m²] as applicable, and values of K then are calculated (open circles in Figure 11-3) using Eq. (11-4) for each of the trial values of K_{rel} generated as shown in Figure 11-3.

Assuming that the effective hydraulic conductivity, K , at a particular timestep is equivalent to the percolation rate at the same timestep, UZFT compares the percolation rate with each of the trial solutions of Eq. (11-4) to identify the value of K that is the most similar to the percolation rate. In the example shown in Figure 11-3, the percolation rate at this timestep is 1×10^{-6} m/yr. The resulting S_w for this layer at this timestep is 0.25, as estimated from the corresponding K and K_{rel} .

The trial conductivity calculations are repeated to obtain the saturation for all layers in each timestep, and the results are used to calculate the time-varying water velocity in each layer for that timestep [Eq. (11-2)]. From the time-varying velocities, the time-varying groundwater travel times are determined for each hydrostratigraphic layer using

$$t_{gw}(t) = \frac{X}{v(t)} \quad (11-5)$$

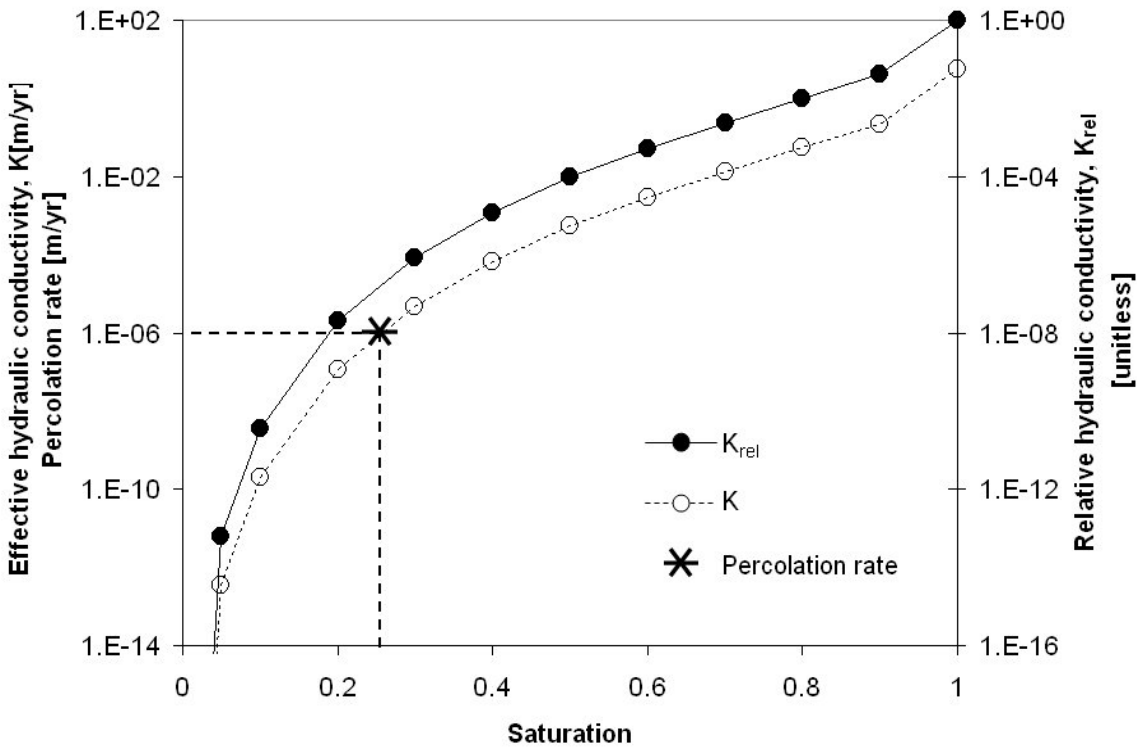


Figure 11-3. Relation Between Effective Hydraulic Conductivity, Percolation Rate, and Saturation

where

$t_{gw}(t)$	—	time-varying groundwater travel time [yr] at time t
x	—	layer thickness, as specified by the <i>tpa.inp</i> parameter <i>UNIT_Thickness_#Subarea</i> [m]
$v(t)$	—	time-varying velocity for the hydrostratigraphic unit [m/yr] at time t

The average groundwater travel time for each hydrostratigraphic layer is determined as a weighted average of the time-varying groundwater travel times over the timeframe of interest. A simple trapezoidal integration of the groundwater travel time is used for the calculation. In addition, the average groundwater travel time is summed for all hydrostratigraphic layers in the subarea to obtain the total groundwater travel time for the unsaturated zone in that subarea.

11.3.2.4 Simplified Flow Model

UZFT uses the average groundwater travel time in each hydrostratigraphic layer to select which layers satisfy a set of selection criteria that maintain the computational efficiency of NEFMKS. That is, layers with an average groundwater travel time less than 20 years or with a travel time less than 10 percent of the total travel time for that subarea are not included as layers (“legs”) in the NEFMKS input file. The use of the 20-year threshold for travel time avoids having a large number of iterations with smaller timesteps that potentially cause instability problems in NEFMKS. Considering total simulation timeframes of many thousands or hundreds of thousands of years, the 20-year minimum threshold for the travel time in each unsaturated zone layer is considered reasonable.

As noted, UZFT assigns matrix flow properties to the hydrostratigraphic layer with the largest matrix K_{sat} so that NEFMKS will always include calculations for at least one layer with transport in the rock matrix. However, there are some cases (e.g., high percolation rates applied to a thin, highly conductive layer) where this layer would otherwise be excluded because it did not meet the imposed minimum travel time selection criteria. In such a case, UZFT increases the thickness of the layer fractionally to obtain an average groundwater travel time equal to or slightly greater than 20 years through the layer. The small increase in thickness is not expected to have an impact on overall performance.

To reduce the computational time in NEFMKS simulations, NEFMKS is invoked either once in each subarea, using one set of constant advective velocities, or a limited number of times based on relative changes in velocity over consecutive timesteps. The choice for implementing constant or time-varying velocities for each leg is determined by the value of a flag, *UZVelocity* (0=average, 1=time-dependent), as specified in *tpa.inp*, where 0 = constant velocities and 1 = time-varying velocities. The constant NEFMKS velocities for each leg are based on the averaged groundwater travel time for the corresponding hydrostratigraphic layer divided by the length (i.e., layer thickness) of that leg. For the time-varying velocities, the user specifies a minimum fractional change in velocity by adjusting the value of the parameter specified as *UnsaturatedZoneMinimumVelocityChangeFactor[Fraction]* in *tpa.inp*. UZFT compares velocities calculated by Eq. (11-2) at each timestep with the last saved velocity in the NEFMKS input file. UZFT only changes the NEFMKS velocity at a particular timestep if the relative difference in velocity is greater than the user-specified fractional amount. The time-varying velocities selected by this process are written to *nefi.vel* for input to NEFMKS for each of the NEFMKS transport

layers (legs). The total groundwater travel time for each subarea is written to *gwttuzsz.res* as an intermediate result for the unsaturated zone.

11.3.3 Radionuclide Transport

In TPA Version 5.1, radionuclides are transported through the unsaturated zone as dissolved species (which includes reversible attachment to naturally occurring colloids) or as irreversibly bound colloidal species. Different retardation factors are applied in UZFT to describe either condition. For most radionuclides, including all aqueous phase (dissolved) radionuclides, transport occurs by advection and longitudinal dispersion, and is modified by sorption onto stationary minerals and onto mobile, naturally occurring colloidal particles. Accordingly, the transport model includes retardation factors for colloids that address the potential effects of radionuclides sorbing to colloids and of colloids sorbing to stationary surfaces.

In addition, the radionuclide source term assumes that a fraction of the mass of certain radioelements is irreversibly bound to colloidal particles that originated in the engineered barrier system (Chapter 10). The irreversibly bound radionuclides are modeled as unique species (J-species) and are transported through the unsaturated zone using properties of the colloidal particles, rather than the transport properties of the elements themselves. The J-species radionuclides are subject to retardation by reversible sorption of their host colloids and by permanent filtration in the rock matrix.

11.3.3.1 Radionuclide Retardation Factors

Sorption values for all radionuclides in UZFT are provided in the form of distribution coefficients (K_D) or their corresponding retardation factors (R_D). Depending on the radionuclide species and whether the flow within a unit is in matrix or in fractures, UZFT assigns a retardation factor that is (i) supplied as a sampled parameter value from *tpa.inp*, (ii) calculated from an input K_D , or (iii) calculated from input water chemistry parameters. After R_D has been calculated, UZFT modifies it to account for reversible sorption associated with mobile, naturally occurring groundwater colloids.

In the porous matrix of a rock, the retardation factor can be calculated from the K_D and from the porosity and density of the matrix by the expression

$$R_D = 1 + \frac{\rho_g(1 - \phi)K_D}{\phi} \quad (11-6)$$

where

R_D	—	retardation factor for a specified radionuclide for transport in matrix in the absence of groundwater colloids [unitless]
ρ_g	—	grain density of the solid phase (mass of solid phase relative to its volume) as specified by the <i>tpa.inp</i> parameter MatrixGrainDensity_UNIT[kg/m ³]
ϕ	—	porosity of the solid phase, as specified by the <i>tpa.inp</i> parameter MatrixPorosity_UNIT [unitless]

K_D — distribution coefficient for radionuclide sorption onto the porous rock matrix, calculated for americium, neptunium, plutonium, thorium, uranium, and curium from the response surface curves in *coefkdeq.dat* and sampled for all other radionuclides from *tpa.inp* as specified by the parameter $\text{MatrixKD\_UNIT\_RN}[\text{m}^3/\text{kg}]^7$

For the modeled actinide species, K_D values are calculated separately for each realization, using a response surface approach to correlate the K_D with sampled values for water chemistry (pH and the partial pressure of dissolved carbon dioxide, PCO_2 , which is a measure of the groundwater carbonate concentration). The sorption response surfaces were developed by applying surface complexation models to experimental data for a wide range of geochemical conditions to generate a set of effective surface area normalized distribution coefficients (K_A) (Turner, et al., 2002). The K_A values are converted to K_D values using the effective surface area properties of the individual hydrostratigraphic units (McMurry and Bertetti, 2005). Parameters describing the response surfaces that are used to obtain K_A values for the actinides are provided in *coefkdeq.dat*. This auxiliary input data file contains coefficients that define sets of curves representing the best fifth order polynomial fits to the surface complexation model predictions of sorption at specific PCO_2 values according to the expression

$$\text{Log } K_A = a + b \text{ pH} + c \text{ pH}^2 + d \text{ pH}^3 + e \text{ pH}^4 + f \text{ pH}^5 \quad (11-7)$$

where a – f represent the coefficients. Distributions of pH and PCO_2 , as specified by the *tpa.inp* parameters $\text{pH\_AllUZ\_SZLayers}[\text{StandardUnits}]$ and $\text{LogCO2PartialPressure\_AllUZ\_SZLayers}[\text{atm}]$, were developed from site-specific hydrochemical data (McMurry and Bertetti, 2005).

For sorption in the rock matrix, K_D is calculated from K_A by

$$K_D = K_A \text{ ESA} \quad (11-8)$$

where

K_D — distribution coefficient for sorption of the dissolved radionuclide onto the porous rock matrix [m^3/kg]
 K_A — surface area normalized distribution coefficient [m^3/m^2]
 ESA — effective surface area of the porous matrix [m^2/kg]

The effective surface area is the ratio of the total available area of mineral grains for radionuclide sorption to the mass of mineral grains. When the pore space is assumed to be spherical, this ratio can be determined from the equation (Arthur, 1996)

$$\text{ESA} = \frac{3\phi}{\rho_g(1-\phi)r} \quad (11-9)$$

⁷Where the term “RN” appears in a formal *tpa.inp* parameter name in this chapter, it refers to a specified radioelement (i.e., radionuclide).

where

ESA	—	effective surface area of the porous matrix [m^2/kg]
ρ_g	—	grain density of the solid phase (mass of solid phase relative to its volume), as specified by the <i>tpa.inp</i> parameter MatrixGrainDensity_UNIT [kg/m^3]
ϕ	—	porosity, as specified by the <i>tpa.inp</i> parameter MatrixPorosity_UNIT [unitless]
r	—	mean pore radius, as specified by the <i>tpa.inp</i> parameter MatrixPoreRadius_UNIT [m]

UZFT then converts the calculated K_D value to an R_D value using Eq. (11-6).

For sorption in fractures, the retardation factor, R_D , for all radionuclides except the actinides is sampled directly from *tpa.inp* as FractureRD_UNIT_RN. For the actinides, the retardation factor is calculated using the K_A value obtained from Eq. (11-7) and is based on an assumed constant-aperture fracture

$$R_D = 1 + \left(\frac{2K_A}{b} \right) f \quad (11-10)$$

where

R_D	—	retardation factor for a specified radionuclide in the absence of groundwater colloids [unitless]
K_A	—	surface area normalized distribution coefficient [m^3/m^2]
b	—	fracture aperture, as specified by the <i>tpa.inp</i> parameter FractureAperture_UNIT [m]
f	—	fracture force factor, as specified by the <i>tpa.inp</i> parameter UZFractureForceFactorForKdToRd [unitless]

The fracture force factor, f , is a special UZFT parameter that controls whether or not sorption in fractures is included for actinides. If the fracture force factor is zero (the reference case value), Eq. (11-10) returns a value of 1 (i.e., no retardation) for R_D .

Although the capability to model sorption in fractures is included in UZFT, implementation of this option in TPA Version 5.1 may produce little or no sorption due to the flux-splitting procedure in TPA Version 5.1 that UZFT follows to construct a simplified flow model for NEFMKS transport calculations. When modeling sorption in fractures, the user should carefully examine the results of each realization to ensure that the conditions were modeled as expected. In particular, if the percolation rate is greater than the matrix conductivity of the layer with the largest matrix saturated hydraulic conductivity, UZFT diverts the excess percolation flux to a bypass fraction that is not included in the NEFMKS transport calculations. No sorption at all—in fractures or in matrix—is modeled for any radionuclides in the bypass fraction.

11.3.3.2 Colloid-Associated Transport

The final step in calculating retardation factors in UZFT is to modify the previously calculated R_D values for each radionuclide to account for sorption onto mobile colloids. Naturally occurring colloids are assumed to be present in water in the fractures and matrix of all hydrostratigraphic units. The colloid concentration, C_c , in the matrix and fractures for each unit is sampled from distributions in *tpa.inp* as specified by the parameters for MatrixColloidConcentration_UNIT and FractureColloidConcentration_UNIT.

The net effect of reversible sorption to colloids is to adjust the retardation factor for radionuclide transport. The resulting retardation factor, R_D^{eff} , is calculated as

$$R_D^{eff} = \frac{R_D + (K_0 R_c)}{(1 + K_0)} = R_D \frac{1 + K_0(R_c/R_D)}{(1 + K_0)} \quad (11-11)$$

where

- R_D^{eff} — retardation factor for the transport of a particular radionuclide in the presence of colloids [unitless]
- K_0 — dimensionless distribution coefficient for sorption onto colloids [unitless]
- R_c — retardation factor specifically associated with colloid transport, as specified by the *tpa.inp* parameter MatrixColloidRetardationFactor_UNIT [unitless] or FractureColloidRetardationFactor_UNIT [unitless]
- R_D — retardation factor in the absence of colloids, calculated from Eq. (11-6) for matrix sorption, calculated from Eq. (11-10) for fracture sorption of actinides, and sampled from *tpa.inp* for fracture sorption of all other radionuclides as the parameter FractureRD_UNIT_RN [unitless]

Equation (11-11) indicates that if the radionuclides and the colloids both undergo the same retardation, colloids will have no additional effect on transport, and so $R_D^{eff} = R_D$. If the radionuclides sorb to the rock matrix or fracture walls more strongly than the colloids themselves do, R_c is less than R_D , so $R_D^{eff} < R_D$, and the effect of colloids in the system is to enhance transport compared to the retardation that would be observed if colloids were not present.

The dimensionless distribution coefficient for colloid sorption, K_0 , can be written as

$$K_0 = C_c ESA_c K_A \quad (11-12)$$

where

- K_0 — dimensionless distribution coefficient for colloid sorption [unitless]
- C_c — colloid concentration, as specified by the *tpa.inp* parameter MatrixColloidConcentration_UNIT[kg/m³] or FractureColloidConcentration_UNIT[kg/m³]

- ESA_C — effective surface area for sorption of colloids [m^2/kg]
 K_A — surface area normalized distribution coefficient [m^3/m^2]

The effective surface area for sorption of colloids, ESA_C , is defined as the ratio of the total area available for sorption to the colloid mass. For transport through the rock matrix, this value is assumed to be proportional to the effective surface area of the rock matrix, ESA , such that $ESA_C = F \times ESA$, where F is the sampled parameter `SurfaceAreaFactor_UNIT` as specified in *tpa.inp*. Because K_D is the product of K_A and ESA (Eq. 11-8), Eq. (11-12) is rewritten in TPA Version 5.1 as

$$K_0 = C_C F K_D \quad (11-13)$$

where

- K_0 — dimensionless distribution coefficient for colloid sorption [unitless]
 C_C — colloid concentration, as specified by the *tpa.inp* parameter `MatrixColloidConcentration_UNIT` [kg/m^3] or `FractureColloidConcentration_UNIT` [kg/m^3]
 F — ratio of the colloid surface area to the rock matrix surface area, as specified by the *tpa.inp* parameter `SurfaceAreaFactor_UNIT` [unitless]
 K_D — distribution coefficient for radionuclide sorption onto the porous rock matrix (m^3/kg), calculated for americium, neptunium, plutonium, thorium, uranium, and curium from the surface response curves in *coefkdeq.dat* and sampled from *tpa.inp* for all other radionuclides as specified by the parameter `MatrixKD_UNIT_RN` [m^3/kg]

For transport in fractures, the effective surface area of colloids (ESA_C) in Eq. (11-12) in all of the hydrostratigraphic units is assumed to have an estimated value of 4×10^5 [m^2/kg], based on the Yucca Mountain-specific measurements of Kingston and Whitbeck (1991). For radionuclide transport in fractures, *tpa.inp* provides R_D values, `FractureRD_UNIT_RN`, instead of K_D values for the non-actinides. Similarly, fracture retardation factors for the actinides are calculated in each TPA Version 5.1 realization. Substituting for K_A from Eq. (11-10) into Eq. (11-12) results in

$$K_0 = 2 \times 10^5 (m^2/kg) b C_C (R_D - 1) \quad (11-14)$$

where

- K_0 — dimensionless distribution coefficient for colloid sorption [unitless]
 C_C — colloid concentration in fractures, as specified by the *tpa.inp* parameter `FractureColloidConcentration_UNIT` [kg/m^3]
 R_D — retardation factor associated with the radionuclide in the absence of colloids, calculated from Eq. (11-10) for fracture sorption of actinides and as specified by the *tpa.inp* parameter `FractureRD_UNIT_RN` for all other radionuclides
 b — fracture aperture, as specified by the *tpa.inp* parameter `FractureAperture_UNIT` [m]

Equation (11-11) applies an adjustment for colloids if fracture retardation factors other than 1.0 are specified by the user.

TPA Version 5.1 also incorporates explicit modeling of the transport of radionuclides that are irreversibly attached to colloids originating from the waste form or waste package corrosion products. Radionuclides that are irreversibly associated with colloids (J-species) are considered to be permanently attached to and remain with the colloid throughout the simulation, and the transport fate of the colloid determines the transport of the radionuclide. The colloid retardation factor, R_c , for each hydrostratigraphic layer is provided directly to UZFT as specified by the *tpa.inp* parameter MatrixColloidRetardationFactor_UNIT[m³/kg] or FractureColloidRetardationFactor_UNIT[m³/kg]. UZFT also assumes that a fraction of the J-species radionuclides will be permanently removed from transport by filtration of the colloidal particles in the rock matrix. From parameter values specified in *tpa.inp*, UZFT identifies which hydrostratigraphic layer, of those that are present (i.e., nonzero thickness) in the subarea, has the maximum value for the specified parameter PermanentLossColloidFilterFactor_UNIT. The parameter is a measure of how effectively colloids would be removed by filtration during transport through the matrix of this layer. UZFT uses this maximum value to calculate the fraction of J-species lost by filtration in the unsaturated zone. Where J-species radionuclides are removed from transport by permanent filtration, they and their progeny are not included in the unsaturated zone release rates.

11.4 Input Parameters in *tpa.inp*

Table 11-1 lists the input and correlated parameter values to UZFT in *tpa.inp* and *tpa_include.inp* that are included in the reference data set for TPA Version 5.1.

Because many of the UZFT layer properties must be defined individually for matrix flow conditions and for fracture flow conditions for each of the seven hydrostratigraphic layers in the unsaturated zone, Table 11-1 contains more than 300 separate parameters. A more concise list of the UZFT parameters, grouped by their properties and root names, is provided as a summary in Table 11-2.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (Disclaimer: The listed input parameter distributions and values were provided for the release of the TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	UZVelocity(0=average, 1=time-dependent)	Option to use an average velocity for each transport leg throughout the NEFMKS calculations for the unsaturated zone, instead of using a set of time-dependent velocities read from <i>nefl.vel</i> [unitless]	iflag 1	Options are 0 = average velocities or 1 = time-dependent velocities. The reference case value of 1, which allows for the use of time-dependent velocities in NEFTAN, is assigned because it is consistent with previous versions of TPA. (See also UnsaturatedZoneMinimumVelocityChangeFactor).
UZFT	PermanentLossColloidFilter Factor_TS_w_[]	Fraction of radionuclides irreversibly attached (J-species) to colloids that are permanently removed by filtration in the Topopah Spring unit [unitless]	constant 0.65	This value is used in the calculations only if the specified fraction is the largest of any layer in the subarea (Pickett, 2007). The filter factor for a single layer was chosen assuming no other layers are present.
UZFT	PermanentLossColloidFilter Factor_CHnv[]	Fraction of radionuclides irreversibly attached (J-species) to colloids that are permanently removed by filtration in the Calico Hills vitric unit [unitless]	constant 0.57	This value is used to apply colloid filtration to any portion of flow that bypasses the NEFMKS transport calculations (i.e., the bypass fraction). This value is applied to colloid filtration in the matrix fraction only if the specified fraction is the largest of any layer in the subarea (Pickett, 2007). The filter factor for a single layer was chosen assuming no other layers are present.
UZFT	PermanentLossColloidFilter Factor_CHnz[]	Fraction of radionuclides irreversibly attached (J-species) to colloids that are permanently removed by filtration in the Calico Hills zeolitic unit [unitless]	constant 0.75	This value is used in the calculations only if the specified fraction is the largest of any layer in the subarea (Pickett, 2007). The filter factor for a single layer was chosen assuming no other layers are present.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	PermanentLossColloidFilter Factor_PPw_[]	Fraction of radionuclides irreversibly attached (J-species) to colloids that are permanently removed by filtration in the Prow Pass welded unit [unitless]	constant 0.41	This value is used in the calculations only if the specified fraction is the largest of any layer in the subarea (Pickett, 2007). The filter factor for a single layer was chosen assuming no other layers are present.
UZFT	PermanentLossColloidFilter Factor_UCF_[]	Fraction of radionuclides irreversibly attached (J-species) to colloids that are permanently removed by filtration in the Upper Crater Flat unit [unitless]	constant 0.51	This value is used in the calculations only if the specified fraction is the largest of any layer in the subarea (Pickett, 2007). The filter factor for a single layer was chosen assuming no other layers are present.
UZFT	PermanentLossColloidFilter Factor_BFw_[]	Fraction of radionuclides irreversibly attached (J-species) to colloids that are permanently removed by filtration in the Bullfrog welded unit [unitless]	constant 0.66	This value is used in the calculations only if the specified fraction is the largest of any layer in the subarea (Pickett, 2007). The filter factor for a single layer was chosen assuming no other layers are present.
UZFT	PermanentLossColloidFilter Factor_UFZ_[]	Fraction of radionuclides irreversibly attached (J-species) to colloids that are permanently removed by filtration in the optional Unsaturated Fault Zone unit [unitless]	constant 0.0	This value is used in the calculations only if the specified fraction is the largest of any layer in the subarea. Assumes no colloid filtration in fault zone.
UZFT	InletArea__1SubArea[m2] InletArea__2SubArea[m2] InletArea__3SubArea[m2] InletArea__4SubArea[m2] InletArea__5SubArea[m2] InletArea__6SubArea[m2] InletArea__7SubArea[m2] InletArea__8SubArea[m2] InletArea__9SubArea[m2] InletArea__10SubArea[m2]	A Inlet area for each subarea, as numbered. Written to <i>nefi.inp</i> as mixing zone (first leg) information [m ²]	constant 5.4e5	The same value is assigned to each subarea. NEFTRAN looks for a value for the inlet area, so a positive real number is provided; however, the value is not used in the NEFMKS calculation because the velocities are input from an external file.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	UZFractureForceFactorFor KdToRd	f This factor controls the calculation of retardation factors in fractures for reversible sorption of actinides (americium, neptunium, plutonium, thorium, uranium, and curium)	constant 0.0	The only values that should be used for this parameter are 0.0 or 1.0. Reference case value is 0.0 (no retardation by sorption in fractures), but user can modify to 1.0, in which case a retardation factor, R_D , is calculated from a surface response function for each actinide (i.e., sorption allowed in fractures).
UZFT	MatrixKD_TSw_l[m3/kg] MatrixKD_CHnv_l[m3/kg] MatrixKD_CHnz_l[m3/kg] MatrixKD_PPw_l[m3/kg] MatrixKD_UCF_l[m3/kg] MatrixKD_BFw_l[m3/kg] MatrixKD_UFZ_l[m3/kg]	K_D Matrix sorption coefficient, K_D , of iodine (I) for each of the hydrostratigraphic units [m ³ /kg]	constant 0.0	No significant retardation for iodine is expected, as is consistent for anionic species. This is also a bounding value and has no uncertainty. Data are from Bechtel SAIC Company, LLC (2001a). The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	MatrixKD_TSw_Tc[m3/kg] MatrixKD_CHnvTc[m3/kg] MatrixKD_CHnzTc[m3/kg] MatrixKD_PPw_Tc[m3/kg] MatrixKD_UCF_Tc[m3/kg] MatrixKD_BFw_Tc[m3/kg] MatrixKD_UFZ_Tc[m3/kg]	K_D Matrix sorption coefficient, K_D , of technetium (Tc) for each of the hydrostratigraphic units [m ³ /kg]	constant 0.0	Assume no retardation for technetium. Consistent with experimental evidence (Bechtel SAIC Company, LLC, 2001a). The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_TSw_Cl[m3/kg] MatrixKD_CHnvCl[m3/kg] MatrixKD_CHnzCl[m3/kg] MatrixKD_PPw_Cl[m3/kg] MatrixKD_UCF_Cl[m3/kg] MatrixKD_BFw_Cl[m3/kg] MatrixKD_UFZ_Cl[m3/kg]	K_D Matrix sorption coefficient, K_D , of chlorine (Cl) for each of the hydrostratigraphic units [m ³ /kg]	constant 0.0	No significant retardation for chlorine is expected, as is consistent for anionic species. This is also a bounding value and has no uncertainty. Data from Bechtel SAIC Company, LLC (2001a). The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	MatrixKD_TSw_Ra[m3/kg]	K_D Matrix sorption coefficient, K_D , of radium (Ra) for the Topopah Spring welded tuff [m ³ /kg]	constant 0.325	Tuffs in the Topopah Spring welded hydrostratigraphic unit are mostly vitric (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) gives K_D values for radium sorption onto vitric tuff that range from 0.05 to 0.6 m ³ /kg in a uniform distribution. The mean expected value is used here (constant value).
UZFT	MatrixKD_CHnvRa[m3/kg]	K_D Matrix sorption coefficient, K_D , of radium (Ra) for the Calico Hills vitric tuff [m ³ /kg]	constant 0.325	Tuffs in the Calico Hills nonwelded vitric hydrostratigraphic unit have vitric layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) gives K_D values for radium sorption onto vitric tuff that range from 0.05 to 0.6 m ³ /kg in a uniform distribution. The mean expected value is used here (constant value).
UZFT	MatrixKD_CHnzRa[m3/kg]	K_D Matrix sorption coefficient, K_D , of radium (Ra) for the Calico Hills zeolitic tuff [m ³ /kg]	constant 3.0	Tuffs in the Calico Hills nonwelded zeolitic hydrostratigraphic unit have zeolitic layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) has a K_D range for radium in zeolitic rocks of 1.0 to 5.0 m ³ /kg (uniform distribution). The mean expected value is used here.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_PPw_Ra[m3/kg]	K_D Matrix sorption coefficient, K_D , of radium (Ra) for the Prow Pass welded tuff [m ³ /kg]	constant 0.55	The Prow Pass tuffs have both zeolitic and devitrified characteristics (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) has K_D s for radium for zeolitic layers ranging from 1.0 to 5.0 m ³ /kg (uniform distribution). The range of K_D s for radium for devitrified layers is lower [0.1 to 1.0 m ³ /kg (uniform distribution)]. The mean expected K_D for devitrified layers is used here.
UZFT	MatrixKD_UCF_Ra[m3/kg]	K_D Matrix sorption coefficient, K_D , of radium (Ra) for the Upper Crater Flat tuff [m ³ /kg]	constant 0.55	The Upper Crater Flat hydrostratigraphic unit represents the non- to partially welded, devitrified, and zeolitized Crater Flat tuffs that occur above the water table in each potential repository subarea. Bechtel SAIC Company, LLC (2004a) has K_D s for radium for zeolitic layers ranging from 1.0 to 5.0 m ³ /kg (uniform distribution). Range of K_D s for radium for devitrified layers is lower [0.1 to 1.0 m ³ /kg (uniform distribution)]. The mean expected K_D for devitrified layers is used here.
UZFT	MatrixKD_BFw_Ra[m3/kg]	K_D Matrix sorption coefficient, K_D , of radium (Ra) for the Bullfrog welded tuff [m ³ /kg]	constant 0.55	The tuffs that compose the Bullfrog welded unit have vitric, zeolitic, and devitrified characteristics. The unit as a whole, however, appears to have significant devitrified zones (Bechtel SAIC Company, LLC, 2002). In Bechtel SAIC Company, LLC (2004a), the range of K_D s for radium in devitrified layers is 0.1 to 1.0 m ³ /kg (uniform distribution). The mean expected K_D for devitrified layers is used here.
UZFT	MatrixKD_UFZ_Ra[m3/kg]	K_D Matrix sorption coefficient, K_D , of radium (Ra) for the optional Unsaturated Fault zone tuff [m ³ /kg]	constant 0.325	The Unsaturated Fault Zone is a hypothetical unit TPA Version 5.1 uses to represent a fault zone. Vitric sorption properties are used.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_TSw_Pb[m3/kg] MatrixKD_CHnvPb[m3/kg] MatrixKD_CHnzPb[m3/kg] MatrixKD_PPw_Pb[m3/kg] MatrixKD_UCF_Pb[m3/kg] MatrixKD_BFw_Pb[m3/kg] MatrixKD_UFZ_Pb[m3/kg]	K_D Matrix sorption coefficient, K_D , of lead (Pb) for each of the hydrostratigraphic units [m ³ /kg]	constant 0.3	Bechtel SAIC Company, LLC (2001a) has same range of K_{Ds} for lead for all rock types [0.1 to 0.5 m ³ /kg (uniform distribution)]. The mean expected value is used here. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	MatrixKD_TSw_Cs[m3/kg]	K_D Matrix sorption coefficient, K_D , of cesium (Cs) for the Topopah Spring welded tuff [m ³ /kg]	constant 0.002	Tuffs in the Topopah Spring welded hydrostratigraphic unit are mostly vitric (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) lists cesium K_D values for vitric rocks as a user-defined distribution (0 = 0 percent, 0.002 = 50 percent, 0.1 = 100 percent). The median expected value is used here.
UZFT	MatrixKD_CHnvCs[m3/kg]	K_D Matrix sorption coefficient, K_D , of cesium (Cs) for the Calico Hills Vitric tuff [m ³ /kg]	constant 0.002	Tuffs in the Calico Hills nonwelded vitric hydrostratigraphic unit have vitric layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) lists cesium K_D values for vitric rocks as a user-defined distribution (0 = 0 percent, 0.002 = 50 percent, and 0.1 = 100 percent). The median expected value is used here.
UZFT	MatrixKD_CHnzCs[m3/kg]	K_D Matrix sorption coefficient, K_D , of cesium (Cs) for the Calico Hills zeolitic tuff [m ³ /kg]	constant 5.0	Tuffs in the Calico Hills nonwelded zeolitic hydrostratigraphic unit have zeolitic layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) lists cesium K_{Ds} for zeolitic layers as a user-defined distribution (0.425 = 0 percent, 5.0 = 50 percent, and 20.0 = 100 percent). The median expected value is used here.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_PPw_Cs[m3/kg]	K_D Matrix sorption coefficient, K_D of cesium (Cs) for the Prow Pass welded tuff [m ³ /kg]	constant .008	The Prow Pass tuffs have both zeolitic and devitrified characteristics (Bechtel SAIC Company, LLC, 2002). The lower range of cesium sorption values for these two rock types is used here. Bechtel SAIC Company, LLC (2004a) lists a K_D range of 0.001 to 0.015 m ³ /kg uniform distribution for devitrified rock, for which the mean expected value is used here.
UZFT	MatrixKD_UCF_Cs[m3/kg]	K_D Matrix sorption coefficient, K_D of cesium (Cs) for the Upper Crater Flat tuff [m ³ /kg]	constant .008	The Upper Crater Flat hydrostratigraphic unit represents the non- to partially welded, devitrified, and zeolitized Crater Flat tuffs that occur above the water table in each potential repository subarea. As before for Prow Pass and Bullfrog, the lower of K_D ranges for zeolitic and devitrified rock type are used for Upper Crater Flat. Bechtel SAIC Company, LLC (2004a) lists a K_D range of 0.001 to 0.015 m ³ /kg uniform distribution for devitrified rock, for which the mean expected value is used here.
UZFT	MatrixKD_BFw_Cs[m3/kg]	K_D Matrix sorption coefficient, K_D of cesium (Cs) for the Bullfrog welded tuff [m ³ /kg]	constant .008	The tuffs that comprise the Bullfrog welded tuff have vitric, zeolitic, and devitrified characteristics. The unit as a whole appears to have significant devitrified zones (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) lists a K_D range of 0.001 to 0.015 m ³ /kg uniform distribution for devitrified rock, for which the mean expected value is used here.
UZFT	MatrixKD_UFZ_Cs[m3/kg]	K_D Matrix sorption coefficient, K_D of cesium (Cs) for the optional Unsaturated Fault Zone tuff [m ³ /kg]	constant 0.002	The Unsaturated Fault Zone is a hypothetical unit used by TPA Version 5.1 to represent a fault zone. There is no corresponding data for the Unsaturated Fault Zone in Bechtel SAIC Company, LLC (2002), thus vitric sorption properties are assumed for this layer/region because DOE vitric K_D s are typically more conservative (less sorption than zeolitic or devitrified K_D s). Bechtel SAIC Company, LLC (2004a) lists cesium K_D values for vitric rocks as a user-defined distribution (0 = 0 percent, 0.002 = 50 percent, and 0.1 = 100 percent). The median expected value is used here.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_TSw_Ni[m3/kg]	K_D Matrix sorption coefficient, K_D of nickel (Ni) for the Topopah Spring welded tuff [m ³ /kg]	constant 0.03	Tuffs in the Topopah Spring welded hydrostratigraphic unit are mostly vitric (Bechtel SAIC Company, LLC, 2002). The K_D values from Bechtel Company, LLC (2001a) for nickel sorption onto vitric tuff range from 0 to 0.05 m ³ /kg, beta distribution, expected value 0.03, stdev = 0.01, COV = 0.33. The expected value is used here.
UZFT	MatrixKD_CHnvNi[m3/kg]	K_D Matrix sorption coefficient, K_D of nickel (Ni) for the Calico Hills vitric tuff [m ³ /kg]	constant 0.03	Tuffs in the Calico Hills nonwelded vitric hydrostratigraphic unit have vitric layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). DOE values for nickel K_D s in Bechtel SAIC Company, LLC (2001a) are 0 to 0.05 m ³ /kg in vitric layers, beta distribution, expected value 0.03, stdev = 0.01, COV = 0.33. The expected value is used here.
UZFT	MatrixKD_CHnzNi[m3/kg]	K_D Matrix sorption coefficient, K_D of nickel (Ni) for the Calico Hills zeolitic tuff [m ³ /kg]	constant 0.05	Tuffs in the Calico Hills nonwelded zeolitic hydrostratigraphic unit have zeolitic layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). K_D s for nickel in Bechtel SAIC Company, LLC (2001a) are 0 to 0.2, beta distribution, expected value 0.05, COV = 0.33, stdev = 0.01 for both devitrified and zeolitic rocks. The expected value is used here.
UZFT	MatrixKD_PPw_Ni[m3/kg]	K_D Matrix sorption coefficient, K_D of nickel (Ni) for the Prow Pass welded tuff [m ³ /kg]	constant 0.05	The Prow Pass tuffs have both zeolitic and devitrified characteristics (Bechtel SAIC Company, LLC, 2002). The lower range of Cs sorption values for these two rock types is used here. K_D s for nickel in Bechtel SAIC Company, LLC (2001a) are 0 to 0.2, beta, expected value 0.05, COV = 0.33, stdev = 0.01 for both devitrified and zeolitic rocks. The expected value is used here.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_UCF_Ni[m3/kg]	K_D Matrix sorption coefficient, K_D , of nickel (Ni) for the Upper Crater Flat tuff [m ³ /kg]	constant 0.05	The Upper Crater Flat hydrostratigraphic unit represents the non- to partially welded, devitrified, and zeolitized Crater Flat tuffs that occur above the water table in each potential repository subarea. Similar to Prow Pass welded and Bullfrog welded, the lower of K_D ranges for zeolitic and devitrified rock type will be used for Upper Crater Flat. K_D s for nickel in Bechtel SAIC Company, LLC (2001a) range from 0 to 0.2, beta distribution, expected value 0.05, COV = 0.33, stdev = 0.01 for both devitrified and zeolitic rocks. The expected value is used here.
UZFT	MatrixKD_BFW_Ni[m3/kg]	K_D Matrix sorption coefficient, K_D , of nickel (Ni) for the Bullfrog welded tuff [m ³ /kg]	constant 0.05	The tuffs that comprise the Bullfrog welded tuff have vitric, zeolitic, and devitrified characteristics. The unit as a whole, however, appears to have significant devitrified zones (Bechtel SAIC Company, LLC, 2002). K_D s for nickel in Bechtel SAIC Company, LLC (2001a) for devitrified rocks range from 0 to 0.2, beta distribution, expected value 0.05, COV = 0.33, stdev = 0.01. The expected value is used here.
UZFT	MatrixKD_UFZ_Ni[m3/kg]	K_D Matrix sorption coefficient, K_D , of nickel (Ni) for the optional Unsaturated Fault Zone tuff [m ³ /kg]	constant 0.03	There is no direct information for the hypothetical Unsaturated Fault Zone in Bechtel SAIC Company, LLC (2002). Vitric sorption properties are assumed for this unit because they are conservative compared to zeolitic or devitrified K_D s. Vitric K_D s for nickel in Bechtel SAIC Company, LLC (2001a) range from 0 to 0.2, beta distribution, expected value 0.05, COV = 0.33, stdev = 0.01. The expected value is used here.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_TSw_Se[m3/kg] MatrixKD_CHnvSe[m3/kg] MatrixKD_CHnzSe[m3/kg] MatrixKD_PPw_Se[m3/kg] MatrixKD_UCF_Se[m3/kg] MatrixKD_BFw_Se[m3/kg] MatrixKD_UFZ_Se[m3/kg]	K_D Matrix sorption coefficient, K_D of selenium (Se) for each of the hydrostratigraphic units [m ³ /kg]	constant 0.0001	Bechtel SAIC Company, LLC (2001a) gives the same range for all rock types for selenium $K_{D,S}$, from 0 to 0.001 m ³ /kg, beta distribution, expected value = 0.0001, stdev = 0.0001, COV = 1.0. Expected value is used here (constant). The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	MatrixKD_TSw_Nb[m3/kg]	K_D Matrix sorption coefficient, K_D of niobium (Nb) for the Topopah Spring welded tuff [m ³ /kg]	constant 0.4	Using the trivalent chemical analogy, the DOE median expected K_D value for americium is used in place of a K_D for niobium. Tuffs in the Topopah Spring welded hydrostratigraphic unit are mostly vitric (Bechtel SAIC Company, LLC, 2002). Data from Bechtel SAIC Company, LLC (2004a) for sorption onto vitric tuff lists americium K_D values from 0.1 to 1.0 m ³ /kg in a piecewise distribution range, with 0.1 = 0 percent, 0.4 = 50 percent, and 1.0 = 100 percent. Only the median expected value is used here (constant value).
UZFT	MatrixKD_CHnvNb[m3/kg]	K_D Matrix sorption coefficient, K_D of niobium (Nb) for the Calico Hills vitric tuff [m ³ /kg]	constant 0.4	Using the trivalent chemical analogy, K_D s for americium are used in place of K_D s for niobium. Tuffs in the Calico Hills nonwelded vitric hydrostratigraphic unit have vitric layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). Data from Bechtel SAIC Company, LLC (2004a) for sorption onto vitric tuff lists americium K_D values from 0.1 to 1.0 m ³ /kg in a piecewise distribution range, with 0.1 = 0 percent, 0.4 = 50 percent, and 1.0 = 100 percent. Only the median expected value is used here (constant value).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_CHnzNb[m3/kg]	K_D Matrix sorption coefficient, K_D , of niobium (Nb) for the Calico Hills zeolitic tuff [m ³ /kg]	constant 5.5	Using the trivalent chemical analogy, K_D s for americium are used in place of K_D s for niobium. Tuffs in the Calico Hills nonwelded zeolitic hydrostratigraphic unit have zeolitic layer properties with respect to sorption (Bechtel SAIC Company, LLC, 2002). Data from Bechtel SAIC Company, LLC (2004a) for sorption onto zeolitic tuff lists americium K_D values from 1.0 to 10.0 m ³ /kg in a uniform distribution. The mean expected value of 5.5 is used here (constant value).
UZFT	MatrixKD_PPw_Nb[m3/kg]	K_D Matrix sorption coefficient, K_D , of niobium (Nb) for the Prow Pass welded tuff [m ³ /kg]	constant 5.5	Using the trivalent chemical analogy, K_D s for americium are used in place of K_D s for niobium. The Prow Pass tuffs have both zeolitic and devitrified characteristics (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) lists zeolitic and devitrified K_D s for americium ranging from 1.0 to 10.0 m ³ /kg (uniform distribution). The mean expected K_D value of 5.5 for the zeolitic layers is used here (constant value).
UZFT	MatrixKD_UCF_Nb[m3/kg]	K_D Matrix sorption coefficient, K_D , of niobium (Nb) for the Upper Crater Flat tuff [m ³ /kg]	constant 5.5	Using the trivalent chemical analogy, K_D s for americium are used in place of K_D s or niobium. The Upper Crater Flat hydrostratigraphic unit represents the non- to partially welded, devitrified, and zeolitized Crater Flat tuffs that occur above the water table in each potential repository subarea. Bechtel SAIC Company, LLC (2004a) lists zeolitic and devitrified K_D s for americium ranging from 1.0 to 10.0 m ³ /kg (uniform distribution). The mean expected K_D value of 5.5 is used here (constant value).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixKD_BFW_Nb[m3/kg]	K_D Matrix sorption coefficient, K_D of niobium (Nb) for the Bullfrog welded tuff [m ³ /kg]	constant 5.5	Using the trivalent chemical analogy, K_D s for americium are used in place of K_D s for niobium. The tuffs that comprise the Bullfrog welded tuff have vitric, zeolitic, and devitrified characteristics. The unit as a whole appears to have significant devitrified zones (Bechtel SAIC Company, LLC, 2002). Bechtel SAIC Company, LLC (2004a) lists devitrified K_D s for americium ranging from 1.0 to 10.0 m ³ /kg (uniform distribution). The mean expected K_D value of 5.5 is used here (constant value).
UZFT	MatrixKD_UFZ_Nb[m3/kg]	K_D Matrix sorption coefficient, K_D of niobium (Nb) for the optional Unsaturated Fault Zone tuff [m ³ /kg]	constant 0.4	Using the trivalent chemical analogy, K_D s for americium are used in place of K_D s for niobium. There is no direct information for the hypothetical Unsaturated Fault Zone in Bechtel SAIC Company, LLC (2002). Vitric sorption properties are assumed for this unit because they are conservative compared to zeolitic or devitrified K_D s. Data from Bechtel SAIC Company, LLC (2004a) for sorption onto vitric tuff lists americium K_D values from 0.1 to 1.0 m ³ /kg in a piecewise distribution range, with 0.1 = 0 percent, 0.4 = 50 percent, and 1.0 = 100 percent. Only the median expected value is used here (constant value).
UZFT	FractureRD_TSw_I FractureRD_CHNvI FractureRD_CHNzI FractureRD_PPw_I FractureRD_UCF_I FractureRD_BFW_I FractureRD_UFZ_I	R_D Fracture retardation factor, R_D , for iodine (I) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHNv = Calico Hills vitric tuff CHNz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFW = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureRD_TSw_Tc FractureRD_CHnvTc FractureRD_CHnzTc FractureRD_PPw_Tc FractureRD_UCF_Tc FractureRD_BFw_Tc FractureRD_UFZ_Tc	R_D Fracture retardation factor, R_D , for technetium (Tc) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
	FractureRD_TSw_Ci FractureRD_CHnvCi FractureRD_CHnzCi FractureRD_PPw_Ci FractureRD_UCF_Ci FractureRD_BFw_Ci FractureRD_UFZ_Ci	R_D Fracture retardation factor, R_D , for chlorine (Ci) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureRD_TSw_Ra	R_D Fracture retardation factor, R_D , for radium (Ra) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
	FractureRD_CHnvRa			
	FractureRD_CHnzRa			
	FractureRD_PPw_Ra			
	FractureRD_UCF_Ra			
	FractureRD_BFw_Ra			
	FractureRD_UFZ_Ra			
UZFT	FractureRD_TSw_Pb	R_D Fracture retardation factor, R_D , for lead (Pb) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
	FractureRD_CHnvPb			
	FractureRD_CHnzPb			
	FractureRD_PPw_Pb			
	FractureRD_UCF_Pb			
	FractureRD_BFw_Pb			
	FractureRD_UFZ_Pb			

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureRD_TSw_Cs	R_D Fracture retardation factor, R_D , for cesium (Cs) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
	FractureRD_CHnvCs			
	FractureRD_CHnzCs			
	FractureRD_PPw_Cs			
	FractureRD_UCF_Cs			
	FractureRD_BFw_Cs			
	FractureRD_UFZ_Cs			
UZFT	FractureRD_TSw_Ni	R_D Fracture retardation factor, R_D , for nickel (Ni) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
	FractureRD_CHnvNi			
	FractureRD_CHnzNi			
	FractureRD_PPw_Ni			
	FractureRD_UCF_Ni			
	FractureRD_BFw_Ni			
	FractureRD_UFZ_Ni			

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureRD_TSw_Se FractureRD_CHnvSe FractureRD_CHnzSe FractureRD_PPw_Se FractureRD_UCF_Se FractureRD_BFw_Se FractureRD_UFZ_Se	R_D Fracture retardation factor, R_D , for selenium (Se) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	FractureRD_TSw_Nb FractureRD_CHnvNb FractureRD_CHnzNb FractureRD_PPw_Nb FractureRD_UCF_Nb FractureRD_BFw_Nb FractureRD_UFZ_Nb	R_D Fracture retardation factor, R_D , for niobium (Nb) in each of the hydrostratigraphic units [unitless]	constant 1.0	Value assumes no fracture retardation ($K_D = 0$, $R_D = 1$). All layers, all nuclides. Also a bounding assumption for fracture transport. The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	MatrixPoreRadius_TSw_m	r The matrix pore radius for this hydrostratigraphic unit is used, along with matrix porosity and matrix grain density, to calculate the effective surface area available for matrix sorption [m]	constant 5.0e-8	The specified constant value is consistent with the estimated median value based on moisture retention curves used by DOE, from work by Travis and Nuttall (1987). Bechtel SAIC Company, LLC (2004b) indicates a more complex distribution of pore sizes for various rock units (see comments for other hydrostratigraphic layers below), but there is a general agreement with the specified value. To minimize surface area uncertainties, the 5e-8 value is retained for all layers pending more detailed characterization.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixPoreRadius_CHnv[m]	r The matrix pore radius for this hydrostratigraphic unit is used, along with matrix porosity and matrix grain density, to calculate the effective surface area available for matrix sorption [m]	constant 5.0e-8	Based on review of Bechtel SAIC Company, LLC (2004b), the median value for CHnv is closer to 4.5e-7, but to minimize surface area uncertainties, the generalized parameter value of 5.e-8, consistent with estimates from moisture retention curves used by DOE (Travis and Nuttall, 1987), is retained for all layers pending more detailed characterization.
UZFT	MatrixPoreRadius_CHnz [m]	r The matrix pore radius for this hydrostratigraphic unit is used, along with matrix porosity and matrix grain density, to calculate the effective surface area available for matrix sorption [m]	constant 5.0e-8	Based on review of Bechtel SAIC Company, LLC (2004b), the CHnz has a median value of about 5e-8, comparable to TSw but with a much broader distribution. This also corresponds to the generalized value estimated from moisture retention curves used by DOE (Travis and Nuttall, 1987).
UZFT	MatrixPoreRadius_PPw_ [m]	r The matrix pore radius for this hydrostratigraphic unit is used, along with matrix porosity and matrix grain density, to calculate the effective surface area available for matrix sorption [m]	constant 5.0e-8	Based on review of Bechtel SAIC Company, LLC (2004b), there are some Prow Pass tuffs in which 96 percent of the pore sizes are less than 5e-8, whereas in others only 16 percent of the pore sizes are less than 5e-8. The average for Prow Pass is that 53 percent of pore sizes are less than 5e-8, but to minimize surface area uncertainties, the generalized parameter value of 5e-8, consistent with estimates from moisture retention curves used by DOE (Travis and Nuttall, 1987), is retained for all layers pending more detailed characterization.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixPoreRadius_UCF_ [m]	r The matrix pore radius for this hydrostratigraphic unit is used, along with matrix porosity and matrix grain density, to calculate the effective surface area available for matrix sorption [m]	constant 5.0e-8	No DOE information on Upper Crater Flat as such; in TPA Version 5.1, this unit represents non- to partially welded, devitrified, and zeolitized tuffs above the water table in the Crater Flat Group (Winterle, et al., 1999). To minimize surface area uncertainties, the 5e-8 value, estimated from moisture retention curves (Travis and Nuttall, 1987), is retained for all layers pending more detailed characterization.
UZFT	MatrixPoreRadius_BFw_ [m]	r The matrix pore radius for this hydrostratigraphic unit is used, along with matrix porosity and matrix grain density, to calculate the effective surface area available for matrix sorption [m]	constant 5.0e-8	Constant value of 5e-8 is consistent with median value for welded tuffs based on moisture retention curves used by DOE, from work by Travis and Nuttall (1987) and as reported in Bechtel SAIC Company, LLC (2004b). To minimize surface area uncertainties, the 5e-8 value is retained pending more detailed characterization.
UZFT	MatrixPoreRadius_UFZ_ [m]	r The matrix pore radius for this hydrostratigraphic unit is used, along with matrix porosity and matrix grain density, to calculate the effective surface area available for matrix sorption [m]	constant 5.0e-8	This is a hypothetical UZFT unit to represent transport through a fault zone. Constant value of 5e-8 is consistent with the median value used for the other UZ hydrostratigraphic units.
UZFT	FractureAperture_TSw_ [m]	b Width of fracture openings in the Topopah Spring welded tuff unit [m]	constant 1.0e-4	The fracture aperture is used to calculate the surface area in fractures that is available for sorption of actinides or for retardation of colloids during fracture flow. Aperture width is representative of DOE estimates for fracture width in Topopah Spring Welded tuff (0.1–0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureAperture_CHnv[m]	<i>b</i> Width of fracture openings in the Calico Hills nonwelded vitric tuff unit [m]	constant 2.0e-4	The fracture aperture is used to calculate the surface area in fractures that is available for sorption of actinides or for retardation of colloids during fracture flow. Aperture width is representative of DOE estimates for fracture width in Calico Hills nonwelded vitric tuff (0.2–0.3 mm), as estimated from Bechtel SAIC Company, LLC (2003a).
UZFT	FractureAperture_CHnz [m]	<i>b</i> Width of fracture openings in the Calico Hills nonwelded zeolitic tuff unit [m]	constant 2.0e-4	The fracture aperture is used to calculate the surface area in fractures that is available for sorption of actinides or for retardation of colloids during fracture flow. Aperture width is within range of DOE estimates for fracture width in Calico Hills nonwelded zeolitic tuff (0.2–0.3 mm), as estimated from Bechtel SAIC Company, LLC (2003a).
UZFT	FractureAperture_PPw_ [m]	<i>b</i> Width of fracture openings in the Prow Pass welded tuff unit [m]	constant 1.0e-4	The fracture aperture is used to calculate the surface area in fractures that is available for sorption of actinides or for retardation of colloids during fracture flow. Aperture width is representative of DOE estimates for fracture width in Prow Pass welded tuff (0.1–0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003a).
UZFT	FractureAperture_UCF_ [m]	<i>b</i> Width of fracture openings in the Upper Crater Flat tuff unit [m]	constant 1.0e-4	The fracture aperture is used to calculate the surface area in fractures that is available for sorption of actinides or for retardation of colloids during fracture flow. Aperture width is representative of DOE estimates for fracture width in Upper Crater Flat tuffs (0.1–0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003a).
UZFT	FractureAperture_BFw_ [m]	<i>b</i> Width of fracture openings in the Bullfrog welded tuff unit [m]	constant 1.0e-4	The fracture aperture is used to calculate the surface area in fractures that is available for sorption of actinides or for retardation of colloids during fracture flow. Aperture width is representative of DOE estimates for fracture width in Bullfrog welded tuff (0.1–0.2 mm), as estimated from Bechtel SAIC Company, LLC (2003a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureAperture_UFZ_ [m]	b Width of fracture openings in the Unsaturated Fault Zone rocks tuff unit [m]	constant 1.0e-4	The fracture aperture is used to calculate the surface area in fractures that is available for sorption of actinides or for retardation of colloids during fracture flow. Hypothetical unit to model transport through a fault zone. Aperture width uncertain. Constant value of 1e-4 m used to correspond to value used for other units.
UZFT	MatrixGrainDensity_TSw_ [kg/m ³]	ρ_g Matrix grain density for Topopah Spring welded tuff and used for actinides (americium, neptunium, plutonium, thorium, uranium, and curium) to calculate the effective surface area and retardation factors for matrix sorption in this layer [kg/m ³]	constant 2460.0	Based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, should be reviewed for consistency with the purported source materials. However, in the transport calculations, they cancel out so that only matrix porosity is important in determining retardation factor, R_D . Thus, if calculations stay as is, there is no need to change these numbers.
UZFT	MatrixGrainDensity_CHnv [kg/m ³]	ρ_g Matrix grain density for Calico Hills nonwelded vitric tuff and used for (americium, neptunium, plutonium, thorium, uranium, and curium) to calculate the effective surface area and retardation factors for matrix sorption in this layer [kg/m ³]	constant 2260.0	Based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, should be reviewed for consistency with the purported source materials. However, in the transport calculations, they cancel out so that only matrix porosity is important in determining retardation factor, R_D . Thus, if calculations stay as is, there is no need to change these numbers.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixGrainDensity_CHnz [kg/m ³]	ρ_g Matrix grain density for Calico Hills nonwelded zeolitic tuff and used for actinides (americium, neptunium, plutonium, thorium, uranium, and curium) to calculate the effective surface area and retardation factors for matrix sorption in this layer [kg/m ³]	constant 2400.0	Based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, should be reviewed for consistency with the purported source materials. However, in the transport calculations, they cancel out so that only matrix porosity is important in determining retardation factor, R_D . Thus, if calculations stay as is, there is no need to change these numbers.
UZFT	MatrixGrainDensity_PPW_ [kg/m ³]	ρ_g Matrix grain density for Prow Pass welded tuff and used for actinides (americium, neptunium, plutonium, thorium, uranium, and curium) to calculate the effective surface area and retardation factors for matrix sorption in this layer [kg/m ³]	constant 2540.0	Based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, should be reviewed for consistency with the purported source materials. However, in the transport calculations, they cancel out so that only matrix porosity is important in determining retardation factor, R_D . Thus, if calculations stay as is, there is no need to change these numbers.
UZFT	MatrixGrainDensity_UCF_ [kg/m ³]	ρ_g Matrix grain density for Upper Crater Flat tuff and used for actinides (americium, neptunium, plutonium, thorium, uranium, and curium) to calculate the effective surface area and retardation factors for matrix sorption in this layer [kg/m ³]	constant 2420.0	Based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, should be reviewed for consistency with the purported source materials. However, in the transport calculations, they cancel out so that only matrix porosity is important in determining retardation factor, R_D . Thus, if calculations stay as is, there is no need to change these numbers.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixGrainDensity_BFW_ [kg/m ³]	ρ_g Matrix grain density for Bullfrog welded tuff and used for actinides (americium, neptunium, plutonium, thorium, uranium, and curium) to calculate the effective surface area and retardation factors for matrix sorption in this layer [kg/m ³]	constant 2570.0	Based on averaging of subunit data reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, should be reviewed for consistency with the purported source materials. However, in the transport calculations, they cancel out so that only matrix porosity is important in determining retardation factor, R_D . Thus, if calculations stay as is, there is no need to change these numbers.
UZFT	MatrixGrainDensity_UFZ_ [kg/m ³]	ρ_g Matrix grain density for Unsaturated Fault Zone and used for actinides (americium, neptunium, plutonium, thorium, uranium, and curium) to calculate the effective surface area and retardation factors for matrix sorption in this layer [kg/m ³]	constant 2630.0	Hypothetical unit to model transport through a fault zone. Best estimate, based on data from other units reported by Flint (1998). Constant values assumed because little variation exists in reported data. These values, along with porosities for each layer, should be reviewed for consistency with the purported source materials. However, in the transport calculations, they cancel out so that only matrix porosity is important in determining retardation factor, R_D . Thus, if calculations stay as is, there is no need to change these numbers.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
tpa_include.inp (separate input file from tpa.inp)	LogCO2PartialPressure_All UZ_SZLayers[atm]	Concentration (partial pressure) of CO ₂ (in log atm) in groundwaters of the unsaturated and saturated zone, excluding near-field [atm]	usersuppliedpwiseCDF 19 -3.9, 0.0 -3.7, 0.037 -3.5, 0.071 -3.3, 0.124 -3.2, 0.159 -2.9, 0.298 -2.7, 0.413 -2.56, 0.5 -2.4, 0.599 -2.2, 0.713 -1.9, 0.849 -1.8, 0.882 -1.6, 0.933 -1.4, 0.965 -1.2, 0.983 -1.0, 0.993 -0.8, 0.997 -0.6, 0.999 -0.5, 1.0	Values are based on analysis of Yucca Mountain region (site-scale model boundary) water chemistries from Bertetti, et al. (2004) and Bechtel SAIC Company, LLC (2004c), as described in McMurry and Bertetti (2005).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
tpa_include.inp (separate input file from tpa.inp)	pH_AIUZ_SZLayers [StandardUnits]	This is assumed to be the pH value for all water in the saturated zone and the unsaturated zone, excluding the near-field [StandardUnits]	usersuppliedpwiseCDF 18 6.5, 0.0 6.63, 0.018 6.81, 0.036 6.98, 0.067 7.15, 0.114 7.33, 0.185 7.5, 0.273 7.68, 0.385 7.85, 0.5 8.02, 0.615 8.2, 0.727 8.37, 0.815 8.55, 0.886 8.72, 0.933 8.89, 0.964 9.07, 0.982 9.24, 0.992 9.4, 1.0	Values are based on analysis of Yucca Mountain region (site-scale model boundary) water chemistries from Bertetti, et al. (2004) and Bechtel SAIC Company, LLC (2004c) as described in McMurry and Bertetti (2005). User-supplied distribution represents a truncated normal distribution with mean 7.85, std dev of 0.58, min 6.5, and max 9.4.
UZFT	MatrixLongitudinal Dispersivity[FractionOf Layer]	Maximum matrix longitudinal dispersivity, specified as a fraction of layer thickness; used in NEFMKS calculations [FractionOfLayer]	constant 0.06	Based on information from CRWMS M&O (2000b), Gelhar, et al. (1992), and Jury, et al. (1991).
UZFT	FractureLongitudinal Dispersivity[FractionOf Layer]	Maximum fracture longitudinal dispersivity, specified as a fraction of layer thickness; used in NEFMKS calculations [FractionOfLayer]	constant 0.06	Based on information from CRWMS M&O (2000b), Gelhar, et al. (1992), and Jury, et al. (1991).
UZFT	MatrixPermeability_TSw_ [m2]	K Matrix permeability for the Topopah Spring welded tuff unit. [m ²]	lognormal 5.6e-20, 5.6e-18	Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixPermeability_CHnv [m2]	K Matrix permeability for the Calico Hills nonwelded vitric tuff unit [m ²]	lognormal 1.8e-15, 1.8e-13	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the rock matrix. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPermeability_CHnz [m2]	K Matrix permeability for the Calico Hills nonwelded zeolitic tuff unit [m ²]	lognormal 9.8e-19, 9.8e-17	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the rock matrix. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPermeability_PPw_ [m2]	K Matrix permeability for the Prow Pass welded tuff unit [m ²]	lognormal 1.3e-18, 1.3e-16	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the rock matrix. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPermeability_UCF_ [m2]	K Matrix permeability for the Upper Crater Flat tuff unit [m ²]	lognormal 5.4e-19, 5.4e-17	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the rock matrix. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPermeability_BFw_ [m2]	K Matrix permeability for the Bullfrog welded tuff unit [m ²]	lognormal 2.1e-20, 2.1e-18	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the rock matrix. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPermeability_UFZ_ [m2]	K Matrix permeability for the Unsaturated Fault Zone unit [m ²]	lognormal 1.8e-19, 1.8e-16	Hypothetical unit to model transport through a fault zone. This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the rock matrix. Values and distribution generalized from information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPorosity_TS_w_ [m2]	ϕ Matrix porosity for the Topopah Spring welded tuff unit [unitless]	constant 0.08	The porosity value is used to calculate matrix surface area, retardation factors, and groundwater velocity in this layer. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPorosity_CHnv	ϕ Matrix porosity for the Calico Hills nonwelded vitric tuff unit [unitless]	constant 0.32	The porosity value is used to calculate matrix surface area, retardation factors, and groundwater velocity in this layer. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixPorosity_CHnz	ϕ Matrix porosity for the Calico Hills nonwelded zeolitic tuff unit [unitless]	constant 0.24	The porosity value is used to calculate matrix surface area, retardation factors, and groundwater velocity in this layer. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPorosity_PPw_	ϕ Matrix porosity for the Prow Pass welded tuff unit [unitless]	constant 0.25	The porosity value is used to calculate matrix surface area, retardation factors, and groundwater velocity in this layer. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPorosity_UCF_	ϕ Matrix porosity for the Upper Crater Flat tuff unit [unitless]	constant 0.22	The porosity value is used to calculate matrix surface area, retardation factors, and groundwater velocity in this layer. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPorosity_BFw_	ϕ Matrix porosity for Bullfrog welded tuff unit [unitless]	constant 0.10	The porosity value is used to calculate matrix surface area, retardation factors, and groundwater velocity in this layer. Values and distribution based on information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixPorosity_UFZ_	ϕ Matrix porosity for the Unsaturated Fault Zone unit [unitless]	constant 0.12	Hypothetical unit to model transport through a fault zone. The porosity value is used to calculate matrix surface area, retardation factors, and groundwater velocity in this layer. Values and distribution generalized from information in Bechtel SAIC Company, LLC (2004d).
UZFT	MatrixBeta_TS_	β Matrix van Genuchten beta parameter for the Topopah Spring welded tuff unit [unitless]	constant 1.9	This parameter is used to calculate the relative hydraulic conductivity of the rock matrix for a range of water saturations. Mean value based on Flint (1998).
UZFT	MatrixBeta_CHnv	β Matrix van Genuchten beta parameter for the Calico Hills nonwelded vitric tuff unit [unitless]	constant 1.3	This parameter is used to calculate the relative hydraulic conductivity of the rock matrix for a range of water saturations. Mean value based on Flint (1998).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixBeta_CHnz	β Matrix van Genuchten beta parameter for the Calico Hills nonwelded zeolitic tuff unit [unitless]	constant 1.3	This parameter is used to calculate the relative hydraulic conductivity of the rock matrix for a range of water saturations. Mean value based on Flint (1998).
UZFT	MatrixBeta_PPw_	β Matrix van Genuchten beta parameter for the Prow Pass welded tuff unit [unitless]	constant 1.5	This parameter is used to calculate the relative hydraulic conductivity of the rock matrix for a range of water saturations. Mean value based on Flint (1998).
UZFT	MatrixBeta_UCF_	β Matrix van Genuchten beta parameter for the Upper Crater Flat tuff unit [unitless]	constant 2.1	This parameter is used to calculate the relative hydraulic conductivity of the rock matrix for a range of water saturations. Mean value based on Flint (1998).
UZFT	MatrixBeta_BFw_	β Matrix van Genuchten beta parameter for the Bullfrog welded tuff unit [unitless]	constant 2.5	This parameter is used to calculate the relative hydraulic conductivity of the rock matrix for a range of water saturations. Mean value based on Flint (1998).
UZFT	MatrixBeta_UFZ_	β Matrix van Genuchten beta parameter for the Unsaturated Fault Zone unit [unitless]	constant 2.3	Hypothetical unit to model transport through a fault zone. This parameter is used to calculate the relative hydraulic conductivity of the rock matrix for a range of water saturations. Values and distribution generalized from values for other units in Flint (1998).
UZFT	FracturePermeability_TSw_ [m2]	K Permeability in fractures of the Topopah Spring welded tuff unit [m ²]	constant 1.1e-12	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the fractures in this layer. An estimated mean value is used, based on information documented in Bechtel SAIC Company, LLC (2003b).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FracturePermeability_CHnv [m ²]	K Permeability in fractures of the Calico Hills nonwelded vitric tuff unit [m ²]	constant 4.1e-14	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the fractures in this layer. An estimated mean value is used, based on information documented in Bechtel SAIC Company, LLC (2003b).
UZFT	FracturePermeability_CHnz [m ²]	K Permeability in fractures of the Calico Hills nonwelded zeolitic tuff unit [m ²]	constant 4.1e-14	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the fractures in this layer. An estimated mean value is used, based on information documented in Bechtel SAIC Company, LLC (2003b).
UZFT	FracturePermeability_PPw_ [m ²]	K Permeability in fractures of the Prow Pass welded tuff unit [m ²]	constant 2.2e-13	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the fractures in this layer. An estimated mean value is used, based on information documented in Bechtel SAIC Company, LLC (2003b).
UZFT	FracturePermeability_UCF_ [m ²]	K Permeability in fractures of the Upper Crater Flat tuff unit [m ²]	constant 2.5e-14	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the fractures in this layer. An estimated mean value is used, based on information documented in Bechtel SAIC Company, LLC (2003b).
UZFT	FracturePermeability_BFw_ [m ²]	K Permeability in fractures of the Bullfrog welded tuff unit [m ²]	constant 4.3e-13	This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the fractures in this layer. An estimated mean value is used, based on information documented in Bechtel SAIC Company, LLC (2003b).
UZFT	FracturePermeability_UFZ_ [m ²]	K Permeability in fractures of the Unsaturated Fault Zone unit [m ²]	constant 1.0e-12	Hypothetical unit to model transport through a fault zone. This parameter is used to calculate the saturated hydraulic conductivity, K_{sat} , of the fractures in this layer. An estimated mean value is used, generalized from information in Bechtel SAIC Company, LLC (2003b).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FracturePorosity_TSw_	ϕ Porosity associated with fractures for the Topopah Spring welded tuff unit [unitless]	constant 0.03	Used to calculate groundwater velocity in fractures in this layer. Best estimate for mean value, based on estimated mean values from DOE for drift-scale model in Bechtel SAIC Company, LLC (2004d).
UZFT	FracturePorosity_CHnv	ϕ Porosity associated with fractures for the Calico Hills nonwelded vitric tuff unit [unitless]	constant 0.003	Used to calculate groundwater velocity in fractures in this layer. Best estimate for mean value, based on estimated mean values from DOE for drift-scale model in Bechtel SAIC Company, LLC (2004d).
UZFT	FracturePorosity_CHnz	ϕ Porosity associated with fractures for the Calico Hills nonwelded zeolitic tuff unit [unitless]	constant 0.002	Used to calculate groundwater velocity in fractures in this layer. Best estimate for mean value, based on estimated mean values from DOE for drift-scale model in Bechtel SAIC Company, LLC (2004d).
UZFT	FracturePorosity_PPw_	ϕ Porosity associated with fractures for the Prow Pass welded tuff unit [unitless]	constant 0.003	Used to calculate groundwater velocity in fractures in this layer. Best estimate for mean value, based on estimated mean values from DOE for drift-scale model in Bechtel SAIC Company, LLC (2004d).
UZFT	FracturePorosity_UCF_	ϕ Porosity associated with fractures for the Upper Crater Flat tuff unit [unitless]	constant 0.001	Used to calculate groundwater velocity in fractures in this layer. Best estimate for mean value, based on estimated mean values from DOE for drift-scale model in Bechtel SAIC Company, LLC (2004d).
UZFT	FracturePorosity_BFw_	ϕ Porosity associated with fractures for the Bullfrog welded tuff unit [unitless]	constant 0.003	Used to calculate groundwater velocity in fractures in this layer. Best estimate for mean value, based on estimated mean values from DOE for drift-scale model in Bechtel SAIC Company, LLC (2004d).
UZFT	FracturePorosity_UFZ_	ϕ Porosity associated with fractures for the Unsaturated Fault Zone unit [unitless]	constant 0.006	Hypothetical unit to model transport through a fault zone. Used to calculate groundwater velocity in fractures in this layer. Values and distribution generalized from information in Bechtel SAIC Company, LLC (2004d).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureBeta_TSw_ FractureBeta_CHnv FractureBeta_CHnz FractureBeta_PPw_ FractureBeta_UCF_ FractureBeta_BFw_ FractureBeta_UFZ_	β Fracture van Genuchten beta parameter for each of the hydrostratigraphic units [unitless]	constant 2.7	This parameter is used to calculate the relative hydraulic conductivity of this layer for a range of water saturations under fracture flow conditions. Selected value is closely linked with related parameters to yield a consistent representation of observations, using data from Bechtel SAIC Company, LLC (2003b, 2001b). The same value is assigned for each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	TSw_Thickness_1SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 1 [m]	constant 53.1	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHnvThickness_1SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 1 [m]	usersupplieddiscrete 2 0, 0.5 4, 0.5	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_1SubArea [m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 1 [m]	constant 108.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_1SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 1 [m]	constant 43.1	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	UCF_Thickness_1SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 1 [m]	constant 44.8	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_1SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 1 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_1SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 1 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_2SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 2 [m]	constant 72.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHInvThickness_2SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 2 [m]	usersupplieddiscrete 2 0, 0.5 5, 0.5	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_2Sub Area[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 2 [m]	constant 125.7	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_2SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 2 [m]	constant 37.2	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_2SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 2 [m]	constant 15.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	BFw_Thickness_2SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 2 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_2SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 2 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_3SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 3 [m]	constant 111.4	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	ChnvThickness_3SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 3 [m]	usersupplieddiscrete 2 0, 0.8 7, 0.2	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_3Sub Area[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 3 [m]	constant 157.4	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_3SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 3 [m]	constant 10.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_3SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 3 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_3SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 3 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	UFZ_Thickness_3SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 3 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_4SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 4 [m]	constant 111.4	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHnvThickness_4SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 4 [m]	usersupplieddiscrete 4 0, 0.2 3.5, 0.3 5.5, 0.4 8.3, 0.1	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_4Sub Area[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 4 [m]	constant 157.4	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_4SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 4 [m]	constant 10.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_4SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 4 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_4SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 4 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	UFZ_Thickness_4SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 4 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_5SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 5 [m]	constant 111.4	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHnvThickness_5SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 5 [m]	triangular 4, 7, 10	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_5Sub Area[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 5 [m]	constant 157.4	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_5SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 5 [m]	constant 10.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_5SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 5 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_5SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 5 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_5SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 5 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	TSw_Thickness_6SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 6 [m]	constant 68.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHnvThickness_6SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 6 [m]	uniform 49, 60	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_6Sub Area[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 6 [m]	constant 89.2	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_6SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 6 [m]	constant 47.7	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_6SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 6 [m]	constant 52.2	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_6SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 6 [m]	constant 15.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_6SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 6 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_7SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 7 [m]	constant 112.6	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	CHnvThickness_7SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 7 [m]	triangular 51, 61, 68	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_7Sub Area[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 7 [m]	constant 101.2	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_7SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 7 [m]	constant 45.7	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_7SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 7 [m]	constant 37.1	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFW_Thickness_7SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 7 [m]	constant 3.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_7SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 7 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_8SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 8 [m]	constant 170.1	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHnvThickness_8SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 8 [m]	usersupplieddiscrete 2 2.5, 0.6 3.5, 0.4	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	CH_Total_Thickness_8SubArea[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 8 [m]	constant 119.3	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_8SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 8 [m]	constant 31.7	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_8SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 8 [m]	constant 3.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_8SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 8 [m]	constant 0.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_8SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 8 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_9SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 9 [m]	constant 140.4	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHInvThickness_9SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 9 [m]	usersupplieddiscrete 4 4, 0.6 20, 0.1 50, 0.1 70, 0.2	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	CH_Total_Thickness_9SubArea[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 9 [m]	constant 104.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	PPw_Thickness_9SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 9 [m]	constant 46.2	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_9SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 9. [m]	constant 33.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_9SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 9 [m]	constant 5.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_9SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 9 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	TSw_Thickness_10SubArea [m]	X Thickness of the Topopah Spring welded tuff unit in Subarea 10 [m]	constant 116.5	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	CHInvThickness_10SubArea [m]	X Thickness of the Calico Hills nonwelded vitric tuff unit in Subarea 10 [m]	triangular 51, 85, 93	The range of thicknesses is for Calico Hills nonwelded tuffs containing less than 15 wt% zeolites, based on the DOE Mineralogic Model (Bechtel SAIC Company, LLC, 2002).
UZFT	CH_Total_Thickness_10SubArea[m]	X Total thickness (vitric and zeolitic units) of the Calico Hills nonwelded tuffs in Subarea 10 [m]	constant 97.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	PPw_Thickness_10SubArea [m]	X Thickness of the Prow Pass welded tuff unit in Subarea 10 [m]	constant 57.5	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UCF_Thickness_10SubArea [m]	X Thickness of the Upper Crater Flat unit in Subarea 10 [m]	constant 58.3	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	BFw_Thickness_10SubArea [m]	X Thickness of the Bullfrog welded tuff unit in Subarea 10 [m]	constant 15.0	Thickness is averaged from five locations in the subarea, derived from Geologic Framework Model 3.1 (CRWMS M&O, 2000a).
UZFT	UFZ_Thickness_10SubArea [m]	X Thickness of the Unsaturated Fault Zone unit in Subarea 10 [m]	constant 0.0	Hypothetical fault zone. The thickness value is set to zero because ordinarily this unit is not used.
UZFT	UnsaturatedZoneMinimum VelocityChangeFactor [Fraction]	This parameter reduces the number of velocity changes that are used in the NEFMKS transport calculations [unitless]	constant 0.4	Equivalent to a program control switch to balance NEFMKS computing efficiency with a useful level of detail in modeled results. The previously accepted velocity will continue to be used unless the provisional new velocity changes by at least this fraction of the previously accepted velocity. The minimum timespan over which velocity does not change is 500 years. The specified constant is based on expert opinion and experience with TPA Version 5.1 simulations.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	SurfaceAreaFactor_TS_w_[] SurfaceAreaFactor_CHnv[] SurfaceAreaFactor_CHnz[] SurfaceAreaFactor_PPw_[] SurfaceAreaFactor_UCF_[] SurfaceAreaFactor_BFw_[] SurfaceAreaFactor_UFZ_[]	Ratio of colloid surface area to rock matrix surface area [unitless]	constant 590.0	The same value for this parameter has been assigned to each hydrostratigraphic layer. The parameter is fairly well constrained and was derived using site-specific data (Contardi, et al., 2001). Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
UZFT	FractureColloidRetardation Factor_TS_w_[] FractureColloidRetardation Factor_CHnv[] FractureColloidRetardation Factor_CHnz[] FractureColloidRetardation Factor_PPw_[] FractureColloidRetardation Factor_UCF_[] FractureColloidRetardation Factor_BFw_[] FractureColloidRetardation Factor_UFZ_[]	R_c Retardation factor for transport of colloids in fractures [unitless]	constant 1.0	Value assumes no retardation of colloids in fractures. The same value is assigned to each hydrostratigraphic layer. Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixColloidRetardation Factor_TS _w [] MatrixColloidRetardation Factor_CH _{nv} [] MatrixColloidRetardation Factor_CH _{nz} [] MatrixColloidRetardation Factor_PP _w [] MatrixColloidRetardation Factor_UCF>[] MatrixColloidRetardation Factor_BF _w [] MatrixColloidRetardation Factor_UFZ>[]	R_c Retardation factor for transport of colloids in the matrix [unitless]	usersuppliedpwiseCDF 20 1.0, 0.0 1.01, 0.01 1.5, 0.07 2.0, 0.12 4.0, 0.22 6.0, 0.29 8.0, 0.33 14.4, 0.4 22.14, 0.45 34.0, 0.5 56.15, 0.55 92.85, 0.6 153.5, 0.65 253.9, 0.0 419.7, 0.75 694.0, 0.8 1148.0, 0.85 1897.0, 0.9 3138.0, 0.95 5188.0, 1.0	Modified from DOE distribution (Bechtel SAIC Company, LLC, 2003c, Table 7). Linearly interpolated in log space between tabulated values and with DOE truncation removed. Presumes 1 percent are unretarded. The same distribution and values are assigned to each hydrostratigraphic layer. Layer Names: TS _w = Topopah Spring welded tuff CH _{nv} = Calico Hills vitric tuff CH _{nz} = Calico Hills zeolitic tuff PP _w = Prow Pass tuff UCF = Upper Crater Flat tuffs BF _w = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	FractureColloid Concentration_TSw_ [kg/m ³]	C _c Concentration of colloids in fractures [kg/m ³]	usersuppliedpwiseCDF	This parameter is used for fracture flow conditions to calculate a modified retardation factor to account for the effect of radionuclide transport by reversible attachment to colloids. The same distribution and values are assigned to each hydrostratigraphic layer. Based on data from Table 6-4 of Bechtel SAIC Company, LLC (2005); linearly interpolated in log space. Best available information on Yucca Mountain region groundwater colloid concentrations (Bechtel SAIC Company, LLC, 2005). Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff UFZ = Unsaturated Fault Zone (hypothetical unit)
	FractureColloid Concentration_CHnv[kg/m ³]		16	
	FractureColloid Concentration_CHnz[kg/m ³]		1.0e-6, 0.0	
	FractureColloid Concentration_PPw_ [kg/m ³]		2.51e-6, 0.1	
	FractureColloid Concentration_UCF_ [kg/m ³]		6.31e-6, 0.2	
	FractureColloid Concentration_BFw_ [kg/m ³]		1.58e-5, 0.3	
	FractureColloid Concentration_UFZ_ [kg/m ³]		3.98e-5, 0.4	
			1.0e-4, 0.5	
			2.51e-4, 0.6	
			6.31e-4, 0.7	
			1.0e-3, 0.75	
			2.15e-3, 0.8	
			4.64e-3, 0.85	
			1.0e-2, 0.9	
			2.24e-2, 0.94	
			5.0e-2, 0.98	
			0.1, 0.99	
			0.2, 1.0	

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
UZFT	MatrixColloidConcentration_ TSw_[kg/m3] MatrixColloidConcentration_ Chnv[kg/m3] MatrixColloidConcentration_ CHnz[kg/m3] MatrixColloidConcentration_ PPw_[kg/m3] MatrixColloidConcentration_ UCF_[kg/m3] MatrixColloidConcentration_ BFw_[kg/m3]	C_c Concentration of colloids in the rock matrix [kg/m ³]	usersuppliedpwiseCDF 16 1.0e-6, 0.0 2.51e-6, 0.1 6.31e-6, 0.2 1.58e-5, 0.3 3.98e-5, 0.4 1.0e-4, 0.5 2.51e-4, 0.6 6.31e-4, 0.7 1.0e-3, 0.75 2.15e-3, 0.8 4.64e-3, 0.85 1.0e-2, 0.9 2.24e-2, 0.94 5.0e-2, 0.98 0.1, 0.99 0.2, 1.0	This parameter is used for matrix flow conditions to calculate a modified retardation factor to account for the effect of radionuclide transport by reversible attachment to colloids. The same distribution and values are assigned to each of the listed hydrostratigraphic layers. Based on data from Table 6-4 of Bechtel SAIC Company, LLC (2005); linearly interpolated in log space. Best available information on Yucca Mountain region groundwater colloid concentrations (Bechtel SAIC Company, LLC, 2005). Layer Names: TSw = Topopah Spring welded tuff CHnv = Calico Hills vitric tuff CHnz = Calico Hills zeolitic tuff PPw = Prow Pass tuff UCF = Upper Crater Flat tuffs BFw = Bullfrog welded tuff
UZFT	MatrixColloidConcentration_ UFZ_[kg/m3]	C_c Concentration of colloids in the rock matrix of the hypothetical Unsaturated Fault Zone [kg/m ³]	constant 0.0	This parameter is used for matrix flow conditions to calculate a modified retardation factor to account for the effect of radionuclide transport by reversible attachment to colloids. In the hypothetical fault zone, it is assumed there are no colloids in the matrix for this layer.
UZFT	UZInitialCourantNumber[]	Ratio of a timestep to a cell residence time; refers to the portion of a cell that a solute will traverse by advection in one timestep [unitless]	constant 0.15	Used in NEFMKS calculations to improve accuracy and decrease numerical dispersion. Selected value is based on expert opinion and experiences with TPA Version 5.1 simulations.

Table 11-1. Reference Data for Parameters of tpa.inp Used by UZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Correlated Parameters	Independent Variable LogCD2PartialPressure_All UZ_SZLayers[atm] Dependent Variable ph_allUZ_SZLayers [standardUtility]	Correlation between CO ₂ partial pressure and pH of water in all unsaturated and saturated zone units	correlateinputs -0.95	Correlation for pH and PCO ₂ derived from analysis of geochemical data (104 sample points) specific to the Yucca Mountain region. Data are from Bechtel SAIC Company, LLC (2004b) and Bertetti, et al. (2004). The development of the correlations is discussed in McMurry and Beertetti (2005).

Table 11-2. Guide to Input Parameters Used by UZFT		
Type	Parameter Name	Attributes
User Option Flags	UZVelocity	0 = use average velocities 1 = use time-dependent velocities
	f UZFractureForceFactorForKdToRd	0 = no actinide sorption in fractures 1 = actinide sorption allowed in fractures
General Parameters for NEFMKS Calculations	UZInitialCourantNumber[]	
	UnsaturatedZoneMinimumVelocityChangeFactor [Fraction]	
	MatrixLongitudinalDispersivity[FractionOfLayer]	
	FractureLongitudinalDispersivity[FractionOfLayer]	
Subarea Dimensions and Layer Thicknesses	A InletArea_#SubArea[m ²]	Values defined for each subarea (#)
	x UNIT_Thickness_#SubArea[m]	Values defined for each layer (UNIT) and subarea (#)
Hydrologic Layer Properties	K MatrixPermeability_UNIT[m ²]	Values defined for each layer (UNIT)
	ϕ MatrixPorosity_UNIT	
	β MatrixBeta_UNIT	
	K FracturePermeability_UNIT[m ²]	
	ϕ FracturePorosity_UNIT	
	β FractureBeta_UNIT	
Sorption-Related Layer Properties	K_D MatrixKD_UNIT_RN[m ³ /kg]	Values defined for each radionuclide (RN) and layer (UNIT)
	R_D FractureRD_UNIT_RN	
	ρ_g MatrixGrainDensity_UNIT[kg/m ³]	Values defined for each layer (UNIT)
	r MatrixPoreRadius_UNIT[m]	
	b FractureAperture_UNIT[m]	

Table 11-2. Guide to Input Parameters Used by UZFT (continued)		
Type	Parameter Name	Attributes
Colloid-Associated Transport Layer Properties	PermanentLossColloidFilterFactor_ <i>UNIT</i>]	Values defined for each layer (<i>UNIT</i>)
	R_C FractureColloidRetardationFactor_ <i>UNIT</i>]	
	R_C MatrixColloidRetardationFactor_ <i>UNIT</i>]	
	C_C FractureColloidConcentration_ <i>UNIT</i> [kg/m ³]	
	C_C MatrixColloidConcentration_ <i>UNIT</i> [kg/m ³]	
	SurfaceAreaFactor_ <i>UNIT</i>]	
Water Chemistry Properties	pH_AllUZ_SZLayers[StandardUnits]	Same value is used by UZFT and SZFT; sampled from values in <i>tpa_include.inp</i>
	LogCO2PartialPressure_AllUZ_SZLayers[atm]	Same value is used by UZFT and SZFT; sampled from values in <i>tpa_include.inp</i>

11.5 Auxiliary Input Data and External Process Models

As discussed in Section 11.3.3.1, *coefkdeq.dat* is an auxiliary input data file that contains polynomial coefficients for Eq. (11-7) and valid pH ranges for discrete PCO₂ concentrations. These data define the surface response functions for actinide K_A values.

The unsaturated zone transport calculations are performed by NEFMKS (Olague, et al., 1991), which uses a series of one-dimensional transport paths (legs) that are defined by their length (i.e., layer thickness), velocity, porosity, dispersion length, and retardation factors. NEFMKS simulates advection and hydrodynamic dispersion of radionuclides using a distributed velocity method, which is similar to a particle-tracking approach where discrete particles are used to simulate contaminant movement. The executable file and source code are provided in the */codes* subfolder.

11.6 Intermediate Outputs and Information Passed to Other Modules

Table 11-3 lists and describes the intermediate output files that are created during execution of UZFT. The input and output files NEFMKS uses for unsaturated zone transport calculations are overwritten each time a subarea calculation is performed in UZFT. The NEFMKS input and output files also are overwritten during execution of SZFT for saturated zone transport calculations (Chapter 12). To preserve a record of NEFMKS input and output files for the unsaturated zone, UZFT saves a copy of each with the root name *nefiuz*, as indicated in Table 11-3.

Table 11-3. Intermediate Output Files Created During Execution of UZFT	
Output File	Contents
<i>cumrel.res</i>	UZFT contributes to this primary output file (Chapter 19), which reports cumulative releases over the simulation period from the engineered barrier system, unsaturated zone, and saturated zone. The results are summed over all subareas as quantity of releases (C_i) for each radionuclide and are reported for every realization in the simulation.
<i>cumrel_c.res</i>	UZFT contributes to this primary output file (Chapter 19), which reports cumulative releases over the compliance period from the engineered barrier system, unsaturated zone, and saturated zone. The results are summed as quantity of releases (C_i) for each radionuclide over all subareas and are reported for every realization in the simulation.
<i>gwtuzsz.res</i>	For each subarea and each realization, this file provides the average groundwater travel times for the unsaturated zone and saturated zone. It also provides the combined travel time for both zones. The file is described further in Chapter 19.
<i>nefiuz.inp</i>	This is a copy of <i>nefi.inp</i> , the main input file for NEFMKS for unsaturated zone transport calculations. It defines unsaturated zone flow path and transport characteristics, including (i) number of NEFMKS legs and leg lengths, (ii) calculated dispersivity for each leg, (iii) decay chain attributes and (iv) colloid-adjusted retardation factors (R_D) for each transport leg. This file is overwritten each time a subarea calculation is performed. At the end of a simulation, <i>nefiuz.inp</i> will contain the input information for the unsaturated zone transport calculation for the last subarea of the last realization.
<i>sotnef.dat</i> <i>nefiuz.src</i>	The file <i>sotnef.dat</i> is written by UZFT as an input file for NEFMKS transport calculations. The file provides NEFMKS with the time-dependent source term (radionuclide releases) data from EBSREL, after adjusting the source term to account for (i) flux splitting, if there is a bypass fraction at that timestep and (ii) the filtration of colloids in the unsaturated zone rock matrix (i.e., less of J-species). UZFT saves a copy of <i>sotnef.dat</i> as <i>nefiuz.src</i> , which is a more informative file name. Both files are overwritten each time a subarea calculation is performed by UZFT. In addition, <i>sotnef.dat</i> is overwritten by SZFT during saturated zone transport calculations (Chapter 12). At the end of a simulation, <i>nefiuz.src</i> will reflect the input source term information for the unsaturated zone transport calculation for the last subarea of the last realization, and <i>sotnef.dat</i> will reflect the corresponding saturated zone transport calculation for that subarea and realization.
<i>nefiuz.vel</i>	This is a copy of <i>nefi.vel</i> , an input file for NEFMKS. It provides the unsaturated zone time-varying water velocities that were developed for NEFMKS using hydrologic parameters and selection criteria specified in <i>tpa.inp</i> and the time history of deep percolation determined in UZFLOW. Velocities in <i>nefiuz.vel</i> are reported in feet per year [1 ft = 0.305 m]. If the flag UZVelocity[0 or 1] in <i>tpa.inp</i> is set to 0 (i.e., constant velocities), the time-varying velocities are not used in NEFMKS, but the values are still listed in <i>nefiuz.vel</i> . This file is overwritten each time a subarea calculation is performed. At the end of a simulation, <i>nefiuz.vel</i> will contain the input velocity for the unsaturated zone transport calculation for the last subarea of the last realization.
<i>nefiuz.dis</i>	This is a copy of <i>nefi.dis</i> , an output file that provides a time history of radionuclide discharge from the unsaturated zone during the simulation period for each radionuclide decay chain specified in <i>tpa.inp</i> , as calculated by NEFMKS. This file is overwritten each time a subarea calculation is performed. At end of a simulation, <i>nefiuz.dis</i> will contain the radionuclide releases for the last unsaturated zone subarea calculated by NEFMKS in the last realization. Note that if UZFT applies flux splitting in the calculations for this subarea, the radionuclide releases reported in <i>nefiuz.dis</i> will include only the fraction of the flow that was used in the NEFMKS transport calculations. However, a time history for the combined (matrix fraction plus bypass fraction) unsaturated zone radionuclide releases is provided in the intermediate output file <i>nefiisz.src</i> (Chapter 10).

Table 11-3. Intermediate Output Files Created During Execution of UZFT (continued)	
Output File	Contents
<i>nefiuz.out</i>	This is a copy of <i>nefi.out</i> output file that contains a summary of NEFMKS input and output, including the average or the time-dependent velocities that are passed to NEFMKS depending on which value is specified in <i>tpa.inp</i> for the parameter UZVelocity[0=average,1=time-dependent]. The file is overwritten each time a subarea calculation is performed. At the end of a simulation, <i>nefiuz.out</i> will contain the output for the unsaturated transport calculation for the last subarea of the last realization.
<i>nefi.rel</i>	This file reports cumulative releases from the unsaturated zone for each radionuclide over the simulation period. It is used to develop the primary output file <i>cumrel.res</i> , which provides the total radionuclide releases in the engineered barrier system, unsaturated zone, and saturated zone for all subareas in a simulation. The <i>nefi.rel</i> file is overwritten each time a subarea calculation is performed in UZFT. The file also is overwritten when transport calculations are executed in SZFT (Chapter 12), so the last-saved copy of <i>nefi.rel</i> typically does not contain information about the unsaturated zone.
<i>uz_kdrd.out</i>	For every realization in a simulation, this file shows the matrix and fracture sorption coefficient (K_D) values calculated by UZFT for six actinides (americium, neptunium, plutonium, thorium, uranium and curium) for every hydrostratigraphic layer in the unsaturated zone. It also shows the calculated fracture retardation factors (R_D) for the same actinides and lists the sampled parameter values from <i>tpa.inp</i> used in K_D and R_D calculations. The calculated values in <i>uz_kdrd.out</i> are not adjusted for the effects of sorption to colloids. Results are shown only for the first subarea processed in each realization.
<i>uz_revers.out</i>	This file reports the adjusted retardation factors (R_D^{eff}) for all radionuclides after corrections to account for effects of reversible sorption to colloids. For each radionuclide, values are reported for each subarea in each realization, but the values are calculated only for the specific hydrostratigraphic layers that were used as transport legs in NEFMKS.

In addition to the files listed in Table 11-3, the user can specify that data passed to and from UZFT is saved separately for specific realizations. This function is implemented in two steps in the *tpa.inp* input block titled <<Output Printer Options>>. First, the user sets the output mode parameter OutputMode(0=None,1=All,2=UserDefined) to a value of 1 or 2. When set to 1, optional output files will be saved for all realizations in a simulation; when set to 2, the files will be saved for realizations starting from the one specified by the *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by the parameter UserDefinedUpperRealizationAppended. Second, from a numbered list in the <<Output Printer Options>> block, the user specifies a value for the *tpa.inp* parameter SelectAppendFiles that will generate the optional output files of interest.

If the parameter SelectAppendFiles remains set at its reference value of 0, note that setting the parameter OutputMode(0=None,1=All,2=UserDefined) to a value of 1 or 2 will cause numerous optional output files to be saved for many modules besides UZFT. Some of these files can be very large and can quickly fill up available memory if all intermediate outputs are specified for all realizations. If only the UZFT optional outputs are desired, it is important to set the SelectAppendFiles parameter in the <<Output Printer Options>> appropriately. The choices that apply specifically to UZFT are Option 8, which produces *uzft.rlt* and *uzft.ech*, and Option 16, which includes the UZFT optional output file *nefiuz.cum*. The contents of these files are described in Table 11-4.

Table 11-4. Optional Intermediate Output Files Created During Execution of UZFT	
Output File	Description
<i>uzft.rlt</i>	This optional output file gives the radionuclide release rate from the unsaturated zone, in curies per year, for each radionuclide, at each timestep, in each subarea, for each specified realization.
<i>uzft.ech</i>	This optional output file shows (i) the volumetric flow rate to the unsaturated zone, in cubic meters per year, and (ii) the radionuclide release rates from the potential repository, in curies per year, that were provided as input to UZFT at each timestep and for each subarea in each realization.
<i>nefiuz.cum</i>	This optional output file reproduces the contents of every <i>nefiuz.inp</i> file generated during a simulation (i.e., <i>nefiuz.inp</i> for each subarea in each realization).

11.7 Techniques for Understanding Module Performance

Although there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of the flow and transport processes modeled by UZFT. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques (e.g., Mohanty, et al., 2004) may be useful to understand their effects on system-level performance.

In addition, “pinch-point” techniques, where output or intermediate results produced by UZFT can be understood in combination with output or intermediate results from other modules (e.g., EBSREL and SZFT), may help to evaluate subsystem processes. A useful intermediate results file for these comparisons is *nefiuz.out*, which contains a summary of all NEFMKS input and output for the unsaturated transport calculation. This file is detailed (many columns of data) and shows only the calculations for the last subarea, but it allows a user to compare starting conditions (radionuclide release rates from EBSREL) with the end results of the NEFMKS unsaturated zone transport calculations (radionuclide release rates from NEFMKS to SZFT). Note that in simulations where flux splitting occurs in UZFT, the NEFMKS transport calculations do not include the radionuclides in the bypass flow fraction, so the releases reported by *nefiuz.out* will be less than the total releases from the unsaturated zone to the saturated zone. However, the time history of the total (combined matrix fraction and bypass fraction) radionuclide releases from UZFT to SZFT is provided by *nefiisz.src* (Chapter 12).

The importance of individual parameters with respect to particular subsystem processes can be examined by repetitively varying an input parameter and analyzing results from various output and intermediate result files. A single parameter importance analysis may be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, single parameter importance analyses may be performed by repetitively specifying smaller ranges within the parameter’s original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges; the user should exercise care in interpreting results from simulations in which input data are altered beyond their intended ranges.

Key input parameters specified in *tpa.inp* that may significantly influence UZFT flow and transport results include CHnvThickness_#SubArea[m], which provides the thickness of the Calico Hills vitric unit, an important layer for matrix flow conditions in UZFT; MatrixPermeability_UNIT[m²], which for each hydrostratigraphic layer affects flow velocities and the selection of transport legs for NEFMKS; and the parameter PermanentLossColloidFilterFactor_UNIT[], which affects the modeled proportion of J-species radionuclides that are permanently removed from transport by filtration in the unsaturated zone.

Variations in the parameters that describe groundwater pH and dissolved CO₂ concentrations, pH_AllUZ_SZLayers[StandardUnits] and LogCO2PartialPressure_AllUZ_SZLayers[atm], are important in terms of their influence on radionuclide release rates from the unsaturated zone because the retardation factors calculated for actinides from K_A values are correlated with these parameters. In adjusting sorption properties, the user should be aware that the distributions in *tpa_include.inp* for pH_AllUZ_SZLayers[StandardUnits] and LogCO2PartialPressure_AllUZ_SZLayers[atm] are carefully tailored to site data, and effective ranges within *coefkdeq.dat* are optimized to this data. Therefore, modifying pH or PCO₂ distributions or their correlation may produce unintended results in calculated K_A values. In addition, because the pH and PCO₂ parameters are correlated, a TPA Version 5.1 run must specify an adequate number of realizations to actuate the correlation feature. If the correlation feature is not invoked, TPA Version 5.1 may produce multiple unintended K_A values of 0, resulting in no sorption of actinides.

Adjusting parameter values in *tpa.inp* allows the user to examine the effect of including or deleting certain processes from the model. Examples of these approaches include the following:

- To minimize the effects of flow and transport in the unsaturated zone, use the *tpa.inp* parameters UNIT_Thickness_#SubArea[m] to set the thickness of the Calico Hills nonwelded vitric layer to zero and to set the thickness of the other layers in a subarea to small values to minimize travel time in the unsaturated zone. This will cause most radionuclides to bypass the unsaturated zone without significant retardation.
- To bypass all flow and transport in the unsaturated zone, set the thickness to zero for all hydrostratigraphic layers in all subareas, as specified by the *tpa.inp* parameter UNIT_Thickness_#SubArea[m]. NEFMKS is not invoked, and radionuclide releases from EBSREL are provided directly to SZFT.
- If the hydrostratigraphic unit Unsaturated Fault Zone, which represents a fast flow pathway from the potential repository to the water table, is to be used to evaluate alternative flow and transport pathways in a simulation, this layer must replace all the other hydrostratigraphic layers in a particular subarea. In such a case, the fault zone thickness as specified by the *tpa.inp* parameter UFZ_Thickness_#SubArea[m] for the subarea of interest can be changed from its reference case value of zero to a value equal to the total unsaturated zone thickness for that subarea. The thicknesses of all the other layers for the subarea then should be set to zero.
- To examine the effect of sorption in fractures, a number of parameters in *tpa.inp* must be changed from their reference case values. The *tpa.inp* parameter specified as

UZFractureForceFactorForKdToRd must be set to 1.0, which enables fracture retardation factor (R_D) calculations for actinides in UZFT. For all other radionuclides, the user must provide separate R_D values for each of the *tpa.inp* parameters specified as FractureRD_UNIT_RN and FractureColloidRetardationFactor_UNIT_RN[] that are not equal to one. (An R_D of 1.0 corresponds to no retardation by sorption in fractures.) These are the minimum actions needed to model sorption in fractures in UZFT, but the modeled results must be interpreted carefully to ensure that the intended option was implemented for each realization. For example, although many of the hydrostratigraphic layers are assigned fracture flow properties, they also are likely to have short (i.e., less than the 20-year minimum) average groundwater travel times, meaning that these fracture-flow layers are not included in the NEFMKS flow and transport calculations. If there are no layers with fracture flow properties in the NEFMKS simplified flow model, no sorption in fractures for that subarea would be modeled even if the user had implemented the fracture sorption option. Another complication would arise if the NEFMKS input file included two or more hydrostratigraphic layers in which at least one layer had fracture flow properties, but the percolation flux and radionuclide releases that were provided to NEFMKS as input values had undergone flux splitting by UZFT into a matrix fraction and a bypass fraction. In this case, the NEFMKS transport modeling would include fracture sorption effects, but only for the portion of the flux that was allowed to pass through the matrix layer (i.e., the matrix fraction of the flux splitting). The bypass fraction, which is diverted directly to the base of the unsaturated zone, would not be affected by sorption modeling, regardless of whether fracture sorption was implemented.

- To remove the effect of reversible sorption of aqueous (dissolved) radionuclides in the matrix, all of the relevant K_D values for the non-actinides must be reset to values of zero for the parameters specified in *tpa.inp* as MatrixKD_UNIT_RN[m³/kg]. Because mean values (as constants) have been specified as the reference case K_D values in *tpa.inp* for these radionuclides, a user also may choose to perform sensitivity tests to examine the effects of a distribution range or extreme values for these K_D values. However, any changes to the parameter values should be consistent with layer properties (i.e., changes should reflect the mineralogy of each hydrostratigraphic unit). For the actinides, matrix retardation factors (R_D) are calculated based on the sampled pH and PCO₂ values, the K_A values determined from *coefkdeq.dat*, and the calculated specific surface area for each hydrostratigraphic unit. There is no direct way to turn off matrix sorption for the actinides by changing K_D or R_D values.
- To examine the effects of reversible sorption associated with colloids in the matrix, the results of a normal realization (e.g., a realization based on the mean value input file, *tpameans.out*) can be compared with an equivalent realization in which the concentration of naturally occurring colloids, specified in *tpa.inp* as the parameter MatrixColloidConcentration_UNIT[kg/m³], is set to zero in *tpa.inp* for all hydrostratigraphic layers.
- To remove the effect of sorption for J-species radionuclides, the parameters specified in *tpa.inp* as MatrixColloidRetardationFactor_UNIT can be set to one for all hydrostratigraphic layers.

- To examine the effect of no filtration of J-species radionuclides in the rock matrix, the colloid filtration factor specified in *tpa.inp* as the parameter PermanentLossColloidFiltrationFactor_UNIT[] can be set to zero for all hydrostratigraphic layers.

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12 SATURATED ZONE FLOW AND TRANSPORT (SZFT)

The Saturated Zone Flow and Transport module (SZFT)¹ describes radionuclide transport in the saturated zone beginning from the location where flow paths from the unsaturated zone reach the water table below the repository and ending at a user-specified distance downstream from the repository area. SZFT (i) receives time-dependent radionuclide mass flux input calculated by the Unsaturated Zone Flow and Transport module (UZFT)² (Chapter 11) and climate state information provided by the Climate and Infiltration module (UZFLOW)³ (Chapter 5); (ii) creates input files for the Network Flow and Transport in Time-Dependent Velocity Field standalone code (NEFMKS)⁴ [which is based on the models of the NEFTRAN II flow and transport code (Olague, et al., 1991)] that solves the advection-dispersion equation for transport of aqueous radionuclides and decay chains provided by UZFT; and (iii) provides time-dependent radionuclide mass arrival (Ci/yr) to calculate receptor doses from groundwater pathways, Dose Conversion Analysis for Groundwater module (DCAGW)⁵ (Chapter 17). SZFT is executed for each repository subarea specified in any TPA Version 5.1 realization for the reference input case.

12.1 Conceptual Model

12.1.1 Hydrogeology

In the TPA Version 5.1 conceptual model, potential releases of aqueous radionuclides from a potential repository located in the unsaturated zone at Yucca Mountain would migrate downward through the unsaturated zone and eventually reach the water table beneath the repository—the starting location for radionuclide transport simulation in the saturated zone. The saturated zone beneath the repository is located in variably welded, fractured volcanic tuff rock. Modeling of groundwater flow paths originating beneath Yucca Mountain (Winterle, 2003) suggests flow paths in the saturated zone are initially to the east-southeast before turning due south (see Figure 12-1). Flow paths are conceptualized as eventually transitioning from the fractured volcanic tuff aquifer system to an alluvial basin aquifer system. Groundwater withdrawals at the receptor location are assumed to occur from the alluvial aquifer system.

The volcanic tuffs are conceptualized as highly fractured with low rock matrix permeability. Flow occurs mainly in fracture networks, and water in the rock matrix pores is assumed to be

¹The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

²The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

³The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

⁴The Network Flow and Transport in Time-Dependent Velocity Fields standalone code is referenced frequently throughout this report. The abbreviation NEFMKS will be used.

⁵The Dose Conversion Analysis for Groundwater module is referenced frequently throughout this report. The abbreviation DCAGW will be used.

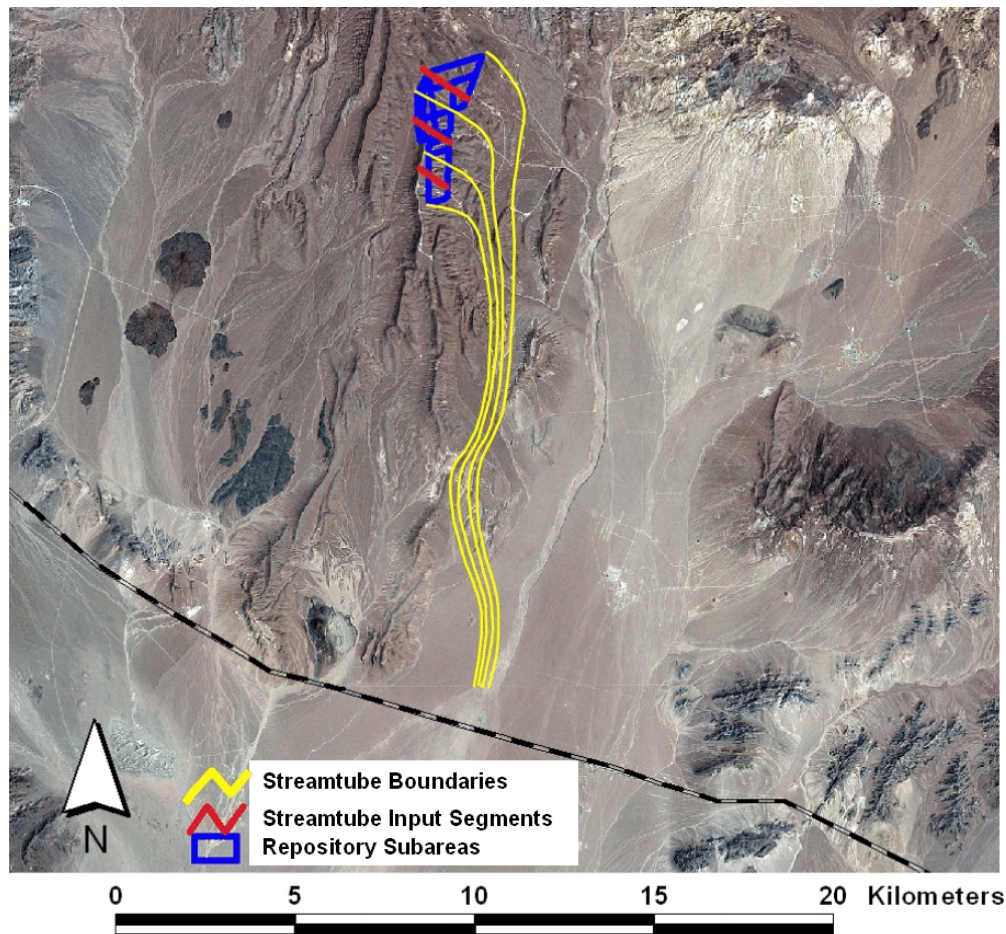


Figure 12-1. Map of the Yucca Mountain Region Depicting Approximate Locations of Streamtubes, Streamtube Input Segments, and Repository Subareas as Defined in SZFT of TPA Version 5.1

stagnant. Accordingly, flow in the volcanic aquifer is treated as a dual-porosity system in which radionuclides are transported in fracture networks but can migrate via diffusion into the rock matrix. Flow in the alluvial aquifer system is conceptualized as occurring in heterogeneous fine- to coarse-grained fluvial channel sediments and is treated as a single-porosity flow system. This conceptual model for differing flow conditions in the tuff and alluvial aquifer systems is consistent with the hydrogeologic description of the area by Luckey, et al. (1996) and the results of saturated zone testing (Bechtel SAIC Company, LLC, 2003a).

Because of the different flow properties of the volcanic tuff and alluvial aquifers, SZFT divides the total flow path into separate transport “legs” representing flow in the two different flow systems.

12.1.2 Groundwater Flow and Radionuclide Transport

In the conceptual model, radionuclides are transported through the unsaturated zone either as dissolved species or in association with colloids {i.e., small solid particles characteristically ranging in size from 10^{-9} to 10^{-6} m [1 m = 3.28 ft]}. SZFT considers colloids that originate in the natural environment (e.g., colloid-sized clay particles) or by degradation of the waste form or engineered barriers (e.g., colloidal iron oxyhydroxide corrosion products). Radionuclide transport processes considered in SZFT include (i) advective transport with longitudinal dispersion, (ii) reversible sorption of dissolved radionuclides to host rock, (iii) diffusion of dissolved radionuclides from the fractures to the matrix in the tuff aquifer, (iv) migration of radionuclides reversibly or irreversibly attached to colloids, and (v) radionuclide decay and ingrowth of progeny nuclides. The radionuclides included in SZFT are represented by a subset of 15 elements from the waste form inventory (Chapter 4, Section 4.6). The specific radionuclides considered in the transport abstraction are those that would be present in sufficient amounts and that would be sufficiently long lived and mobile in groundwater to be of interest in postclosure performance assessment calculations (McMurry and Bertetti, 2005).

Advective transport of radionuclides is a function of groundwater flux rates and effective porosity of the flow system. For a given flux, a smaller effective porosity will result in higher flow velocity. Spatial variations in flow velocity produce longitudinal dispersion that results in some contaminants traveling faster or slower than the mean flow velocity. Molecular-scale Fickian diffusion can also have the same result but is expected to be insignificant compared to macroscale dispersion over a transport distance of several kilometers.

Sorption of radionuclides to host rock and alluvial sediments can delay the migration of some aqueous-phase species. Elements such as iodine and technetium that form anions in aqueous solutions have little affinity for sorption to silicic rocks and sediments and generally will travel at the advective velocity in groundwater. Other elements such as the actinides (americium, neptunium, plutonium, thorium, uranium, and curium) have varying affinities for sorption, depending on geochemical conditions. Because of their relative importance to performance and the influence of groundwater chemistry—primarily pH and dissolved carbon dioxide concentration (PCO_2)—on their sorption behavior, these actinides are modeled in more detail than other elements. Dissolved species and colloids tracked as species may be retarded by sorption onto rock matrix or fractures.

Radionuclides are associated with colloids either by attachment to a colloid surface (reversible or irreversible sorption) or as an intrinsic part of the colloid itself. Examples of intrinsic association include (i) colloid-sized pieces of vitrified waste or spent fuel spalled from a waste form or (ii) a secondary precipitate of an oversaturated radionuclide-bearing phase such as thorium oxide (ThO_2). In the model, radionuclides that are strongly sorbed to a colloid (i.e., corrosion product colloids) and those that are an intrinsic part of a waste form colloid are considered to be irreversibly bound to the colloid. Only four elements—curium, thorium, americium, and plutonium—are assumed to bind irreversibly to colloids, and all such colloids are assumed to originate in the waste package. In contrast to irreversible attachment, reversible sorption onto colloids is conceptually equivalent to reversible sorption onto other solid phases (e.g., glass shards, clays, zeolites). Similarly, colloids themselves may be retarded by sorption to solid surfaces depending on the composition, size, and surface charge of the colloid.

12.2 Model Support and Assumptions

The conceptual model of groundwater flow paths in TPA Version 5.1 is based on the hydrogeologic site description provided by Luckey, et al. (1996). Results of modeling and additional data collection (e.g., Bechtel SAIC Company, LLC, 2003a,b) are generally consistent with that site description and provide additional information related to uncertainties in important hydrogeologic parameter inputs, such as effective porosity and groundwater flux, and the relative travel distances in tuff and alluvium. The reference case input values for groundwater flux in each of the three saturated zone streamtubes are based on modeling by Winterle (2003).

The approach of assuming linear, empirically determined equilibrium distribution coefficients to model sorption of radionuclides to mineral surfaces is a well documented and generally accepted approach for approximating the effects of sorption on delaying radionuclide transport in groundwater. The approach neglects effects such as slow sorption kinetics and geochemical heterogeneity along the flow path, and thus distribution coefficients and retardation coefficients need to be selected prudently and an appropriate range of uncertainty needs to be considered to ensure the assessment of radionuclide sorption in total system performance is reasonable. Bertetti, et al. (2004) and McMurry and Bertetti (2005) document the basis for radionuclide sorption parameters in TPA Version 5.1 in detail.

The following are some of the key general assumptions used in the TPA Version 5.1 abstraction of saturated zone flow and transport.

- Flow in the tuff and alluvial aquifer systems occurs in the direction of the horizontal hydraulic gradient (i.e., flow anisotropy is not explicitly included, but its potential effects are considered in uncertainty distributions for parameters that affect flow velocity and distance to the tuff–alluvium interface).
- Volcanic tuff layers can be treated as a single rock type in which flow occurs predominantly in fracture networks. This assumption ignores the potential that a significant component of matrix flow may occur in some volcanic tuff units.
- Climate change during the period of repository performance has no effect on the regional groundwater flow direction.
- The velocity field can be adequately modeled by dividing the region into three flow tubes whose lateral boundaries are defined by streamlines emanating from either edge of the repository.
- Radionuclides entering a flow tube are uniformly mixed across the width of the flow tube.
- The longitudinal dispersivity is related to the length of the transport path and assumes variations in velocity fields are Gaussian. Longitudinal macrodispersivity is generally assumed to increase with the scale of the contaminant plume until an asymptotic upper bound is attained (Gelhar, 1993). Consequently, the dispersion length is calculated as a fraction of the flow path length.
- Although temporal changes in the flow field caused by climatic change and variations in pumping rates may affect transport, SZFT assumes that a steady-state representation of

the streamtubes is sufficient (although the capability exists to update the velocity input to NEFMKS as a function of climate state).

- There is no explicit accounting for effects of lateral dispersion on vertical spreading of the plume in the streamtube approach. Vertical dispersion would likely reduce *in-situ* radionuclide concentrations or reduce the fraction of mass captured by the pumping well. Further, it is assumed for dose calculations (Chapter 17) that all radionuclide mass transported by groundwater will be captured by well pumping at the receptor location.
- The linear K_d approach used in SZFT assumes that the sorption process is reversible, has reached equilibrium, and is independent of variations in water chemistry or mineralogy. These assumptions may only be partially met in the saturated zone of Yucca Mountain (Chapman and McKinley, 1987) because sorption may vary in response to changes in groundwater chemistry, temperature, properties of the solid substrate on which sorption occurs, or concentration of the radionuclide. Groundwater and mineral substrates are assumed to maintain their present ranges of chemical and mineralogical compositions over time. In recognition of the uncertainty and variability associated with the K_d approach, performance assessment calculations typically sample K_d values from a range of values that are appropriate to sorption for the expected variation in conditions. For the important actinide elements, variations in water chemistry are included explicitly in the calculation of K_d for each realization. The linear approach also assumes that there are an unlimited number of sorption sites; this implicit assumption appears reasonable for the saturated zone near Yucca Mountain because solubility limits and dilution effects suggest that the concentrations of radionuclides and other species that may compete for sorption sites will be low relative to the large number of available mineral sorption sites.
- NEFMKS uses a first-order rate constant to simulate the effect of diffusive exchange of solutes between fractures and matrix. This approach assumes that solute concentrations within the nonflowing matrix domain reflect a well-mixed system (i.e., the effect of time-varying concentration gradients within the matrix is not considered). This assumption may not be valid in flow systems with rapid advective transport combined with slow diffusive exchange rates and large blocks of matrix between flowing intervals. In such cases, the result of this assumption can be that downstream solute concentrations are underestimated at early times and overestimated at late times (van Genuchten, 1985). To counter this effect, a partial penetration fraction parameter was added to allow the capability to limit the fraction of matrix available for penetration by diffusion (Section 12.3).
- For reversible colloid sorption, the time scale for attachment/detachment to colloids is assumed to be small compared to transport time (i.e., attachment kinetics are neglected). Also, equilibrium partitioning of the radionuclides is assumed to occur among three phases: aqueous, colloid bound, and sorbed to the host rock. These assumptions may not be valid if sorption is kinetically controlled and is slow. Relatively slow sorption of plutonium on inorganic colloids has been observed in several experiments (e.g., Lu, et al., 2000). However, based on available estimates of kinetic sorption rates (e.g., Painter, et al., 2002) and travel times in alluvium that generally are expected to exceed 100 years (e.g., Winterle, 2003), the colloid-bound plutonium in the

alluvial aquifer is in the fast reversible (equilibrium) range consistent with these assumptions.

- Colloid filtration is not considered for the saturated zone flow and transport abstraction. All colloids not filtered by the unsaturated zone are assumed to travel unfiltered through the saturated zone. This approach may overestimate colloid transport; however, the mechanics of colloid filtration over long transport distances presently are not well understood. Therefore, credit for colloid filtration in the saturated zone is not taken. The user may, however, evaluate the effects of additional colloid filtration in the saturated zone by simply increasing the colloid filtration factors for the unsaturated zone to account for total effective filtration. The abstraction does include retardation of irreversibly (and reversibly) sorbed colloid species to account for temporary attachments and detachments that may occur along the flow paths.

12.3 Implementation of Conceptual Model in TPA Version 5.1

SZFT is called once for each subarea in every realization for a reference case simulation. A key function of SZFT is to build the input files NEFMKS needs to simulate flow and transport in the volcanic tuff and alluvium aquifers. The general flow of information to and within SZFT is illustrated in Figure 12-2. To accomplish this task, SZFT provides the following types of calculation information to NEFMKS: (i) a time history of radionuclide mass entering the saturated zone, (ii) radionuclide and decay chain information, (iii) flow path characteristics, (iv) time-dependent flow velocity information, (v) radionuclide transport parameters for each radionuclide species, and (vi) matrix diffusion rates (volcanic tuff aquifer only).

12.3.1 Radionuclide Source Input

Time varying radionuclide source input is calculated by UZFT for each subarea and passed to SZFT. SZFT formats this data and writes it to *sotnef.dat*, which NEFMKS uses as an input file. SZFT copies *sotnef.dat* to *nefiisz.src*, which is not used but has a file name that is more intuitive relative to the information contained within it. Both *sotnef.dat* and *nefiisz.src* are overwritten each time SZFT is called; at the end of a TPA Version 5.1 run, these files will reflect the source term provided to SZFT for the last subarea of the last realization.

12.3.2 Flow Model for NEFMKS

12.3.2.1 Flow Path Characteristics

The characteristics of the one-dimensional streamtubes used in the NEFMKS calculations are specified in *strmtube.dat*. The northernmost and southernmost streamtube boundaries were selected to be tangential to the respective ends of the repository footprint. All water passing beneath the repository must flow through one or more of these streamtubes. For each subarea in a TPA Version 5.1 realization, SZFT calculates which of the streamtubes is closest to the centroid of the subarea based on the distance to the nearest inlet centerline defined in *strmtube.dat*.

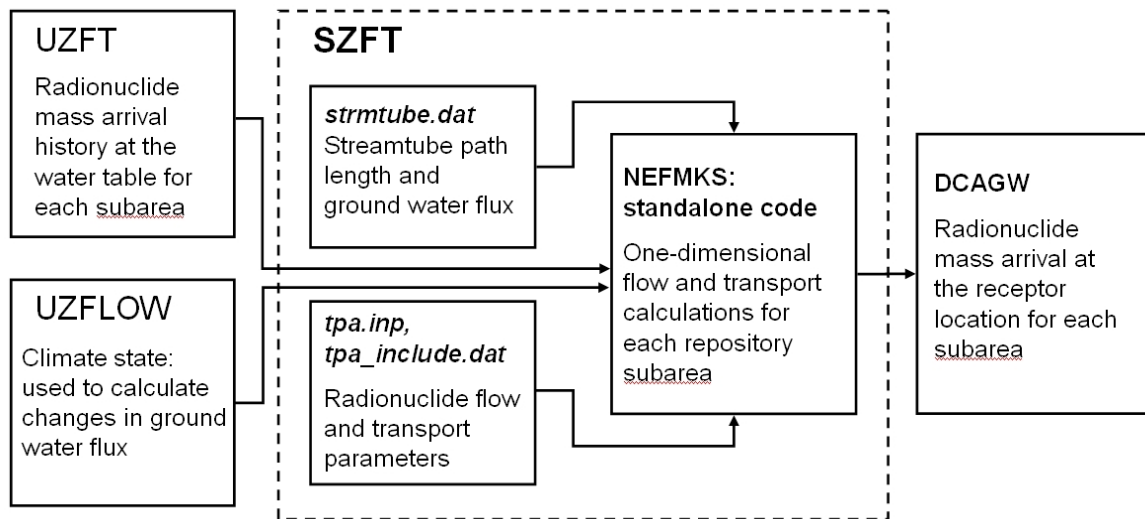


Figure 12-2. Information Flow Diagram for SZFT

Based on the information provided in *strmtube.dat*, SZFT divides each streamtube into three transport “legs” by default. Leg 1 is a mixing leg that represents the initial transport distance beneath the repository area where flow is assumed to occur in fractured tuff. Leg 2 represents flow in the volcanic tuff aquifer system from the downstream repository edge to the tuff–alluvium transition. Leg 3 represents flow in alluvium for the remainder of the total transport distance. The flow distance in Leg 1 will be fixed for each subarea in a realization, depending on the distance from the subarea centroid to the streamtube centerline. Although the total transport distance in each streamtube is fixed, the portions of the transport distance in the tuff and alluvium legs are treated as uncertain by sampling values of the *tpa.inp* input parameter DistanceToTuffAlluviumInterface[km]. This transport leg information is formatted by SZFT and supplied to *nefii.inp* for input to NEFMKS.

The user can split the tuff and alluvium transport legs into separate NEFMKS runs. The associated input parameter is SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes). To run the reference case with a single NEFMKS calculation, this parameter is set to 0. To run separate NEFMKS calculations for the tuff and alluvium legs, set to 1. Under certain combinations of parameter values, this mode can run faster as a result of separating fast and slow velocity zones into separate calculations. In most cases, however, the normal mode should be used, unless special conditions arise that cause problems with long run times for NEFMKS or the analyst wishes to separately evaluate the relative contributions of tuff and alluvium on saturated zone radionuclide transport.

12.3.2.2 Flow Velocity and Groundwater Travel Times

SZFT calculates groundwater velocity history during the simulation period and writes it to *nefii.vel* for input to NEFMKS. At each timestep and for each leg, time-dependent velocity, $v(t)$ [m/yr], is calculated by

$$v(t) = \frac{q_{in} a(t)}{W b_w \phi_{eff}} \quad (12-1)$$

where

- q_{in} — input streamtube flux representing the volume of water per year per meter of depth below the water table specified in *strmtube.dat* [m²/yr]
- $a(t)$ — velocity multiplier to allow increased flux as a function of climate state
- W — input streamtube width specified in *strmtube.dat* [m]
- b_w — input parameter, StreamTubeWidthMultiplier[], used to adjust calculated velocity to account for combined uncertainties related to streamtube dimensions and input fluxes [unitless]
- ϕ_{eff} — effective flow porosity of volcanic tuff (FracturePorosity_STFF) or alluvium (AlluviumMatrixPorosity_SAV) [unitless]

The parameter $a(t)$ allows for consideration of time-varying changes in velocity as a function of the climate state. This function is used if the SZFluxMultiplierAtGlacialMaximum[] input parameter is set to a value greater than 1.0. If the user specifies a value greater than 1.0, SZFT will calculate velocity at each timestep based on the time-dependent climate state specified in *climato2.dat* (Chapter 5). The streamtube input flux will be multiplied by the specified value when the maximum glacial climate state is reached and by linearly scaled values when the climate state is intermediate between initial climate and the glacial maximum. SZFT only writes an updated velocity value to *nefii.vel* if the fractional change in velocity from the previous timestep is greater than the value specified by the input parameter SaturatedZoneMinimumVelocityChangeFactor[Fraction].

SZFT will make other adjustments to the groundwater velocities specified for the tuff and alluvium transport legs if the computed total travel times for each leg are less than the values specified by the input parameters MinimumResidenceTime_STFF[yr] for the tuff leg and MinimumResidenceTime_SAV[yr] for the alluvium leg. This adjustment is made because the computational efficiency of NEFMKS is sensitive to the ratio of leg length to velocity. The reference data set for TPA Version 5.1 specifies minimum travel times of 10 years for the tuff leg and 100 years for the alluvium leg.

From the time-varying velocities, the time-varying groundwater travel times are determined for each hydrostratigraphic layer using

$$t_{gw}(t) = \frac{L}{v(t)} \quad (12-2)$$

where

- $t_{gw}(t)$ — time-varying groundwater travel time [yr] at time t
- L — streamtube length, tube_length [m] specified in *strmtube.dat*
- $v(t)$ — time-varying velocity for the transport leg [m/yr] at time t

The average groundwater travel time for each transport leg is determined as a weighted average of the time-varying groundwater travel times over the timeframe of interest. A simple trapezoidal integration of the groundwater travel time is used for the calculation. In addition, the average groundwater travel time is summed for all transport legs originating from each subarea to obtain the total groundwater travel time for the saturated zone. The total groundwater travel time for each subarea is written to *gwttuzsz.res* as an intermediate result.

Spatial variability in flow velocity between different repository regions is accounted by the use of separate streamtubes with different spatial dimensions and input fluxes. Within each streamtube, spatial variability in the velocity field is accounted by the use of a dispersion term in the one-dimensional advection-dispersion equation solved by NEFMKS (Olague, et al., 1991). NEFMKS calculates a longitudinal dispersion coefficient [m^2/yr] by multiplying the flow velocity by a dispersion length. SZFT calculates this dispersion length for each transport leg by multiplying the transport distance in each leg by the input parameters MixingZoneDispersionFraction for the initial mixing leg, DispersionFraction_STFF for the tuff leg, and DispersionFraction_SAV for the alluvium leg.

12.3.3 Radionuclide Transport Parameters

In TPA Version 5.1, radionuclides are transported through the saturated zone by advection and longitudinal dispersion, modified by reversible sorption onto stationary minerals and onto mobile, naturally occurring colloidal particles. Radionuclides are modeled as either dissolved species or irreversibly bound colloidal species. Different retardation factors are applied in SZFT to describe either species. Reversible colloids are incorporated through modification of the dissolved species' retardation factors. For irreversibly bound colloidal species, a fraction of the mass for specified radionuclides is assumed to be irreversibly associated with colloidal particles originating in the engineered barrier system (Chapter 10). The radionuclides associated with these colloids are modeled as unique species (J-species) and are transported through the saturated zone using properties of the colloidal particles, rather than the transport properties of the elements themselves.

12.3.3.1 Radionuclide Retardation Factors

Sorption values for all radionuclides in SZFT are also provided in the form of retardation factors (R_D)—unlike UZFT in which sorption values are provided as distribution or sorption coefficients (K_D). In porous media (e.g., in sediments or the porous matrix of a rock), the retardation factor can be calculated from the K_D and from the porosity and density of the host solid phase by the expression

$$R_D = 1 + \frac{\rho_g(1 - \phi_m)K_D}{\phi_m} \quad (12-3)$$

where

R_D — retardation factor, Immobilerd_STFF_RN⁶ or AlluviumMatrixRD_SAV_RN
[unitless]

⁶Where the term “__RN” appears in a formal *tpa.inp* parameter name in this chapter, it refers to a particular radioelement (i.e., radionuclide) as listed in Table 12-1 (Section 12.4).

- ρ_g — grain density of the solid phase, ImmobileGrainDensity_STFF[kg/m³] or AlluviumMatrixGrainDensity_SAV[kg/m³]
- ϕ_m — porosity of the solid phase, ImmobilePorosity_STFF or AlluviumTotalPorosity_SAV [unitless]
- K_D — distribution coefficient [m³/kg]

With the exception of the actinides (americium, neptunium, plutonium, thorium, uranium, and curium), R_D values are provided directly to SZFT by *tpa.inp*. Separate R_D values are entered for tuff fracture surfaces (FractureRD_STFF_RN), tuff rock matrix (ImmobileRd_STFF_RN), and saturated alluvium (AlluviumMatrixRD_SAV_RN). SZFT formats values of R_D for all radionuclides and supplies them to *nefii.inp* for use in NEFMKS.

An important difference between TPA Version 4.0 and TPA Version 5.1 is that for TPA Version 5.1, the sorption coefficients for the actinides americium, neptunium, plutonium, thorium, uranium, and curium are determined from sorption response surfaces that correlate K_D (and R_D) values with variations in groundwater chemistry (specifically pH and PCO₂). The sorption response surfaces were developed by applying surface complexation models to experimental data over a wide range of geochemical conditions to generate a set of effective surface area normalized distribution coefficients (K_A) (McMurry and Bertetti, 2005; Turner, et al., 2002), which are in turn converted to K_D and then R_D values using the specific surface area properties of the saturated fractured tuff and the saturated alluvium. Parameters describing the response surfaces that are used to obtain K_A values for the actinides are provided in *coefkdeq.dat*. This auxiliary input data file contains coefficients that define sets of curves representing the best fifth-order polynomial fits to the surface complexation model predictions of sorption at specific PCO₂ values according to the expression

$$\text{Log } K_A = a + b \text{ pH} + c \text{ pH}^2 + d \text{ pH}^3 + e \text{ pH}^4 + f \text{ pH}^5 \quad (12-4)$$

where a–f represent the coefficients. Because the pH and PCO₂ parameters are correlated and the polynomial coefficients are carefully tailored to specific and realistic ranges of pH and PCO₂, it is important to specify an adequate number of realizations to actuate the correlation feature within TPA Version 5.1. If the correlation feature is not invoked, the codes may produce unintended K_A values of zero. Within SZFT, K_A is related to K_D by the equation

$$K_D = K_A \text{ ESA} \quad (12-5)$$

where

- K_D — distribution coefficient [m³/kg]
- K_A — surface area normalized distribution coefficient [m³/m²]
- ESA — effective surface area

The effective surface area either is given as a measured property AlluviumMatrixSpecificSurfaceArea [m²/kg] (saturated alluvium) or it can be derived (saturated fractured tuff) from the geometric relationship (Arthur, 1996)

$$ESA = \frac{3\phi_m}{\rho_g(1 - \phi_m)r} \quad (12-6)$$

where

ESA	—	effective surface area [m ² /kg]
ρ_g	—	grain density of the saturated fractured tuff, ImmobileGrainDensity_STFF [kg/m ³]
ϕ_m	—	porosity of the saturated fractured tuff, ImmobilePorosity_STFF [unitless]
r	—	mean pore radius of the saturated fractured tuff, ImmobilePoreRadius_STFF [m]

SZFT then converts the calculated K_D value to an R_D value using Eq. (12-4) and supplies it to NEFMKS via *nefii.inp*.

The parameter SZFractureForceFactorForKdToRd must be set to a value of 1.0 to enable the fracture R_D calculations for the actinides. Actinide fracture R_D values are determined using the equation

$$R_D = 1 + \left(\frac{2K_A}{b} \right) f \quad (12-7)$$

where

R_D	—	retardation factor [unitless]
K_A	—	surface area normalized distribution coefficient [m ³ /m ²]
b	—	saturated tuff fracture aperture width, FractureAperture_STFF[m]
f	—	fracture force factor, SZFractureForceFactorforkdtoRd [unitless]

12.3.3.2 Colloid-Associated Transport

TPA Version 5.1 also incorporates explicit modeling of the transport of radionuclides that may be attached or associated with colloids present in the groundwater. The two types of colloids modeled by TPA Version 5.1 are irreversible and reversible colloids. Irreversible colloids are representative of colloids originating from the waste form or waste package corrosion products. Radionuclides associated with irreversible colloids are permanently attached to and remain with the colloids throughout the simulation. Irreversible colloids are defined as separate radionuclide species (J-species) and may be retarded in the saturated zone based on specified retardation factors for saturated zone layers {ColloidRetardationFactor_STFF[] and ColloidRetardationFactor_SAV_[]}.

Radionuclides associated with reversible colloids (natural system colloids present in the groundwater) may sorb and desorb from the colloids during the simulation. To account for radionuclide migration associated with reversible attachment to colloids, SZFT adjusts the

retardation factors for each species to include the effects of potentially enhanced transport of colloids. The retardation factor adjustment is a function of colloid concentration {ColloidConcentration_STFF[kg/m³] and ColloidConcentration_SAV_[kg/m³]} in each geologic layer and a dimensionless surface area factor {SurfaceAreaFactor_STFF[] and SurfaceAreaFactor_SAV[]}, which provides an adjustment for the much greater surface area of the colloids relative to the host rock in each layer. This colloid retardation factor adjustment is determined by first calculating a dimensionless colloid distribution coefficient (K_0) using the expression

$$K_0 = \frac{C_c F \phi_m (R_D - 1)}{\rho_g (1 - \phi)} \quad (12-8)$$

where

K_0	—	dimensionless colloid distribution coefficient [unitless]
ρ_g	—	grain density of the solid phase, ImmobileGrainDensity_STFF[kg/m ³] or AlluviumMatrixGrainDensity_SAV[kg/m ³]
ϕ_m	—	porosity of the solid phase, ImmobilePorosity_STFF or AlluviumTotalPorosity_SAV [unitless]
F	—	dimensionless factor accounting for surface area differences between solid phase and colloid, SurfaceAreaFactor_STFF[] or SurfaceAreaFactor_SAV[]
C_c	—	colloid concentration in groundwater, ColloidConcentration_STFF[kg/m ³] or ColloidConcentration_SAV_[kg/m ³]
R_D	—	retardation factor for the radionuclide

For the saturated tuff fractures and the saturated alluvium (mobile phases), the K_0 is then used to adjust the R_D for each radionuclide using the expression

$$R_D^{eff} = \frac{R_D + (K_0 R_c)}{(1 + K_0)} \quad (12-9)$$

where

R_D^{eff}	—	retardation factor adjusted for the effects of reversible colloids [unitless]
K_0	—	dimensionless colloid distribution coefficient [unitless]
R_c	—	retardation factor for colloids, ColloidRetardationFactor_STFF[] or ColloidRetardationFactor_SAV_[] [unitless]
R_D	—	retardation factor for the radionuclide [unitless]

While in saturated tuff matrix (immobile phase), the adjusted, effective R_D is calculated by

$$R_D^{eff} = \frac{R_D}{1 + K_0} \quad (12-10)$$

where

- R_D^{eff} — retardation factor adjusted for the effects of reversible colloids [unitless]
- K_0 — dimensionless colloid distribution coefficient [unitless]
- R_D — retardation factor for the radionuclide [unitless]

Although the effects of colloid-associated transport implemented in TPA Version 5.1 generally result in enhanced migration of radionuclides, especially those that are strongly sorbing, radionuclides with low R_D values may experience slower migration due to the effects of colloid-associated transport. Results of the changes to retardation factors due to the application of the reversible colloid transport model are reported in a generated output file, *sz_reverse.out*.

12.3.3.3 Matrix Diffusion

NEFMKS can account for the migration of dissolved contaminants from flowing pores and fractures into the immobile water within the rock matrix pores. The governing equation used in NEFMKS to account for the rate of change of concentration in the immobile phase is (Olague, et al., 1991)

$$\phi_m R_D \frac{\partial C_s(x,t)}{\partial t} = \beta [C_d(x,t) - C_s(x,t)] \quad (12-11)$$

where

- ϕ_m — immobile (stagnant) matrix porosity, ImmobilePorosity_STFF [unitless]
- R_D — retardation factor for diffusion in stagnant matrix region
ImmobileRd_STFF_RN [unitless]
- C_s — volume-averaged solute concentration in stagnant region [kg/m³]
- x — distance in direction of flow [m]
- t — time [yr]
- β — mass-transfer rate coefficient [1/yr], calculated
- C_d — dynamic (mobile) solute concentration [kg/m³]

This process is commonly referred to as matrix diffusion. The mass transfer rate coefficient, β [1/yr], defines the rate of exchange between the flowing fracture region and the stagnant matrix region as a linear function of the difference in solute concentration. The value of β is a function of several factors that may affect the diffusive exchange rate using the following formula

$$\beta = \frac{\phi_s D}{0.28 \left(\frac{f}{2n} \right)^2} \quad (12-12)$$

where

D	—	effective matrix diffusion coefficient, DiffusionRate_STFF [m ² /yr]
f	—	fraction of immobile porosity in which matrix diffusion occurs, ImmobilePorosityPenetrationFraction_STFF [unitless]
ϕ_s	—	effective immobile (stagnant) matrix porosity [unitless]
n	—	number of fractures per meter, FracturesPerMeter_STFF[1/m]
0.28	—	shape factor used for parallel planar matrix blocks (van Genuchten, 1985) [unitless]

Eq. (12-12) is based on a formula derived by van Genuchten (1985) for estimating first-order, mass-transfer coefficients according to rates of diffusion and flow system geometry. Because Eq. (12-11) is based on an implicit assumption that solute concentrations are uniformly distributed throughout the matrix region, the original formula of van Genuchten was modified to include the factor f to allow consideration of cases in which matrix blocks may not be fully permeated by diffusing solutes (e.g., if time scales for transport to the receptor location are short relative to the time scale for diffusion to the matrix block center). When values lower than 1.0 are used, the value of f also is used to scale the effective immobile porosity of tuff matrix to a lower value using the formula

$$\phi_s = f \phi_m \quad (12-13)$$

where

ϕ_m	—	volcanic tuff rock matrix porosity, ImmobilePorosity_STFF [unitless]

The penetration fraction is difficult to estimate because it is a nonlinear function of several variables, including matrix block size, advection velocity, and solute-specific diffusion rates. The van Genuchten (1985) approach for estimating β was developed to permit the first-order rate transfer approach [Eq. (12-11), assuming $f = 1.0$] to match solute mean breakthrough times that would be calculated if an analytical solution that explicitly considers solute concentration gradients within the matrix was used (e.g., Sudicky and Frind, 1982). The effect of setting ImmobilePorosityPenetrationFraction_STFF to a value less than 1.0 is to reduce the mass transfer rate, which may improve the transport calculation match to earliest solute arrival times, but also may result in overestimating peak solute concentrations at later times. The user who wishes to evaluate the effects of partial matrix penetration should consider correlation to the fracture spacing parameter FracturesPerMeter_STFF[1/m] because wider spacing of flowing fractures would reduce the ability of solutes to fully penetrate the matrix.

To account for the effects of reversible radionuclide sorption to colloids on diffusion, the mass transfer rate coefficient, β , and the immobile matrix retardation factor, R_D , must be adjusted to account for the portion of the species bound to colloids that cannot diffuse into the rock matrix.

Pickett and Dam (2003), following Contardi, et al. (2001), developed an approach to calculate a modified rate coefficient, β^{eff} , using the equation

$$\beta^{eff} = \frac{\beta}{1 + K_0} \quad (12-14)$$

and a modified matrix retardation factor R_D^{eff} , calculated from

$$R_D^{eff} = \frac{R_D}{1 + K_0} \quad (12-15)$$

K_0 is given by

$$K_0 = \frac{C F \phi_s (R_D - 1)}{\rho_g (1 - \phi_s)} \quad (12-16)$$

where

- C — colloid concentration in fractures, ColloidConcentration_STFF[kg/m³]
- F — dimensionless factor accounting for surface area differences between matrix and colloid, SurfaceAreaFactor_STFF[]
- ρ_g — matrix grain density, ImmobileGrainDensity_STFF[kg/m³]

For colloids that form irreversible attachments to colloids (i.e., J-species), matrix diffusion is disabled by setting β equal to zero for all J-species.

12.4 Input Parameters in *tpa.inp* (and *tpa_include.inp*)

Table 12-1 lists the input and correlated parameter values to SZFT from *tpa.inp* and *tpa_include.inp* that are included in the reference data set for TPA Version 5.1.

12.5 Auxiliary Input Data and External Process Models

Auxiliary input data files used by SZFT provide detailed information on one-dimensional streamtubes and streamtube input fluxes used in the transport calculations and information to define the surface response functions for actinide K_A values. Table 12-2 lists and describes the auxiliary input data files for SZFT. NEFMKS is used to calculate flow and transport. Olague, et al. (1991) detail the theory and operation of NEFMKS.

Table 12-1. Reference Data for Parameters of <i>tpa.inp</i> Used by SZFT <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	ImmobilePorosityPenetration Fraction_STFF	f Effective fraction of saturated rock matrix accessible to matrix diffusion during the time scale for transport from source to receptor, used to calculate effective immobile porosity and the matrix diffusion mass-transfer rate coefficient in NEFMKS [unitless]	constant 1.0	Value of 1.0 provides no adjustment to matrix diffusion rate constant; best for representing mean solute breakthrough time. Lower values can better estimate earliest solute arrival times when fracture spacings are large, but also may overestimate peak concentration. If a distribution is desired, user should consider strong correlation to FracturesPerMeter_STFF.
SZFT	FracturesPerMeter_STFF [1/m]	n Effective spacing between transmissive zones in the tuff aquifer, used to calculate the matrix diffusion mass-transfer rate coefficient in NEFMKS [1/m]	uniform 0.05, 1.0	Lower bound based on transmissive interval spacing of 20 m [65.6 ft] from well observations; upper bound based on estimated spacings of connected fractures (see Winterle, et al., 2000).
SZFT	MixingZoneDispersion Fraction	Dispersion fraction of the mixing zone (SZ)-longitudinal dispersion specified as a fraction of the path length [unitless]	constant 0.01	A constant value is used because this parameter has a negligible effect on repository performance estimates (e.g., Mohanty, et al., 2004). Value is based on low end of the range of observed values for longitudinal dispersivity (e.g., Gelhar, et al., 1992).
SZFT	DispersionFraction_STFF	Dispersion fraction of tuff (SZ)-longitudinal dispersion specified as a fraction of the path length [unitless]	constant 0.01	A constant value is used because this parameter has a negligible effect on repository performance estimates (e.g., Mohanty, et al., 2004). Value is based on low end of the range of observed values for longitudinal dispersivity (e.g., Gelhar, et al., 1992).
SZFT	DispersionFraction_SAV	Dispersion fraction of Amargosa Valley (SZ)-longitudinal dispersion specified as a fraction of the path length [unitless]	constant 0.1	Based on de Marsily (1986) citing work of Lallemant-Barrés and Peaudcerf (1978).

Table 12-1. Reference Data for Parameters of <i>tpa.inp</i> Used by SZFT (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	FracturePorosity_STFF	ϕ_{eff} Effective fracture porosity of the saturated tuff (i.e., volume fraction through which the bulk of flow occurs) [unitless]	loguniform 1.0e-3, 1.0e-2	Based on CNWRA best estimates (Farrell, et al., 2000; Mohanty, et al., 2000, Chapter 10).
SZFT	DiffusionRate_STFF	D Effective diffusion coefficient in saturated tuff [m ² /yr]	constant 1.0e-3	Consistent with diffusion coefficient reported for TcO ₄ anion by Triay, et al. (1996); constant value used because uncertainty is small compared to uncertainty considered for FracturesPerMeter_STFF, which also has a stronger effect on matrix diffusion rate.
SZFT	DistanceToTuffAlluviumInterface[km]	Distance to tuff alluvium interface [km]	uniform 12.0, 17.0	Location of tuff–alluvium interface is fairly well constrained by Nye County well data; uncertainty range also reflects potential effects of horizontal anisotropy and depth at which flow path transition occurs.
SZFT	StreamTubeWidthMultiplier[]	b_w Accounts for uncertainty in groundwater flux and geometry of flow path [unitless]	uniform 0.5, 2.0	Best estimate based on experience from groundwater flow modeling; accounts for uncertainties in groundwater flux and geometry of flow path.
SZFT	SZFluxMultiplierAtGlacialMaximum[]	Factor to account for the proportion of increased saturated zone streamtube flux at glacial maximum (wettest) climate state [unitless]	constant 1.0	Constant value to 1.0 is appropriate because <i>strmtube.dat</i> based on a scenario of increased flux during potential future wetter climate. Analyses by Winterle (2003) suggest groundwater travel times may not be significantly different following a water table rise.
SZFT	SZFractureForceFactorForKdToRd	User option to turn sorption on/off in fractures for americium, neptunium, plutonium, thorium, uranium, and curium ; if SZFFFFKTR = 0, then $R_0 = 1$ (no sorption in fractures) [unitless]	constant 0.0	Program control switch to investigate retardation effects in fractures. This applies to saturated tuff layer only. Acceptable values are 0 (no retardation) or 1 (retardation).

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	FractureRD_STFF_I FractureRD_STFF_Tc FractureRD_STFF_Ci FractureRD_STFF_Pb FractureRD_STFF-Cs FractureRD_STFF_Ni FractureRD_STFF_Se FractureRD_STFF_Nb FractureRD_STFF_Ra	R_D Retardation factor for iodine, technetium, chlorine, lead, cesium, nickel, selenium, niobium, and radium in saturated tuff fractures [unitless]	constant 1.0	Bounding assumption of no retardation in fractures for unsaturated and saturated zones. All layers, all nuclides. Retardation of dissolved radionuclides is considered to be much more limited in fractures than in the matrix because sorption is assumed to be primarily controlled by the mineral surface area, which is much greater in the rock matrix. Although TPA Version 5.1 has the capability to represent retardation of dissolved radionuclides within fractures, fracture retardation factors are set to 1.0 (i.e., no retardation) in the reference case data set for TPA Version 5.1. It should be noted that sorption of colloids onto fracture surfaces is included in the abstraction because there are site-specific data that indicate this process occurs and the data provide reasonably bounding colloid sorption values for use in the abstraction (Bechtel SAIC Company, LLC, 2004a).
SZFT	AlluviumMatrixRD_SAV_I	R_D Retardation factor for iodine in saturated alluvium [unitless]	constant 1.0	Experimental evidence using iodine and alluvium shows that sorption not significantly different than zero (e.g., Bechtel SAIC Company, LLC, 2003b).
SZFT	AlluviumMatrixRD_SAV_Tc	R_D Retardation factor for technetium in saturated alluvium [unitless]	constant 1.0	Conservative assumption of $K_D = 0$. Confirmed by DOE experimental results (e.g., Bechtel SAIC Company, LLC, 2003b).
SZFT	AlluviumMatrixRD_SAV_Ci	R_D Retardation factor for chlorine in saturated alluvium [unitless]	constant 1.0	Field evidence indicates chlorine behaves conservatively (chemically) in the saturated zone (e.g., Bechtel SAIC Company, LLC, 2004b).
SZFT	AlluviumMatrixRD_SAV_Ra	R_D Retardation factor for radium in saturated alluvium [unitless]	constant 3580.0	K_D values in Bechtel SAIC Company, LLC (2003a) for radium sorption in saturated alluvium are 0.1 to 1 m ³ /kg with a uniform distribution. The mean or "expected" value of 0.55 m ³ /kg is used and has been converted to an R_D of 3,580 using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	AlluviumMatrixRD_SAV_Pb	R_D Retardation factor for lead in saturated alluvium [unitless]	constant 1950.0	Lead sorption value taken from the Bechtel SAIC Company, LLC (2001), which indicates lead K_D s in the saturated zone range from 0.1 to 0.5 m ³ /kg with a uniform distribution (an assumption that devitrified tuff is an adequate analog to STFF and alluvium is also made). The mean or "expected" value of 0.3 m ³ /kg is used and has been converted to an R_D of 1,950 using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .
SZFT	AlluviumMatrixRD_SAV-Cs	R_D Retardation factor for cesium in saturated alluvium [unitless]	constant 4730.0	K_D values in Bechtel SAIC Company, LLC (2003a) for cesium sorption in saturated alluvium are 0.1 to 1 m ³ /kg with a truncated normal distribution (mean = 0.728). The mean or "expected" value of 0.728 m ³ /kg is used and has been converted to an R_D of 4,730 using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .
SZFT	AlluviumMatrixRD_SAV_Ni	R_D Retardation factor for nickel in saturated alluvium [unitless]	constant 650.0	Nickel sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates nickel K_D s in the saturated zone ranging from 0 to 0.2 m ³ /kg with a uniform distribution (an assumption that devitrified tuff is an adequate analog to STFF and alluvium is also made). The mean or "expected" value of 0.1 m ³ /kg is used and has been converted to an R_D of 650 using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .
SZFT	AlluviumMatrixRD_SAV_Se	R_D Retardation factor for selenium in saturated alluvium [unitless]	constant 2.0	Selenium sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates selenium K_D s in the saturated zone ranging from 0 to 0.001 m ³ /kg with a beta distribution (an assumption that devitrified tuff is an adequate analog to STFF and alluvium is also made). The mean or "expected" value of 0.0001 m ³ /kg is used and has been converted to an R_D of 1.65 (rounded to 2) using an alluvium porosity of 0.30 and bulk density of 1,950 kg/m ³ .
SZFT	AlluviumMatrixRD-SAV-Nb	R_D Retardation factor for niobium in tuff saturated fractures [unitless]	constant 1.0	Bounding assumption of no retardation in fractures for unsaturated and saturated zones. All layers, all nuclides.

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	AlluviumMatrixRD_SAV_Nb	R_D Retardation factor for niobium in saturated alluvium [unitless]	constant 35800.0	Using an analog between expected trivalent species Nb^{3+} and Am^{3+} , the americium R_D is substituted for niobium. Values in Bechtel SAIC Company, LLC (2003a) for americium sorption in saturated alluvium are 1.0 to $10.0 \text{ m}^3/\text{kg}$ with a truncated normal distribution (mean = 5.5, stdev = 1.5). The mean or "expected" value of $5.5 \text{ m}^3/\text{kg}$ is used and has been converted to an R_D of 35,800 using an alluvium porosity of 0.30 and bulk density of $1,950 \text{ kg}/\text{m}^3$.
SZFT	FractureAperture_STFFF[m]	b Effective width of fracture apertures for saturated tuff (STFF) layer [m]	constant $1.0\text{e-}4$	Aperture width is representative of DOE estimates for fracture width in tuff layers (0.1–0.2 mm) as estimated from Bechtel SAIC Company, LLC (2003c).
SZFT	AlluviumMatrixGrainDensity_SAV[kg/m3]	ρ_g Grain density of alluvium sediments [kg/m ³]	constant 2520.0	DOE-measured grain density values for alluvium (Bechtel SAIC Company, LLC, 2003a) have small range, 2,490 to $2,550 \text{ kg}/\text{m}^3$. Mean value of $2,520 \text{ kg}/\text{m}^3$ is used.
SZFT	AlluviumMatrixPorosity_SAV	ϕ_{eff} Effective flow porosity of saturated alluvium [unitless]	uniform $1.0\text{e-}1$, $1.5\text{e-}1$	Current DOE range (Bechtel SAIC Company, LLC, 2003a) is truncated normal with min = 0.0, mean = 0.18, and max = 0.30; std dev = 0.051. Field measured value at 19D (Bechtel SAIC Company, LLC, 2003a) is 0.10. Best estimate of USFIC team, using Walker and Eakin (1963) and Fischer (1992), is to use a uniformly distributed range of 0.10 to 0.15.
SZFT	AlluviumTotalPorosity_SAV	ϕ_m Total porosity of saturated alluvium; used for calculating retardation factor for radionuclides in the saturated alluvium layer [unitless]	uniform 0.15, 0.3	Range based on alluvium porosity data from DOE (Bechtel SAIC Company, LLC, 2003a).
SZFT	AlluviumMatrixSpecificSurfaceArea[m2/kg]	ESA Specific surface area of alluvium; used for calculating retardation factor for radionuclides in the saturated alluvium layer [m ² /kg]	uniform $0.9\text{e}3$, $3.1\text{e}3$	Range based on analysis of surface area data from Fortymile Wash wells (Bertetti, et al., 2004) using mesopore and micropore analysis (BET method). Subsequent statistical analyses and experimental evidence suggest that the 10-percent effective range should be applied with little or no contribution from other minerals (McMurry and Bertetti, 2005).

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	ImmobileRd_STFF_I	R_D Retardation factor for iodine in saturated tuff matrix during matrix diffusion [unitless]	constant 1.0	Experimental evidence using iodine and alluvium shows that iodine sorption is not significantly different than zero (e.g., Bechtel SAIC Company, LLC, 2003b).
SZFT	ImmobileRd_STFF_Tc	R_D Retardation factor for technetium in saturated tuff matrix during matrix diffusion [unitless]	constant 1.0	Conservative assumption of $K_D = \text{zero}$. Confirmed by DOE experimental results (e.g., Bechtel SAIC Company, LLC, 2003b).
SZFT	ImmobileRd_STFF_Cl	R_D Retardation factor for chlorine in saturated tuff matrix during matrix diffusion [unitless]	constant 1.0	Field evidence indicates chlorine behaves conservatively (chemically) in the saturated zone (e.g., Bechtel SAIC Company, LLC, 2004b).
SZFT	ImmobileRd_STFF_Ra	R_D Retardation factor for radium in saturated tuff matrix during matrix diffusion [unitless]	constant 5400.0	Values in Bechtel SAIC Company, LLC (2003a) for radium sorption in saturated tuff are 0.1 to 1 m ³ /kg with a uniform distribution. The mean or "expected" value of 0.55 m ³ /kg is used and has been converted to an R_D of 5,400 using a porosity of 0.20 and bulk density of 1,976 kg/m ³ for the STFF.
SZFT	ImmobileRd_STFF_Pb	R_D Retardation factor for lead in saturated tuff matrix during matrix diffusion [unitless]	constant 3000.0	Lead sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates lead K_D s in the saturated zone ranging from 0.1 to 0.5 m ³ /kg with a uniform distribution (an assumption that devitrified tuff is an adequate analog to STFF and alluvium is also made). The mean or "expected" value of 0.3 m ³ /kg is used and has been converted to an R_D of 3,000 using an STFF porosity of 0.20 and bulk density of 1,976 kg/m ³ .
SZFT	ImmobileRd_STFF-Cs	R_D Retardation factor for cesium in saturated tuff matrix during matrix diffusion [unitless]	constant 7200.0	Used cesium sorption values from Bechtel SAIC Company, LLC (2003a) for alluvium as there should be little difference between alluvium and devitrified tuff for cesium retention. The range for alluvium is 0.1 to 1 m ³ /kg with a mean value of 0.728 m ³ /kg. Converted to an R_D of 7,200 for the STFF using a porosity of 0.20 and a bulk density of 1,976 kg/m ³ .

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	ImmobileRd_STFF_Ni	R_D Retardation factor for nickel in saturated tuff matrix during matrix diffusion [unitless]	constant 990.0	Nickel sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates nickel K_D s in the saturated zone ranging from 0 to 0.2 m ³ /kg with a uniform distribution (an assumption that devitrified tuff is an adequate analog to STFF and alluvium is also made). The mean or "expected" value of 0.1 m ³ /kg is used and has been converted to an R_D of 990 using an STFF porosity of 0.20 and bulk density of 1,976 kg/m ³ .
SZFT	ImmobileRd_STFF_Se	R_D Retardation factor for selenium in saturated tuff matrix during matrix diffusion [unitless]	constant 2.0	Selenium sorption value taken from Bechtel SAIC Company, LLC (2001), which indicates selenium K_D s in the saturated zone ranging from 0 to 0.001 m ³ /kg with a beta distribution (an assumption that devitrified tuff is an adequate analog to STFF and alluvium is also made). The mean or "expected" value of 0.0001 m ³ /kg is used and has been converted to an R_D of 1.98 (rounded to 2) using an STFF porosity of 0.20 and bulk density of 1,976 kg/m ³ .
SZFT	ImmobileRd_STFF_Nb	R_D Retardation factor for niobium in saturated tuff matrix during matrix diffusion [unitless]	constant 54300.0	Using an analogy between expected trivalent species Nb ³⁺ and Am ³⁺ , the Am retardation factor is substituted for Nb. Values in Saturated Zone Flow and Transport Analysis/Model Report (Bechtel SAIC Company, LLC, 2003a) for Am sorption in STFF are 1.0 to 10.0 m ³ /kg with a truncated normal distribution (mean = 5.5, standard deviation = 1.5). The mean ("expected") K_D value of 5.5 m ³ /kg for the devitrified layers is used and has been converted to a retardation factor of 54300.0 assuming a bulk density of 1,976 kg/m ³ and porosity of 0.20 for the STFF.
SZFT	ImmobileGrainDensity_STFF[kg/m3]	ρ_g Matrix grain density of saturated tuff [kg/m ³]	constant 2470.0	DOE data (Bechtel SAIC Company, LLC, 2003a) indicate that average grain density of layers that would make up STFF are not significantly different from 2,470 kg/m ³ .
SZFT	ImmobilePorosity_STFF	ϕ_m Matrix porosity in saturated tuff [unitless]	constant 0.2	Average matrix porosity used by DOE in Bechtel SAIC Company, LLC (2003a) is 0.22. A small range is evident but not likely to have significant effects.

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	ImmobilePoreRadius_STFF [m]	r Estimated pore radius of saturated tuff matrix [m]	constant 5.0e-8	Pore radius is used along with porosity and density to calculate surface area for each hydrostratigraphic layer. The constant value of 5e-8 is consistent with median value based on moisture retention curves used by DOE from work by Travis and Nuttall (1987). Bechtel SAIC Company, LLC (2004c) indicates a more complex distribution of pore sizes for various rock units, but there is a general agreement with the 5e-8 m value. To minimize surface area uncertainties, the 5e-8 m value is retained pending more detailed characterization.
SZFT	MinimumResidenceTime_STFF [yr]	Minimum residence time in tuff [yr]	constant 10.0	Used for code efficiency reasons. NEFMKS model is very sensitive to contiguous leg-to-velocity ratios. Value is reasonable based groundwater flux on order of 1 m/yr, minimum effective fracture porosity of 0.001, and travel distance greater than 10 km.
SZFT	MinimumResidenceTime_SAV [yr]	Minimum residence time in alluvium [yr]	constant 100.0	Used for code efficiency reasons. NEFMKS model is very sensitive to contiguous leg length-to-velocity ratios. Value is reasonable based groundwater flux on order of 1 m/yr, minimum effective alluvium porosity of 0.1, and travel distance greater than 1 km.
SZFT	SaturatedZoneMinimumVelocityChangeFactor [Fraction]	Timesteps for the NEFMKS velocity file are ignored unless the difference in the velocity with that of the preceding timestep exceeds the minimum velocity change factor [unitless]	constant 0.1	Value selected for code efficiency reasons. The underlying model for NEFMKS is very sensitive to contiguous timestep to velocity ratios. A 10-percent velocity change requirement is reasonable. Not used in reference case in which saturated zone velocity remains constant throughout the simulation time.
SZFT	SurfaceAreaFactor_SAV[] SurfaceAreaFactor_STFF[]	F Ratio of colloid to formation surface area [unitless]	constant 590.0	Parameter is fairly well constrained; derived using site-specific data (Contardi, et al., 2001).

Table 12-1. Reference Data for Parameters of <i>tpa.inp</i> Used by SZFT (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	ColloidRetardationFactor_SAV_[]	R_c Colloid retardation factor in alluvium [unitless]	usersuppliedpwisecdf 20 1.0, 0.0 1.01, 0.01 1.5, 0.07 2.0, 0.12 4.0, 0.22 6.0, 0.29 8.0, 0.33 14.4, 0.4 22.14, 0.45 34.0, 0.5 56.15, 0.55 92.85, 0.6 153.5, 0.65 253.9, 0.7 419.7, 0.75 694.0, 0.8 1148.0, 0.85 1897.0, 0.9 3138.0, 0.95 5188.0, 1.0	Modified from DOE distribution (Bechtel SAIC Company, LLC, 2003e, Table 7). Linearly interpolated in log space between tabulated values and with DOE truncation removed. Presumes 1 percent of colloids travel unretarded.

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	ColloidRetardationFactor_STFF_II	R_c Colloid retardation factor in the fractured volcanic leg of saturated zone [unitless]	usersuppliedpwisecdf 15 1.0, 0.0 1.01, 0.01 1.5, 0.04 2.0, 0.06 4.0, 0.12 6.0, 0.15 10.23, 0.25 14.86, 0.35 26.0, 0.5 34.35, 0.6 45.39, 0.7 59.98, 0.8 219.0, 0.9 418.6, 0.95 800.0, 1.0	Modified from DOE distribution (Bechtel SAIC Company, LLC, 2003e, Table 8). Linearly interpolated in log space between tabulated values and with DOE truncation removed. Presumes 1 percent of colloids travel unretarded.
SZFT	ColloidConcentration_SAV_ [kg/m3] ColloidConcentration_STFF (kg/m3)	C Colloid concentration in alluvium and in fractures of the saturated volcanic tuff [kg/m ³]	usersuppliedpwisecdf 16 1.0e-6, 0.0 2.51e-6, 0.1 6.31e-6, 0.2 1.58e-5, 0.3 3.98e-5, 0.4 1.0e-4, 0.5 2.51e-4, 0.6 6.31e-4, 0.7 1.0e-3, 0.75 2.15e-3, 0.8 4.64e-3, 0.85 1.0e-2, 0.9 2.24e-2, 0.94 5.0e-2, 0.98 0.1, 0.99 0.2, 1.0	Based on DOE distribution (Bechtel SAIC Company, LLC (2003e, Table 5). Linearly interpolated in log space.

Table 12-1. Reference Data for Parameters of tpa.inp Used by SZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
SZFT	SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)	Flag: To run separate NEFMKS models for tuff and alluvium, set = 1	iconstant 0	Selects one of two operational modes for the saturated zone flow and transport calculations. To run SZFT in the original normal mode, set = 0. To run SZFT in the new mode where tuff and alluvium legs use a separate NEFMKS runs, set = 1. Under certain combinations of parameter values, this mode can run faster than the original mode. Normal mode is to be used unless special conditions arise that, in the determination of the analyst, require separate runs for the saturated zone legs.
tpa_include.inp (separate input file from tpa.inp)	LogCO2PartialPressure_All UZ_SZLayers[atm]	Log of the partial pressure of aqueous carbon dioxide in all unsaturated and saturated zone layers [atm]	usersuppliedpwiscdf 19 -3.9, 0.0 -3.7, 0.037 -3.5, 0.071 -3.3, 0.124 -3.2, 0.159 -2.9, 0.298 -2.7, 0.413 -2.56, 0.5 -2.4, 0.599 -2.2, 0.713 -1.9, 0.849 -1.8, 0.882 -1.6, 0.933 -1.4, 0.965 -1.2, 0.983 -1.0, 0.993 -0.8, 0.997 -0.6, 0.999 -0.5, 1.0	User-defined distribution to simulate truncated normal distribution derived from geochemical data (104 sample points) specific to the Yucca Mountain region. Data are from Bechtel SAIC Company, LLC (2004b) and Bertetti, et al. (2004). The development of the distributions is discussed in McMurry and Bertetti (2005).

Table 12-1. Reference Data for Parameters of *tpa.inp* Used by SZFT (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
<i>tpa_include.inp</i> (separate input file from <i>tpa.inp</i>)	pH_AIIUZ_SZLayers [StandardUnits]	pH of water in all unsaturated and saturated zone transport layers [-log(activity H ⁺)]	usersuppliedpwiscdf 18 6.5, 0.0 6.63, 0.018 6.81, 0.036 6.98, 0.067 7.15, 0.114 7.33, 0.185 7.5, 0.273 7.68, 0.385 7.85, 0.5 8.02, 0.615 8.2, 0.727 8.37, 0.815 8.55, 0.886 8.72, 0.933 8.89, 0.964 9.07, 0.982 9.24, 0.992 9.4, 1.0	User-defined distribution to simulate truncated normal distribution derived from geochemical data (104 sample points) specific to the Yucca Mountain region. Data are from Bechtel SAIC Company, LLC (2004b) and Bertetti, et al. (2004). The development of the distributions is discussed in McMurry and Bertetti (2005).
Correlated Parameters	Independent Variable: LogCO2PartialPressure_AIIUZ_SZLayers[atm] Dependent Variable: pH_AIIUZ_SZLayers [StandardUnits]	Correlation between CO ₂ partial pressure and pH of water in all unsaturated and saturated zone units	correlateinputs -0.95	Correlation for pH and PCO ₂ derived from analysis of geochemical data (104 sample points) specific to the Yucca Mountain region. Data are from Bechtel SAIC Company, LLC (2004b) and Bertetti, et al. (2004). The development of the correlation is discussed in McMurry and Bertetti (2005).

Table 12-2. Auxiliary Input Data Files Used By SZFT	
File	Contents
<i>strmtube.dat</i>	The reference data set in TPA Version 5.1 defines three streamtubes that emanate from the water table beneath the potential repository footprint and terminate at the regulatory compliance boundary. For each streamtube, <i>strmtube.dat</i> defines (i) an input flux, (ii) a set of three points defining the centerline of the streamtube inlet underneath the repository footprint, and (iii) a set of coordinates defining the width of the streamtubes at discrete distances downstream from the repository edge. For the reference case data set, sources from the unsaturated zones of Subareas 1, 6, 7, 8, and 9 contribute to the central streamtube; Subareas 2, 3, 4, and 5 contribute to the northern streamtube; and Subarea 10 contributes to the southern streamtube.
<i>coefkdeq.dat</i>	<i>coefkdeq.dat</i> contains polynomial coefficients and valid pH ranges for discrete PCO_2 concentrations that define the surface response functions for actinide K_A values.

12.6 Intermediate Outputs and Information Passed to Other Modules

Table 12-3 lists and describes the intermediate output files that are created during execution of SZFT. In addition to the output files listed in Table 12-3, the user can specify that calculated information passed to and from SZFT be saved as intermediate output for specific realizations. This capability can be useful, for example, if the user wishes to evaluate the radionuclide mass inputs and outputs rather than the final dose result. This functionality is implemented in the *tpa.inp* input block titled <<Output Print Options>> by setting the output mode parameter, `OutputMode(0=None,1=All,2=UserDefined)`, to a value of 1 or 2. When set to 1, all optional intermediate output for SZFT will be saved for all realizations. When set to 2, optional intermediate output selected will be saved for realizations starting from *tpa.inp* parameter `UserDefinedLowerRealizationAppended` and ending with the realization specified by *tpa.inp* parameter `UserDefinedUpperRealizationAppended`. The contents of SZFT intermediate output files *szft.rlt* and *szft.ech* are described in Table 12-4.

The user should be aware that setting `OutputMode(0=None,1=All,2=UserDefined)` to 1 or 2 will also cause intermediate output files to be written for numerous other modules if the parameter `SelectAppendFiles` remains set at the default value of 0. Some of these files can be very large and can quickly fill up available memory if all intermediate outputs are specified for all realizations. Therefore, if the user is interested only in the SZFT intermediate outputs, the `SelectAppendFiles` parameter in the <<Output Print Options>> input block should be set to a value of 9 for just *szft.ech* and *szft.rlt*, or 16 for just *nefiisz.cum* and *nefiuz.cum* (Chapter 11).

Table 12-3. Intermediate Output Files Created During Execution of SZFT	
File	Contents
<i>cumrel.res</i> <i>cumrel_c.res</i>	These files report cumulative releases over the simulation period (<i>cumrel.res</i>) or the compliance period (<i>cumrel_c.res</i>) from the engineered barrier system, unsaturated zone, and saturated zone summed over all subareas in terms of Ci for each radionuclide. These files are further described in Chapter 19.
<i>gwtuzsz.res</i>	Groundwater travel times for each subarea for the unsaturated zone, saturated zone, and combined travel time. This file is further described in Chapter 19.
<i>nefiialluv.cum</i>	Saturated alluvium flow and radionuclide transport input parameters for NEFMKS for each subarea in each realization. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .
<i>nefiituff.cum</i>	Saturated tuff flow and radionuclide transport input parameters for NEFMKS for each subarea in each realization. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .
<i>nefiialluv.dis</i>	Contains time histories for radionuclide discharge rates from last saturated alluvium NEFMKS run of a simulation; typically the last subarea of the last realization. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .
<i>nefiisz.dis</i>	This is a copy of the <i>nefii.dis</i> output file produced by NEFMKS during the saturated zone transport calculation. It contains a time history of radionuclide discharge from the saturated zone during the simulation period for each radionuclide decay chain specified in <i>tpa.inp</i> . This file is overwritten each time a subarea calculation is performed; at the end of simulation this file will reflect the saturated zone transport calculation for the last subarea.
<i>nefiituff.dis</i>	Contains time histories for radionuclide discharge rates from last saturated tuff NEFMKS run of a simulation; typically the last subarea of the last realization. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .
<i>nefiialluv.inp</i>	Input information for the saturated alluvium NEFMKS transport calculation for the last subarea. File is overwritten each time a subarea calculation is performed. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .
<i>nefiisz.inp</i>	This is a copy of <i>nefii.inp</i> for NEFMKS; it defines flow path and transport characteristics. This file is overwritten each time a subarea calculation is performed; at the end of simulation, this file will reflect the saturated zone transport calculation for the last subarea.

Table 12-3. Intermediate Output Files Created During Execution of SZFT (continued)	
File	Contents
<i>nefiituff.inp</i>	Input information for the saturated tuff NEFMKS transport calculation for the last subarea. File is overwritten each time a subarea calculation is performed. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .
<i>nefmks.log</i>	Logs calls to NEFMKS by SZFT by printing “szft” once for each call. Used for diagnostics only. Generated only when parameter SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 1 in <i>tpa.inp</i> .
<i>nefiialluv.out</i>	This is a copy of the <i>nefii.out</i> output file produced by <i>nefmks.out</i> during the saturated tuff transport calculation. It contains a summary of all NEFMKS input and output. It is overwritten each time a subarea calculation is performed; at end of simulation, this file will reflect the saturated zone transport calculation for the last subarea. Generated only when parameter SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 1 in <i>tpa.inp</i> .
<i>nefiisz.out</i>	This is a copy of the <i>nefii.out</i> output file produced by NEFMKS during the saturated zone transport calculation. It contains a summary of all <i>nefmks.exe</i> input and output. It is overwritten each time a subarea calculation is performed; at the end of simulation, this file will reflect the saturated zone transport calculation for the last subarea.
<i>nefiituff.out</i>	This is a copy of <i>nefii.out</i> produced by <i>nefmks.out</i> during the saturated tuff transport calculation. It contains a summary of all NEFMKS input and output. It is overwritten each time a subarea calculation is performed; at end of simulation, this file will reflect the saturated zone transport calculation for the last subarea. Generated only when parameter SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 1 in <i>tpa.inp</i> .
<i>sz_kdrd.out</i>	This file provides a report of intermediate results of calculated values for radionuclide distribution coefficients and the sampled parameters contributing to those calculations.
<i>sz_revers.out</i>	This file reports the retardation factors after corrections to account for effects of reversible sorption to colloids. For each radionuclide, values are reported for mobile and immobile regions for both the tuff and alluvium transport legs and for each subarea.

Table 12-3. Intermediate Output Files Created During Execution of SZFT (continued)	
File	Contents
<i>sotnef.dat</i> <i>nefiisz.src</i>	These files are identical: <i>sotnef.dat</i> is an input file for NEFMKS that defines the input source from UZFT, and the file is copied to <i>nefiisz.src</i> because the file name is more intuitive. Both of these files are overwritten each time a subarea calculation is performed; at the end of simulation, this file will reflect the saturated zone transport calculation for the last subarea.
<i>nefi.rel</i>	This is an intermediate output that reports cumulative releases over the simulation period from the saturated zone. This file is overwritten each time a subarea calculation is performed; at the end of each simulation, this file will reflect the saturated zone transport calculation for the last subarea and is used to develop the <i>cumrel.res</i> , which sums releases over all subareas.
<i>nefiuz.src</i>	Input file for NEFMKS transport calculations. The file provides NEFMKS with the time-dependent source term (radionuclide releases) data from EBSREL, after adjusting the source term to account for (i) flux splitting, if there is a bypass fraction at that timestep and (ii) the filtration of colloids in the unsaturated zone rock matrix (i.e., less of J-species). UZFT saves a copy of <i>sotnef.dat</i> as <i>nefiuz.src</i> , which is a more informative file name. Both files are overwritten each time a subarea calculation is performed by UZFT. At the end of a simulation, <i>nefiuz.src</i> will reflect the input source term information for the unsaturated zone transport calculation for the last subarea of the last realization.
<i>nefiialluv.vel</i>	Copy of <i>nefi.vel</i> generated by SZFT for the saturated alluvium transport calculation. Overwritten each time NEFMKS is called. At the end of each simulation, this file will reflect the last subarea of the last realization run. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .
<i>nefiisz.vel</i>	This is a copy of the <i>nefi.vel</i> input file for NEFMKS, which defines the time-varying velocity during the simulation period. This file is overwritten each time a subarea calculation is performed; at the end of simulation, this file will reflect the saturated zone transport calculation for the last subarea.
<i>nefiituff.vel</i>	Copy of <i>nefi.vel</i> generated by SZFT for the saturated tuff transport calculation. Overwritten each time NEFMKS is called. At the end of each simulation, this file will reflect the last subarea of the last realization run. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .

Table 12-4. Optional Intermediate Output Files Created During Execution of SZFT	
File	Description
<i>szft.rlt</i>	The time history of radionuclide releases calculated by SZFT is provided by this file.
<i>szft.ech</i>	UZFT releases passed to SZFT are included in this file.
<i>nefiisz.cum</i>	This file is identical to <i>nefiisz.inp</i> except that information for every timestep is reported.

12.7 Techniques for Understanding Module Performance

While there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of processes modeled by SZFT. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques may be useful to understand their effects on system-level performance (Mohanty, et al., 2004).

In addition, “pinch-point” techniques, where output or intermediate results produced by SZFT can be understood in combination with output or intermediate results from other modules (e.g., UZFT), may help to evaluate subsystem processes. Key output files and intermediate result files useful for these comparison include *nefiisz.out*, which contains a summary of all NEFMKS input and output for the unsaturated transport calculation. This output file is detailed (many columns of data) and shows only the calculations for the last subarea, but it allows a user to compare starting conditions (radionuclide release rates from UZFT) with end results (radionuclide release rates from SZFT) in a single file. For more detailed comparisons of radionuclide transport for each subarea, the user may find it helpful to compare the optional output file *szft.ech*, which contains the UZFT radionuclide release rates passed as input to SZFT for all times, all radionuclides, and all subareas, and *szft.rlt*, which contains the radionuclide release rates that are output from SZFT for all times, all radionuclides, and all subareas. A comparison of the intermediate output files *sz_kdrd.out* and *sz_revers.out* may indicate how significantly retardation factors are affected by the colloid-associated transport modeling.

The importance of individual parameters with respect to particular subsystem processes can be examined by repetitively varying an input parameter and analyzing results from various output and intermediate result files. A single parameter importance analysis may be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, single parameter importance analyses may be performed by repetitively specifying smaller ranges within the parameter’s original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges; the user should exercise care in interpreting results from simulations in which input data are altered beyond their intended ranges.

There are also several parameters that can be varied to alter the effect of key subsystem processes with which they are associated or set to eliminate the effect of individual processes and examine specific aspects of SZFT. For example:

- The effect of matrix diffusion in tuff may be disabled by setting the input parameter value for DiffusionRate_STFF [m^2/yr] to zero.
- Colloid concentration parameters can be set to zero to remove the effect of reversible colloid sorption (ColloidConcentration_STFF [kg/m^3] and ColloidConcentration_SAV [kg/m^3]).
- Retardation factors for any or all radionuclides can be set to 1.0 to remove consideration of the effects of sorption. Modification of R_D or retardation factor for an element requires changes to both layers (STFF and SAV). Values are specified within *tpa.inp* for all elements except six actinides (americium, neptunium, plutonium, thorium, uranium, and curium). Any changes should be consistent with layer properties (i.e., changes should reflect the mineralogy of the STFF or SAV). For the six actinides previously listed, the R_D may be set to 1.0 by resetting the values of ImmobileGrainDensity_STFF [kg/m^3] and AlluviumMatrixGrainDensity [kg/m^3] to 0.0.
- Retardation in saturated tuff fractures may be enabled. To simulate retardation in the fractured tuff for the six actinides, the parameter SZFractureForceFactorForKdToRd must be set to 1 (0 = no, 1 = yes). For other radionuclides, retardation factors for the fractures, FractureRD_STFF_RN, must be changed for each radionuclide.
- The distributions for pH and PCO_2 are carefully tailored to site data and are correlated as described in Section 12.3.3, and effective ranges within *coefkdeq.dat* are optimized to this data. Modification of pH or PCO_2 distributions or their correlation should be done with care to prevent calculation of unintended R_D values for actinides.
- The parameter SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) can be set to 1 to separate transport calculations for flow in tuff and alluvium and evaluate their respective effects on transport.

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13 DIRECT FAULTING DISRUPTIVE EVENT (FAULTO)

This chapter describes an abstracted model for the Direct Faulting Disruptive Event module (FAULTO)¹ in TPA Version 5.1. This abstraction calculates the fraction of subareas and times where waste package failures occur from direct fault disruption within the potential repository. Information is supplied to FAULTO from *tpa.inp* and from the READER utility module (Chapter 4) in the form of drift endpoints to determine how many drifts are intersected and to determine the number of failed waste packages. This information is provided to the Engineered Barrier System Radionuclide Release module (EBSREL)² (Chapter 10). Direct fault disruption is assumed in each realization as a one fault and one time event, and the probability of the faulting event occurring is factored into the analysis as a postprocessing calculation. FAULTO is not executed in the reference case simulation. Refer to the flag setting in Section 13.4 for execution of FAULTO.

13.1 Conceptual Model

FAULTO evaluates the potential for direct waste package rupture from displacements along planar faults. These faults are decoupled in space and time (i.e., only one fault per realization is possible). In FAULTO, faults are conceptualized as near-vertical planar deformation zones with a length and width. All waste packages within these zones are assumed damaged, provided the fault displacement exceeds a threshold displacement value.

It is assumed that waste packages emplaced in the potential repository will be appropriately set back from those faults known to present a potential hazard and that a minimum amount of fault displacement is needed to disrupt a waste package. Thus, FAULTO is designed to evaluate hazards related to faults unaccounted for in the potential repository design, such as (i) new faults, which may form during the period of concern; (ii) hidden faults, which are presently unknown and unmapped within the potential repository; or (iii) underestimated faults, which are mapped faults considered insignificant during design and construction (i.e., where no fault setback was implemented) that could pose a risk over the lifetime of the potential repository.

13.2 Model Support and Assumptions

FAULTO is an abstracted model of the failure of waste packages from instantaneous fault displacements along new, undiscovered, or inadequately characterized faults (Figures 13-1 and 13-2). FAULTO considers the (i) distribution of waste packages within the emplacement drifts, (ii) fault recurrence parameters, (iii) fault geometric parameters, (iv) fault-slip displacement, and (v) the threshold displacement for fault disruption.

Waste packages are assumed to be distributed uniformly throughout the potential repository as a first-order approximation. The potential repository design could influence the extent to which this assumption is acceptable, but using a uniform density of emplaced waste packages is

¹The Direct Faulting Disruptive Event module is referenced frequently throughout this chapter. The abbreviation FAULTO will be used.

²The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

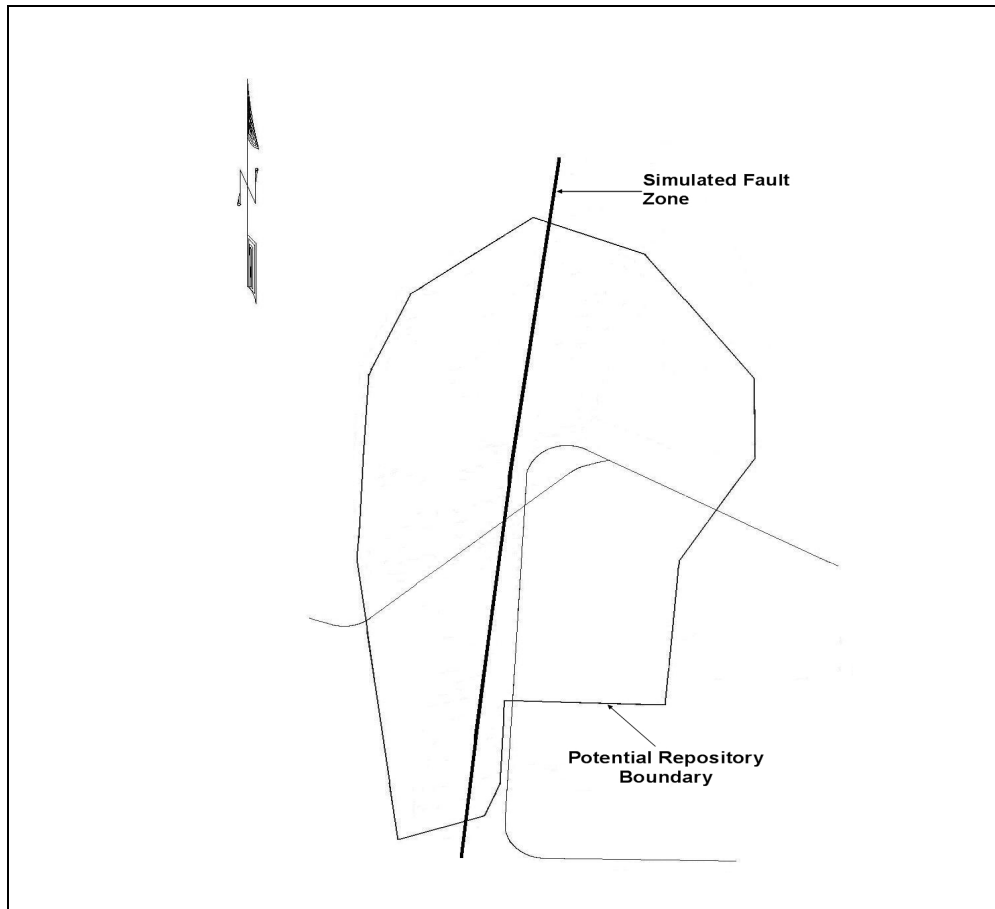


Figure 13-1. Simulated Fault Zone Within the Potential Repository Boundary (CRWMS M&O, 2003)

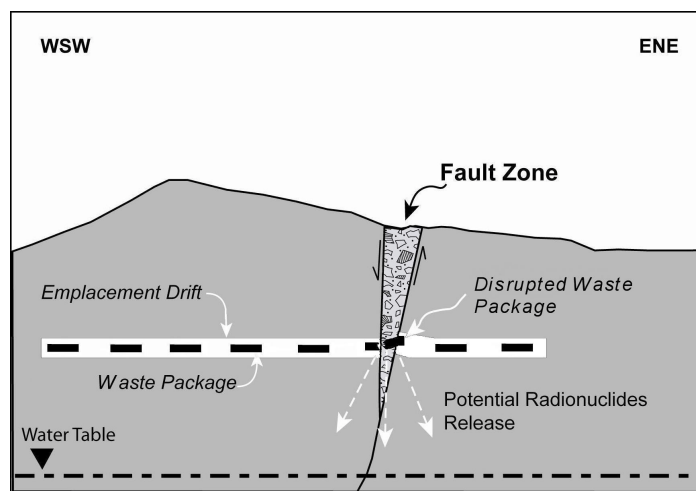


Figure 13-2. Schematic Section Illustrating Potential Waste Package Disruption Caused by a Normal Fault Intersecting an Emplacement Drift (Not to Scale)

acceptable to estimate the significance of fault displacement without speculating on the potential repository design.

The time for the next faulting event is calculated from the effective recurrence rate considering the length and orientation of the mapped faults in the Yucca Mountain region.

The annual probability of faulting in the potential repository region was estimated at 5.0×10^{-6} (Mohanty, et al., 2002). Fifty percent of faulting is assumed to occur on new faults or faults where waste packages are not set back in the potential repository design. This assumption is supportable because geological observations infer that large faulting events in Yucca Mountain will occur on known and mapped faults. For example, paleoseismic studies show that nearly all the large faults at Yucca Mountain produce evidence for repeated earthquake ruptures (U.S. Geological Survey, 1996). The model for the fault orientation, length, width, and displacement is based on field data of the Yucca Mountain region (Stamatakis, et al., 2003).

Specific assumptions associated with the modeling approach for assessing the effects for direct faulting in FAULTO and TPA Version 5.1 follow.

- No links are assumed among faulting, seismicity, rockfall, volcanism, or other effects or causes of faulting. These processes (i.e., seismicity, rockfall, and volcanism) are considered elsewhere in TPA Version 5.1 (Chapters 6 and 14). In FAULTO, only the direct effect of faulting impinging, via a damage zone, on waste packages is considered. In nature, volcanic eruptions are always accompanied by numerous pre- and syneruption earthquakes (Luhr and Simkin, 1993; Fedotov and Markhinin, 1983), and all faulting events that would directly disrupt waste packages would be accompanied by significant seismicity. Because of the generally low probability of these disruptive events, and for simplification purposes, only the direct effect of faulting is considered here.
- It is assumed that when a faulting event occurs, waste package disruption will occur because the fault slip will equal or exceed the user-defined threshold value of fault displacement, and all waste packages intersected by the fault zone (i.e., fault length within the potential repository boundary multiplied by the fault width) are then assumed failed. The threshold displacement is an input parameter in *tpa.inp* that is supplied by the user that allows flexibility to evaluate a range of waste package disruption processes. Although TPA Version 5.1 does not couple the degradation of the waste package strength caused by corrosion or other phenomena with the threshold displacement, the approach is considered reasonable because the *tpa.inp* parameter threshold displacement for FaultDisruptionOfWP[m] can account for these considerations.
- Waste packages intersected by faults are assumed to be completely and immediately failed. As a result of this assumption, the radionuclide inventory of the disrupted waste packages is available for release of radionuclides (Chapter 10).
- Waste package failure in FAULTO is not linked to a waste package mechanical failure approach, as used in the Waste Package Corrosion Failure module (EBSFAIL). While faulting could weaken waste packages and make them more susceptible to corrosion

over time, this simplification is reasonable because the waste package is assumed to fail when the fault displacement exceeds a threshold value.

- The damage zone caused by displacement along a fault is assumed to be restricted within the fault zone boundaries (i.e., no diffuse deformation outside the fault zone).
- Direct fault disruption along a fault zone, as generated by FAULTO, is assumed to cause no fault disruption on other faults, either mapped or uncharacterized, within the potential repository block.
- As described above, 50 percent of faulting is assumed to occur on new faults or faults where waste packages are not set back in the potential repository design. Assuming 50 percent of faulting occurs on new faults is also appropriate. This value requires that varying the percentage of faulting on new faults will only result, generally, in a difference of a factor of two in the effects of direct fault disruption if the parameter values in FAULTO are similar.
- In FAULTO, no correlations are assumed between fault length, fault-zone width, fault orientation, and probable displacement along the fault plane. TPA Version 5.1 initiates a new fault zone within the potential repository based on geometric and recurrence parameters. Geometric parameters include fault-zone location, orientation, strike, length, width, and displacement. Recurrence parameters include recurrence rate, time of faulting event, and cumulative displacement rate. Although in nature these geometric and recurrence properties may be related (i.e., longer faults seem to correlate with wider deformation zones or bigger faults tend to be more active), for simplicity, and from a risk-informed perspective (Stamatakis, et al., 2003), they are specified as independent parameters in TPA Version 5.1.
- TPA Version 5.1 is limited to one faulting event per realization, regardless of the selected recurrence interval. This simplification is acceptable as long as the estimate of recurrence intervals is on the order of 10^5 years, and the time period of interest is 10,000–20,000 years. Otherwise, this limitation reduces the potential consequence of faulting. Nonetheless, a previous evaluation of the risk from faulting (Stamatakis, et al., 2003) suggests that even for longer periods of interest, this limitation may be appropriate, but should be assessed by the user.

Some parameters normally used to fully describe faulting events are not used in FAULTO, including fault-dip angle, number of slip surfaces, partition of fault slip among different slip surfaces, and cumulative displacement rate partitioned among slip surfaces. These parameters were excluded for the following reasons:

- Fault-dip angle is not important because the waste packages are assumed to be emplaced within almost horizontal drifts. Fault dips at the surface at Yucca Mountain are rarely less than 45° . Although the fault intersection area would be increased by lower angle faults, their rarity (i.e., low probability) would result in only a small impact on the fault intersection area. Variations in the fault-dip angle over the vertical dimension of the emplacement drifts will also not affect the consequence.

- The number of slip surfaces of a fault does not affect performance because the entire fault is assumed to have the same maximum displacement. The area affected is the fault width times the trace length of the fault within the footprint of the potential repository. Because the waste packages are assumed to be uniformly distributed in emplacement drifts, only the area affected is important and not the exact location of the slip surfaces within the area affected.
- Cumulative displacement rates for faults at Yucca Mountain (Ghosh, et al., 1997, Table 2-4) are too small to affect the performance of the potential repository over the first 10,000 or 20,000 years. For much longer simulation periods, the value and distribution type of these cumulative fault displacement rates may need to be reevaluated. The user should determine an appropriate value for these cumulative fault displacement rate parameters given that TPA Version 5.1 simulations can be executed for time periods of up to 1 million years.

13.3 Implementation of Conceptual Model in TPA Version 5.1

FAULTING (a standalone external code for simulating direct fault disruption) has been implemented in TPA Version 5.1 as FAULTO, a module to simulate an externally imposed faulting disruptive scenario. A complete technical description of the FAULTING standalone code and equations are detailed in Ghosh, et al. (1997). FAULTO is executed in four major sequential steps as follows:

- Step 1: Parameters are determined from *tpa.inp*, Section 13.4.
- Step 2: Upon testing of the probability of occurrence of a NW fault, assign appropriate fault orientation (either NE or NW), and use appropriate fault length (either NE or NW) to calculate the fault midpoint coordinates.
- Step 3: Depending on the fault orientation, assign values of fault width, fault displacement, and values of cumulative displacement rate to faulting event.
- Step 4: With the defined fault parameters, determine which subareas are intersected by the fault, and calculate the time of failure of waste packages and the fraction of subareas that the fault intersected.

FAULTO does not require inputs from other modules, and all input parameters for FAULTO are specified in *tpa.inp*. To simulate the effects of a faulting disruptive event, the user must set the input parameter FaultingDisruptiveScenarioFlag(yes=1,no=0), as specified in *tpa.inp* to 1. In the reference case, this event flag is set to 0. When this parameter is set to 1, FAULTO calculates the time of waste package failure and the fraction of each potential repository subarea disrupted by direct faulting for subsequent use in radionuclide release calculations in EBSREL.

FAULTO initiates a new fault zone within the potential repository based on sampled geometric and recurrence parameters. A detailed list of parameters is provided in Table 13-1 (Section 13.4). For simplicity, these parameters are specified as independent parameters in TPA Version 5.1. Geometric parameters include fault-zone location (i.e., east-west and north-south coordinates of the center of the fault), fault orientation, fault length, fault-zone width,

and largest credible displacement of the fault. Recurrence parameters include time of faulting event and cumulative displacement rate.

The time of the next faulting event is determined by the *tpa.inp* parameter TimeOfNextFaultingEventInRegionOfInterest[yr]. Calculating the effective recurrence interval for faulting within the potential repository boundary is not straightforward because, unlike point-source events, fault zones are tabular volumes with planar boundaries that have orientation, length, and width. In TPA Version 5.1, fault orientation, fault length, and fault zone width are treated via parameters.

Recurrence rate does not scale directly with change in simulation area. There is a critical simulation region below which the recurrence interval does not increase in proportion to the reduction in the size of the simulation area. If the simulation region is smaller than the critical simulation area, a fault could still initiate outside the critical simulation area and have the necessary length and orientation to intersect the potential repository. To overcome this problem, an empirical solution uses an area of interest larger than the potential repository footprint (Mohanty, et al., 2002). This approach is described in the subsequent paragraph.

The critical simulation region for faulting was developed to include the range of fault orientations and length of faults (e.g., the fault map of Simonds, et al., 1995). Approximately 90 percent of the faults have lengths of 30 km [18.6 mi] or shorter or half-lengths of 15 km [9.3 mi] or shorter. In addition, fault orientations range between N55° W (azimuth 305°) and N25° E (azimuth 25°). Given these constraints, the size of the critical simulation region is 15.2 by 32.8 km [9.4 by 20.4 mi]. The ratio of the critical simulation region area to the area used to estimate faulting recurrence from paleoseismic studies is 2.2 (498.6 divided by 225.0). Thus, the scaled recurrence of the critical simulation region is 5,909 years (13,000 divided by 2.2), yielding a conditional probability for faulting of 1.69×10^{-4} /year.

In FAULTO, the recurrence value is then scaled to only the potential repository footprint to empirically estimate what percentage of faults generated in the critical simulation region would actually intersect the potential repository given a 5,909-year recurrence interval for the critical simulation region (Mohanty, et al., 2002). Previous modeling results show that an average of 3 percent of all simulated faults intersect the potential repository footprint, based on a number of different realizations between 500,000 and 1 million (Mohanty, et al., 2002). Thus, the recurrence interval for faulting within the potential repository itself is 197,000 years (5,909 divided by 0.03) or an annual probability of 5.0×10^{-6} (Mohanty, et al., 2002).

Using the time of the next faulting event for the potential repository footprint (i.e., the effective recurrence interval), as specified by the *tpa.inp* parameter TimeOfNextFaultingEventInRegionOfInterest[yr], FAULTO then uses the midpoint location, fault-zone width, and displacement of a fault in the potential repository. The displacement is assumed to be the same for the entire length of the fault. With the orientation and fault-zone width known, FAULTO calculates the intersection area of the fault with the potential repository. When the displacement exceeds the threshold displacement specified in *tpa.inp*, the fraction of the subareas in the intersection area is reported to CUMFAIL2 (Chapter 4) which converts it to the number of waste packages failed and subsequently reports this quantity to EBSREL. Otherwise, the new time of the fault event when the threshold displacement would be reached is determined by adding the threshold displacement, less the displacement divided by the cumulative displacement rate to the fault event time.

13.4 Input Parameters in *tpa.inp*

FAULTO is run when the event flag `FaultingDisruptiveScenarioFlag(yes=1,no=0)` located in *tpa.inp* is set to 1. Table 13-1 details the 17 input parameters used in FAULTO. Information supplied to FAULTO is located in *tpa.inp* and *drifts.dat*.

13.5 Auxiliary Input Data and External Process Models

FAULTO utilizes no information generated by an external process model. The *drifts.dat* file (Chapter 4) provides the orientation and location of the emplacement drifts within each of the subareas of the potential repository. FAULTO uses this information to determine the intersection area of the fault within the drifts in each subarea.

13.6 Intermediate Outputs and Information Passed to Other Modules

The intermediate output from FAULTO is available in *wpsfail.res*. For all realizations, *wpsfail.res* provides the number of waste packages failed and the time of waste package failure in a simulation. The *wpsfail.res* file is further described in Chapter 19.

In addition to *wpsfail.res*, the user can specify that calculated information passed to and from FAULTO be saved as intermediate output for specific realizations. Table 13-2 describes these optional intermediate output files. To specify the optional intermediate output files, the user can set *tpa.inp* parameter `OutputMode(0=None,1=All,2=UserDefined)` to a value of 1 or 2. When set to 1, all optional intermediate output for FAULTO will be saved for all realizations. When set to 2, optional intermediate output selected will be saved for realizations starting from *tpa.inp* parameter `UserDefinedLowerRealizationAppended` and ending with the realization specified by *tpa.inp* parameter `UserDefinedUpperRealizationAppended`. The user can select FAULTO optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter `SelectAppendFiles` to 5 for *faulto.ech* and *faulto.rlt*.

13.7 Techniques for Understanding Module Performance

While there is no single analysis that best provides insights into subsystem processes, different techniques can be used to better understand the relative effects of a FAULTO-modeled simulated faulting event. Parameters with significant uncertainties are sampled through probabilistic distribution functions. Several parametric sensitivity analyses can be conducted to understand these parameters' effects on system-level performance.

Table 13-1. Reference Data for Parameters of tpa.inp Used by FAULTO <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GLOBAL	FaultingDisruptiveScenarioFlag (yes=1,no=0)	Activates the faulting disruptive scenario calculations	iflag 0	This flag must be changed to 1 for a faulting event to occur. The reference case does not include faulting event, so the flag is set to zero.
FAULTO	TimeOfNextFaultingEventIn RegionOfInterest[yr]	Time of next faulting event [yr]	finite exponential 100.0, 10000.0, 2.0e-5	This is based on the probabilistic seismic hazard analyses for fault displacement and ground motion (CRWMS M&O, 1998).
FAULTO	ThresholdDisplacementForFault DisruptionOfWVP[m]	Threshold fault displacement estimated necessary to disrupt waste package [m]	constant 0.2	In the current design, there are two waste package clearance values: (i) open drifts: minimum clearance between waste package and drift wall is 1 m and (ii) drifts completely filled with rock rubble: minimal clearance between struts supporting drip shields on defense-type waste packages is 20 cm (CRWMS M&O, 2003). Thus the smallest clearance value was selected as the threshold for fault displacement that can cause waste package disruption.
FAULTO	XLocationOffFaultingEventIn RegionOfInterest[m]	X location of center of faulting event in region of interest [m]	uniform 547346.0, 549744.0	The center of the fault is to be located within the potential repository footprint. The westernmost and easternmost easting universal transverse mercator zone 11 coordinates of the footprint are 547346 and 549744, respectively (CRWMS M&O, 2003).
FAULTO	YLocationOffFaultingEventIn RegionOfInterest[m]	Y location of center of faulting event in region of interest [m]	uniform 4076112.4, 4081576.0	The center of the fault is to be located within the potential repository footprint. The southernmost and northernmost northing universal transverse mercator zone 11 coordinates of the footprint are 4076112.4 and 4081576.0, respectively (CRWMS M&O, 2003).

Table 13-1. Reference Data for Parameters of <i>tpa.inp</i> Used by FAULTO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
FAULTO	ProbabilityForNWOrientationOf Faults	Probability for NW orientation of faults [unitless]	constant 0.05	The initial module supported two fault populations (northeast and northwest). More recent data from the Exploratory Studies Facility and Enhanced Characterization of Repository Block show that faults at Yucca Mountain fall within a single distribution, with a mean strike of N10E (Stamatakis, et al., 2003). This probability is thus set low to effectively minimize the northwest set from the computations.
FAULTO	RNtoDetermineFaultOrientation	Random number to determine fault orientation [unitless]	uniform 0.0, 1.0	Based on a low probability of occurrence for the NW-oriented faults, this parameter is not important but remains to provide flexibility in computation.
FAULTO	NWFaultStrikeOrientationMeasured fromNorthClockwise[degrees]	NW strike orientation of fault measured from N clockwise [degrees]	constant - 32.5	Based on a low probability of occurrence for the northwest-oriented faults, this parameter is not important but remains to provide flexibility in computation.
FAULTO	NEFaultStrikeOrientationMeasured fromNorthClockwise[degrees]	NE strike orientation of fault measured from N clockwise [degrees]	constant 10.0	This is the mean value of fault orientations from Yucca Mountain fault data (Stamatakis, et al., 2003). The N10E orientation of fault intersecting the N72E orientation of the drift (CRWMS M&O, 2003) with a 62° angle disrupts an elevated number of waste packages.
FAULTO	NWFaultTraceLength[m]	NW fault trace length [m]	constant 6000.0	Based on a low probability of occurrence for the NW-oriented faults, this parameter is not important but remains to provide flexibility in computation.
FAULTO	NEFaultTraceLength[m]	NE fault trace length [m]	constant 6000.0	This parameter is set at the minimum fault length such that all faults generated by the model will transect the approximately 5,500-m-long potential repository footprint area (Stamatakis, et al., 2003).
FAULTO	NWFaultZoneWidth[m]	NW fault zone width [m]	lognormal 0.01 16, 62.8	Based on a low probability of occurrence for the NW-oriented faults, this parameter is not important but remains to provide flexibility in computation.
FAULTO	NEFaultZoneWidth[m]	NE fault zone width [m]	lognormal 0.01 16, 62.8	This is the best-fit distribution to the DOE exploratory studies facility fault data. (See Stamatakis, et al., 2003 for detailed data analysis.)

Table 13-1. Reference Data for Parameters of <i>tpa.inp</i> Used by FAULTO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
FAULTO	NWAmountOfLargestCredible Displacement[m]	NW fault displacement [m]	constant 0.2	This is set to the same value as the ThresholdDisplacementforFaultDisruptionOfWp[m] to ensure that each fault displacement results in waste package damage. For simulation periods longer than 10,000 years, the value and distribution type may need to be reconsidered to ensure that the effects of direct faulting are not overestimated.
FAULTO	NEAmountOfLargestCredible Displacement[m]	NE fault displacement [m]	constant 0.2	This is set to the same value as the ThresholdDisplacementforFaultDisruptionOfWp[m] to ensure that each fault displacement results in waste package damage. For simulation periods longer than 10,000 years, the value and distribution type may need to be reconsidered to ensure that the effects of direct faulting are not overestimated.
FAULTO	NWCumulativeDisplacement Rate[mm/yr]	NW cumulative displacement rate [mm/yr]	constant 5.0e-5	Given the typical 50,000-year fault recurrence rates at Yucca Mountain, cumulative displacement rates for faults are too small to affect the performance of the potential repository over the next 10,000 or 20,000 years (Ghosh, et al., 1997, Table 2-4) and were not considered important. Thus, this parameter, estimated for a 10,000-year period, is set to a minimum value. For a longer period of interest, the parameter may need to be reevaluated. Because TPA Version 5.1 simulations can be executed for different time periods, for example 1,000 years or 1 million years, a value of the cumulative displacement that simplifies the 10,000-year calculation was used in <i>tpa.inp</i> {see the parameters NWCumulativeDisplacementRate[mm/yr] and NECumulativeDisplacementRate[mm/yr]}. For longer simulation periods, the user should determine an appropriate value for these parameters, for example, by using information from the Electrical Power Research Institute (1993).

Table 13-1. Reference Data for Parameters of <i>tpa.inp</i> Used by FAULTO (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
FAULTO	NECumulativeDisplacementRate[mm/yr]	NE cumulative displacement rate [mm/yr]	constant 5.0e-5	Given the typical 50,000-year fault recurrence rates at Yucca Mountain, cumulative displacement rates for faults are too small to affect the performance of the potential repository over the next 10,000 or 20,000 years (Ghosh, et al., 1997, Table 2-4) and were not considered important. Thus, this parameter, estimated for a 10,000-year period, is set to a minimum value. For a longer period of interest, the parameter may need to be reevaluated. Because TPA Version 5.1 simulations can be executed for different time periods, for example 1,000 years or 1 million years, a value of the cumulative displacement that simplifies the 10,000-year calculation was used in <i>tpa.inp</i> (see the parameters NWCumulativeDisplacementRate[mm/yr] and NECumulativeDisplacementRate[mm/yr]). For longer simulation periods, the user should determine an appropriate value for these parameters, for example, by using information from the Electrical Power Research Institute (1993).

Table 13-2. Optional Intermediate Output Files Created During Execution of FAULTO	
File	Description
<i>faulto.rlt</i>	A file containing the fraction of subareas of waste packages failed by faulting events for all timesteps
<i>faulto.ech</i>	A file containing inputs to FAULTO, including timesteps and number of subareas

In addition, “pinch-point” techniques, wherein output produced from FAULTO can be understood in combination with output or intermediate results from other modules, for example EBSREL, may help to better evaluate subsystem processes. Simulation results from FAULTO are not directly comparable with results from other consequence modules, but the effect of waste package disruption by faulting might be better understood by comparing it with, for example, the effect of waste package disruption by an ascending basaltic magma through a conduit or a dike as simulated in the Igneous Disruptive Event Involving Magma module (VOLCANO). Two key output result files useful for these comparisons are *volcano.rlt* and *faulto.rlt*, which include data on failed waste packages.

Further, single parameter importance analyses can be performed by repetitively varying input parameters associated with particular FAULTO-modeled subsystem processes. Single parameter importance analyses can be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, a single parameter importance analysis can be performed by repetitively specifying smaller ranges within the parameter’s original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges. The user should exercise care in interpreting results from simulations in which inputs are altered beyond their intended ranges. Key input parameters and data that can ultimately influence pathway and dose calculations in FAULTO include geometric parameters such as the width and location of a fault found in *tpa.inp*.

As previously indicated, the width of the fault zone is one of the most important parameters in this module. By adjusting the width of a simulated fault zone within its assigned range, the resulting number and fraction of impacted subareas can be compared. Single parameter importance analyses can also be performed on the center of a simulated fault. For a given orientation and width, the center of a fault zone located on the edges of the potential repository footprint can intersect fewer emplacement drifts than a centrally located fault.

13.8 References

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14 IGNEOUS DISRUPTIVE EVENT INVOLVING MAGMA (VOLCANO)

The Igneous Disruptive Event Involving Magma module (VOLCANO)¹ simulates key potentially disruptive igneous processes related to the intrusion of basaltic magma rising along a dike or conduit within the potential repository footprint and possibly erupting at the surface. It determines the (i) timing of possible future igneous events, (ii) type of igneous event (i.e., intrusive only or intrusive and extrusive), (iii) location and number of failed waste packages, and (iv) mass of waste in metric tons of uranium (MTU)² released via the airborne pathway.

VOLCANO is included in a simulation when the disruptive scenario flag `VolcanismDisruptiveScenarioFlag` (1=yes, 0=no) in *tpa.inp* is set to 1. Information supplied to VOLCANO is located in *tpa.inp* and from the utility module `READER` in the form of drift endpoints (Chapter 4). Output from VOLCANO is used by the Engineered Barrier System Radionuclide Release module (EBSREL)³ (Chapter 10), the Igneous Activity Ash Remobilization module (ASHREMOB)⁴ (Chapter 15), the Igneous Activity Airborne Transport module (ASHPLUMO)⁵ (Chapter 16), and the Igneous Activity Deposition and Evolution of Ash module (ASHRMOVO)⁶ (Chapter 16).

14.1 Conceptual Model

The occurrence of igneous activity is a disruptive scenario with a relatively low annual probability of occurrence but potentially high radiological dose consequence. Models of igneous disruptive events at the potential repository involve the intersection of ascending magma by way of a dike or conduit with a drift(s), the advancement of magma into a drift(s), and the interaction between magma and waste packages. Dike/conduit–drift interactions reflect complexities within the volcanic plumbing and can therefore be difficult to model. For example, magma can ascend to the surface through one main volcanic conduit that exactly intersects a drift (Figure 14-1). Alternatively, secondary conduits can form, some possibly with horizontal magma flow developing between the conduits along the intersected drift(s). Also, magma ascending along a conduit intersecting a drift(s) can flow some distance into the drift before continuing its ascent to the surface along an offset conduit segment. Magma can intrude drifts along dikes several kilometers in length that never actually breach the surface. Because of this phenomenological complexity, VOLCANO is capable of considering a range of potential scenarios for the interaction of magma with waste packages.

¹The Igneous Disruptive Event Involving Magma module is referenced frequently throughout this chapter. The abbreviation VOLCANO will be used.

²Metric tons of uranium is referenced frequently throughout this chapter. The abbreviation MTU will be used.

³The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

⁴The Igneous Activity Ash Remobilization module is referenced frequently throughout this chapter. The abbreviation ASHREMOB will be used.

⁵The Igneous Activity Airborne Transport module is referenced frequently throughout this chapter. The abbreviation ASHPLUMO will be used.

⁶The Igneous Activity Deposition and Evolution of Ash module is referenced frequently throughout this chapter. The abbreviation ASHRMOVO will be used.

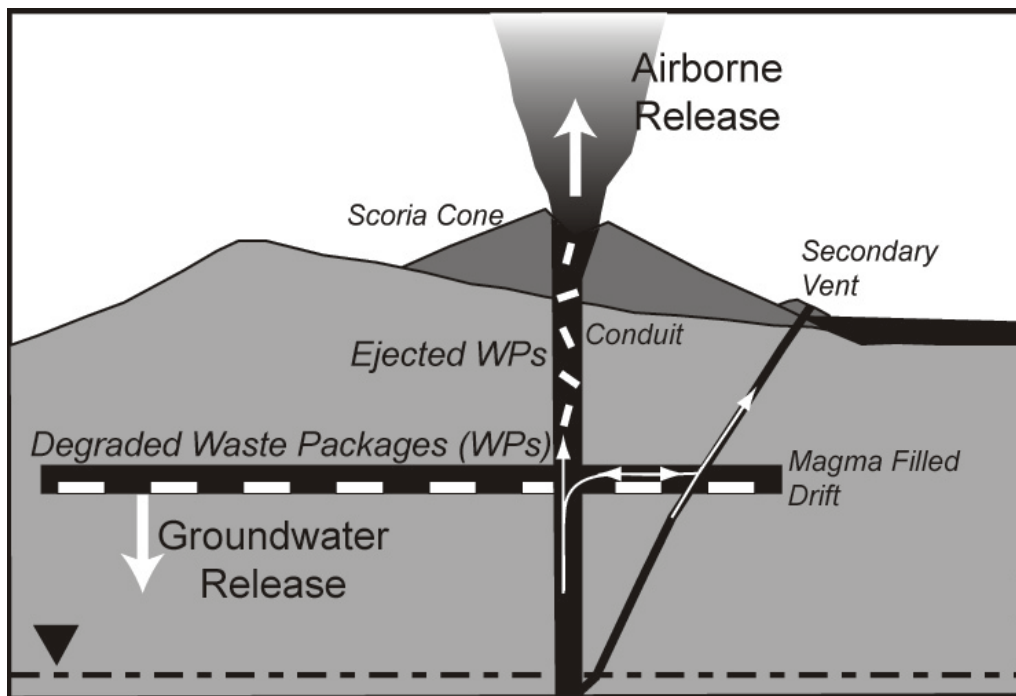


Figure 14-1. Schematic of Magma Ascending Along a Conduit/Dike, Intersecting and Filling a Drift, and Disrupting Waste Packages

Damage to waste packages and release of waste following these various event scenarios can be broadly categorized into two types of igneous events: extrusive or intrusive. Extrusive events involve the continued ascent of magma subsequent to intersection with a drift and an eruption at the surface. During its rise, magma can disrupt waste packages and directly transport high-level waste into the accessible environment via the airborne pathway. Intrusive events, on the other hand, do not include the direct transport of waste to the surface as part of the event. Instead, magma that flows into intersected drifts fails waste packages and makes their contents available for hydrologic transport after the event. An igneous event is always associated with a subsurface intrusion. In any model of repository disruption by igneous activity, magma ascending via a dike/conduit intersects the repository and invades a drift(s); waste packages fail and release waste whether that magma continues its ascent to the surface or not. Extrusive processes do not always occur during an igneous event.

14.2 Model Support and Assumptions

The development of a conduit during a volcanic event that intersects the potential repository can be straightforwardly abstracted for use in performance assessments. Field studies of historically active (Doubik and Hill, 1999) and ancient (Valentine and Groves, 1996) volcanoes show that subvolcanic conduits erode the surrounding wall rock throughout the course of an

eruption and eject this rock from the volcano. In a subsurface geologic repository, the processes of conduit erosion are not likely to differentiate between rock and waste packages. Thus, waste packages intersected by a conduit are expected to fail and their contents ejected.

Abstracting the growth of a dike within the footprint of the potential repository in an igneous intrusive scenario can also be a clear-cut exercise. Although initial dike–drift interactions involve complex magma flow processes, models indicate that pressurized magma will flow rapidly into unconfined drifts and fill intersected drifts with magma (Darteville and Valentine, 2005; Bechtel SAIC Company, LLC, 2004a; Woods, et al., 2002) . Thus, the performance assessment only needs to determine the number of drifts potentially intersected by magma rising along a dike and the number of waste packages per intersected drift; any drift intersected is expected to fill with magma and expose the encountered waste packages to thermo-mechanical stresses that exceed design capacities (NRC, 1999; Bechtel SAIC Company, LLC, 2004b).

VOLCANO is capable of considering magma–drift interactions following a range of alternative magma ascent pathways during intrusive and extrusive activity. To effectively abstract this range of potential event scenarios while maintaining efficiency, there are several important specific assumptions in VOLCANO:

- The event location (i.e., the volcanic conduit or the center of the dike) is assumed to form within the potential repository block consistent with calculated probabilities for volcano formation within the potential repository footprint (Hill and Stamatakis, 2002).
- The timing of an igneous event is modeled by a Poisson process that is homogeneous in time.
- Multiple conduits commonly are observed during historical eruptions [e.g., 1975 Tolbachik (Doubik and Hill, 1999)]. Additionally, observations from the < 5 million year basaltic volcanoes of the Yucca Mountain region suggest multiple conduits formed during single igneous events (NRC, 2005; 1999). Thus, multiple conduits can form during a volcanic disruptive event within the potential repository footprint. The effects of multiple conduits can be evaluated using TPA Version 5.1 by setting the *tpa.inp* parameter VolcanoModel(1=Geometric,2=Distribution) to a value of 2.
- Combined thermo-mechanical effects from magma exposure exceed the capabilities of the waste packages (NRC, 2005; Bechtel SAIC Company, LLC, 2004a,b); thus, all waste packages are assumed to fail when they are engulfed by basaltic magma. Other thermal or degassing processes that affect waste package degradation or affect nondisturbed repository performance do not appear capable of significantly affecting waste package performance (NRC, 2005; Bechtel SAIC Company, LLC, 2004a,b). Thus, these processes are not considered in the current module. Waste packages failed by extrusive processes are confined to the conduit, including horizontal flow in drifts along offset conduits.

- In TPA Version 5.1, waste packages only fail by an igneous disruptive event once. Thus, waste packages failed by VOLCANO are not available to fail again at a later time by another disruptive event [e.g., Direct Faulting Disruptive Event module (FAULTO)⁷ (Chapter 13)].

14.3 Implementation of Conceptual Model in TPA Version 5.1

VOLCANO is activated when VolcanismDisruptiveScenarioFlag(1=yes,0=no) in *tpa.inp* is set to 1. The key function of VOLCANO is to determine waste package failure resulting from igneous activity; VOLCANO uses two different methods for each type of igneous event (i.e., extrusive and intrusive). The first method, herein called the geometric model, abstracts a simplified geometric relationship between ascending magma and the potential repository and therefore uses geometric constraints to calculate the number of waste package failures. However, it is unable to directly account for complexities related to volcanic plumbing such as multiple conduits or magma flow offset horizontally along a drift. Field observations at historical eruption sites suggest these alternative scenarios are common and should be considered a reasonable possibility. To appropriately consider the effects of these various eruption scenarios, a second method was developed which utilizes a user-defined distribution; the distribution model uses process-based constraints to evaluate waste package disruption.

The *tpa.inp* parameter VolcanoModel(1=Geometric,2=Distribution) selects the model. When the *tpa.inp* parameter ExtrusiveEventFlag(extrusive=1,intrusive=0) is set to 1, the model selected by the user is used to determine waste packages failed by both extrusive and intrusive processes (i.e., the user cannot use the distribution model to determine waste packages failed by extrusive processes and the geometric model to determine waste packages failed by intrusive processes in a single realization).

14.3.1 Geometric Model

In the geometric extrusive model, a single volcanic conduit forms that is continuous from a magma source located at some depth below the potential repository to the surface within the potential repository footprint and is centered on a drift. Although the geometry of subvolcanic conduits is often irregular and complex, the information that is relevant to performance assessment is the effective area of rock that is eroded and ejected. This area can be represented by a simple cylinder.

In TPA Version 5.1, the values of *tpa.inp* parameters DiameterOfVolcanicConduit[m] and SubareaOfVolcanicEvent[] determine the effective diameter of the volcanic conduit and the subarea in which the conduit is located, respectively. The diameter is used to calculate the number of failed waste packages and the amount of waste in MTU available for release via the airborne pathway. Considering the length and spacing of the waste packages, the number of waste packages that can be positioned within the diameter of the conduit is derived (Figure 14-2).

⁷The Direct Faulting Disruptive Event module is referenced frequently throughout this chapter. The abbreviation FAULTO will be used.

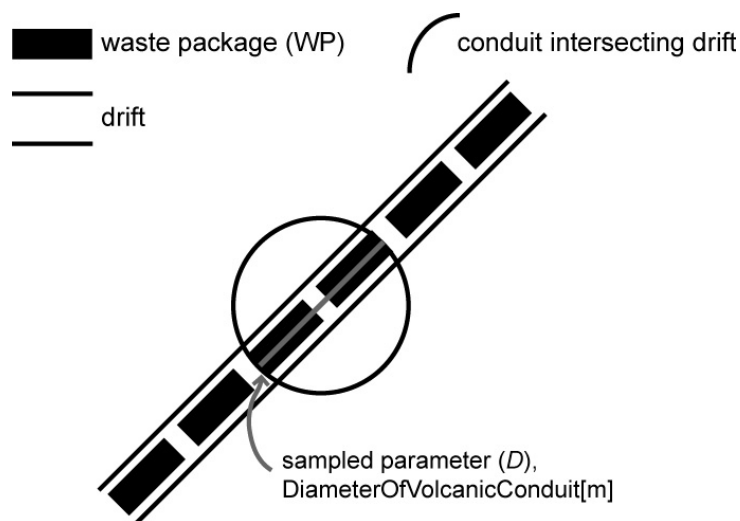


Figure 14-2. Schematic Showing the Derivation of Number of Waste Packages Ejected for an Extrusive Event in the Geometric Model

The total mass of waste ejected is then determined by simply multiplying the number of waste packages by the mass of waste per package

$$X_{\text{ejected}} = (D/S)X_{\text{WP}} \quad (14-1)$$

where

- X_{ejected} — mass of high level waste ejected into the accessible environment following an airborne pathway [MTU]
- D — effective diameter of volcanic conduit as specified by the *tpa.inp* parameter DiameterOfVolcanicConduit[m]
- S — spacing between waste packages in the drift as specified by the *tpa.inp* parameter WPSpacingAlongEmplacementDrift[m], which is defined in the Near-Field Environment module (NFENV)⁸ (Chapter 7)
- X_{WP} — mass of waste in MTU per representative waste package calculated in READER (Chapter 4)

During an intrusive event, magma ascends along a dike through the potential repository footprint and thereby intersects a drift(s). Because of the significant pressure differences between ascending magma and open drifts, magma intersecting a drift will flow into that drift (NRC, 2005; Woods, et al., 2002; Bechtel SAIC Company, LLC, 2004a). The combined thermo-mechanical effects of magma emplacement cause waste packages to fail and allow the contained high-level waste to be released through subsequent hydrologic flow and transport processes.

⁸The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

In the geometric intrusive model, magma fills all drifts intersected by the dike, and all the waste packages within each intersected drift fail. To determine which drifts are intersected, first the event center has to be located along a drift centerline. Drift length is calculated using the endpoints of each drift, and these lengths are summed to find a total drift length. The value of the *tpa.inp* parameter `RNToDetermineCenterOfVolcanicDike[]` is applied to the total drift length to determine the dike center position. This intrusive event location is selected regardless of whether an extrusive event occurred, and if it did occur, regardless of the subarea sampled for conduit formation. Therefore, it is possible that the subareas the dike intersects do not include the subarea with the conduit. After the dike center location is found, the *tpa.inp* parameters `AngleOfVolcanicDikeMeasuredFromNorthClockwise[degrees]` and `LengthOfVolcanicDike[m]` are sampled to determine values for dike angle and length, respectively. The number of failed waste packages per subarea is ascertained using the portion within a subarea of drifts intersected by the dike and assumed filled with magma.

14.3.2 Distribution Model

The distribution extrusive model is an alternative method for assessing the amount of waste released during a volcanic eruption within the potential repository footprint. It was designed to include variations in volcanic plumbing (e.g., secondary conduits) and possible effects of a subsurface repository on conduit development (e.g., an offset conduit) not captured in the geometric extrusive model (Figure 14-1). Rather than constructing a model based on simplified geometries, the distribution extrusive model uses a user-defined distribution to evaluate alternative eruption scenarios.

In the distribution extrusive model, sampling a value for the parameter `SubareaOfVolcanicEvent[]` determines the subarea in which waste packages fail by extrusive processes. The number of waste packages disrupted by conduit flow is determined by sampling a value for the *tpa.inp* parameter `NumberOfWPsEntrainedByEjecta[]`, representing the number of failed waste packages following horizontal magma flow through a drift. The amount of waste released (in MTU) to the accessible environment along an airborne release pathway can be directly determined from the number of disrupted waste packages based on the average MTU per waste package

$$X_{\text{ejected}} = (N_{\text{ex}})X_{\text{WP}} \quad (14-2)$$

where

X_{ejected} — mass of high-level waste ejected into the accessible environment following an airborne pathway [MTU]

N_{ex} — number of waste packages disrupted during extrusive igneous activity as specified by the *tpa.inp* parameter `NumberOfWPsEntrainedByEjecta[]`

X_{WP} — mass of waste in MTU per representative waste package; calculated in READER (Chapter 4)

Similar to the geometric intrusive model, the distribution intrusive model is based on the concept that subsurface igneous intrusions can affect more waste packages than those directly in the path of magma rising along an intersecting conduit/dike. Once ascending magma breaches a drift, it can flow freely into the intersected drift and fill it; waste packages subsequently fail and waste is released via groundwater pathways. The user can evaluate the effects of this process by considering the number of waste packages failed, but not erupted directly, by a

repository-penetrating igneous event through multiple drifts. The value for the *tpa.inp* parameter `NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[]` decides this fraction. It is applied to each subarea to obtain the number of failed waste packages per subarea.

14.4 Input Parameters in *tpa.inp*

Table 14-1 presents the input and correlated parameters VOLCANO uses to determine the time of the igneous event, the type of igneous activity (extrusive and/or intrusive), the amount of waste released due to failure of waste packages by volcanic disruption, and the number of waste package failures per subarea. VOLCANO is run when the event flag `VolcanismDisruptiveScenarioFlag(1=yes,0=no)` in *tpa.inp* is set to 1 (Table 14-2). Information supplied to VOLCANO is located in *tpa.inp* and *drifts.dat* (Chapter 4). VOLCANO also uses the mass of waste in a representative waste package as determined in READER (Chapter 4).

14.5 Auxiliary Input Data and External Process Models

VOLCANO utilizes no auxiliary input data or external process models.

14.6 Intermediate Outputs and Information Passed to Other Modules

VOLCANO defines the source term for high-level waste transport by a basaltic volcanic eruption. It determines the (i) timing of the volcanic event, (ii) amount of waste released via the air pathway (transport by an eruption column), and (iii) fraction of waste packages in a failed subarea disrupted by magma.

VOLCANO records waste package failure time from an igneous event for all subareas in *wpsfail.res*. This file is also used to pass the number of waste packages failed by magma flow into drifts (i.e., igneous intrusions) for all subareas to EBSREL for groundwater source-term calculations; *wpsfail.res* is further described in Chapter 19. The mass of waste (in MTU) ejected by a volcanic event is passed to either ASHPLUMO and then ASHRMOVO or ASHREMOB for ground surface radionuclide release calculations (Figure 14-3). The event flag `AshEvolutionMode[0=no_ashremob,1=ashremob]` in *tpa.inp* determines the destination for the ejected waste (Chapter 15).

In addition to the previously noted output file, the user can specify that calculated information passed to and from VOLCANO be saved as intermediate output for specific realizations. Table 14-3 lists and describes these optional intermediate output files. To specify the optional intermediate output files, the user can set *tpa.inp* parameter `OutputMode(0=None,1=All,2=UserDefined)` to a value of 1 or 2. When set to 1, all optional intermediate output for VOLCANO is saved for all realizations. When set to 2, optional intermediate output selected is saved for realizations starting from *tpa.inp* parameter `UserDefinedLowerRealizationAppended` and ending with the realization specified by *tpa.inp* parameter `UserDefinedUpperRealizationAppended`. The user can select VOLCANO optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter `SelectAppendFiles` to 6 for *volcano.rlt* and *volcano.ech*.

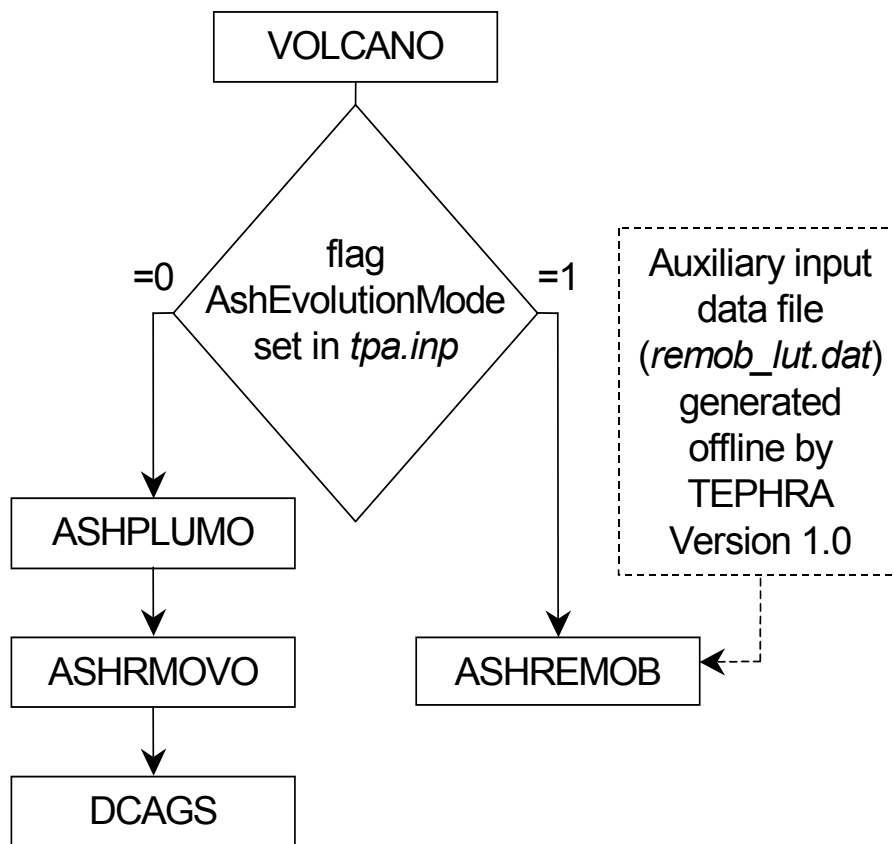


Figure 14-3. Information Flow Diagram for VOLCANO

Table 14-1. Reference Data for Parameters of tpa.inp Used by VOLCANO <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Disruptive Scenario Flags	VolcanismDisruptiveScenario Flag (1=yes, 0=no)	Activates the igneous activity disruptive scenario calculations	iflag 0	This flag must be set to 1 for the igneous disruptive scenario to occur, the nominal scenario does not include disruptive scenarios.
VOLCANO	VolcanoModel (1=Geometric, 2=Distribution)	Use geometric constraints (1) or process-based constraints (2) on waste package disruption	iconstant 1	Program control parameter used to select different methods of calculating the number of waste package failures; geometric model uses geometric constraints, and distribution model uses constraints based on processes (NRC, 2005; Woods, et al., 2002).
VOLCANO	TimeOfNextVolcanicEvent in RegionOfInterest[yr]	Time of next volcanic event [yr]	finite exponential 100.0, 10000.0, 1.0e-7	Technical basis for an estimated probability of volcanic disruption of the potential repository site is explained in NRC (2005, 1999) and Hill and Stamatakos (2002). This distribution is not significantly different than the probabilities being considered between 100 and 10,000 years postclosure. The annual probability of occurrence for igneous events of 10^{-2} was determined from performance assessment and the range of credible models in NRC (1999).

Table 14-1. Reference Data for Parameters of tpa.inp Used by VOLCANO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
VOLCANO	ExtrusiveEventFlag(extrusive=1, intrusive=0)	Flag set to 1 when there is an extrusive event in addition to intrusive event or 0 when there is only an intrusive event	iflag 1	User option.
VOLCANO	SubareaOfVolcanicEvent[]	Subarea where extrusive igneous event occurs [unitless]	iuniform 1, 10	Subarea from which waste packages are ejected.
VOLCANO	RNToDetermineCenterOf VolcanicDike[]	Dike center located randomly along the drift centerlines found in <i>drifts.dat</i> (for VolcanoModel=1) [unitless]	uniform 0.0, 1.0	Selects a location as the basis for a dike of sampled angle and length from a distribution of all points located within the potential repository along the drift centerlines.
VOLCANO	AngleOfVolcanicDikeMeasured FromNorthClockwise[degrees]	Dike angle (for VolcanoModel=1) [degrees]	uniform 0.0, 15.0	The orientation of planar, vertical igneous intrusions (i.e., dikes) at shallow crustal levels is controlled by the three-dimensional distribution of crustal stress (Anderson, 1938; Delaney, et al., 1986). In addition, preexisting crustal structures, such as faults, can serve as conduits for ascending magma at shallow crustal levels (Young, et al., 1994; Jolly and Sanderson, 1997). Although the current direction of maximum horizontal compressive stress at Yucca Mountain is oriented 28° from north, faults at the potential repository site are oriented between 0° and 15° from north (Morris, et al., 1996). This serves as the most likely orientation direction for future igneous intrusions at the potential repository site.

Table 14-1. Reference Data for Parameters of tpa.inp Used by VOLCANO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
VOLCANO	LengthOfVolcanicDike[m]	Length of volcanic dike (for Volcano Model=1) [m]	uniform 2000.0, 11000.0	Few data are available on dike lengths for the Yucca Mountain region. Connor, et al. (1997) summarize volcanic alignment data that are consistent with subsurface dike lengths between 2 and 11 km [1.2 and 6.8 mi] for 5 Myr and younger Yucca Mountain region volcanoes. A detailed geologic map by Gartner and Delaney (1988) of the San Rafael volcanic field, Utah, provides length information for more than 200 basaltic dikes that were originally emplaced 0.5–1.5 km [0.3–0.9 mi] from the surface (Delaney and Gartner, 1997). The length range of 2–8 km [1.2–5.0 mi] accounts for the range observed by Gartner and Delaney (1988) and Yucca Mountain region vent alignment lengths (Connor, et al., 1997).
VOLCANO	DiameterOfVolcanicConduit[m]	D Effective diameter of volcanic conduit (forVolcano Model=1) [m]	uniform 5.0, 50.0	Subsurface conduits for basaltic scoria cone volcanoes have roughly cylindrical conduits with these diameters at depths comparable to the potential repository drifts (NRC, 2005; Doubik and Hill, 1999). Used to calculate number of waste packages ejected during an extrusive event in the geometric model.
VOLCANO	NumberOfWPsEntrainedBy Ejecta[]	N_{ex} Number of waste packages that fail during a volcanic event and are erupted (for VolcanoModel=2) [unitless]	Beta 1.0, 150.0, 1.0, 2.0	User-supplied distribution for an example alternative conceptual model that abstracts a process in which ascending basaltic magma intersects a drift, fills drift with magma, and fractures drift roof to entrain waste in resulting volcanic conduit (NRC, 2005; Woods, et al., 2002). Points of initial magma intersection with drift and breakout through roof can vary randomly (NRC, 1999), entraining 1 to 150 waste packages per drift using simplified panel widths and average waste package spacing of 5.5 m [18.0 ft] (Bechtel SAIC Company, LLC, 2005).

Table 14-1. Reference Data for Parameters of tpa.inp Used by VOLCANO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
VOLCANO	NormalizedMagmalInduced MechanicalFailuresRemainingIn Drift[]	Failure factor applied to all subareas based on number of waste packages that fail during an intrusive event and remain in the intersected drifts (for VolcanoModel=2) [unitless]	usersuppliedpwiscdf 19 0.0, 0.0 8.941e-6, 0.084 0.01788, 0.094 0.05364, 0.117 0.08941, 0.141 0.1252, 0.175 0.1609, 0.213 0.1886, 0.257 0.1887, 0.475 0.2527, 0.562 0.2813, 0.588 0.2814, 0.712 0.4470, 0.781 0.5633, 0.813 0.6974, 0.843 0.8156, 0.881 0.8157, 0.967 0.8444, 0.969 0.8445, 1.0	Example of a user-supplied distribution to abstract an alternative conceptual model in which ascending basaltic magma intersects drifts and fills them with magma, causing all waste packages in each intersected drift to fail (NRC, 2005). Based on panel widths of 500–700 m [1,640–1,970 ft], distribution is calculated using a simplified model of the potential repository footprint with randomly located dikes of length 2–10 km [1.2–6.0 mi]. The maximum number of failed waste packages remaining in the drift is 9,445, which was normalized to a total package count of 11,184 (Bechtel SAIC Company, LLC, 2003).
NFENV	WPSpacingAlongEmplacement Drift[m]	Waste package spacing [m]	constant 5.265	Approximation using design specifications presented in Bechtel SAIC Company, LLC (2005).

Table 14-2. Input Flags Used by VOLCANO	
Input Flag Name	Description
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	This flag activates the igneous activity disruptive scenario calculations.
VolcanoModel(1=Geometric,2=Distribution)	This flag selects the source-term model used to calculate waste package failures by intrusive and extrusive processes. The geometric model is set as the reference case.
ExtrusiveEventFlag(extrusive=1,intrusive=0)	This flag determines the occurrence of an extrusive igneous event. An extrusive event occurs in the reference case. When set to 1, both extrusive and intrusive events occur.

Table 14-3. Optional Intermediate Output Files Created During Execution of VOLCANO	
File	Description
<i>volcano.rlt</i>	A file containing output from VOLCANO: inventory ejected, inventory of intrusive waste package failures by subarea, and fraction of waste packages failed from volcanic activity by time and subarea
<i>volcano.ech</i>	A file containing input to VOLCANO that includes information timesteps

14.7 Techniques for Understanding Module Performance

Many different approaches can be taken to evaluate the effects of disruptive events involving igneous activity simulated by VOLCANO. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques may be useful to understand their effects on system-level performance.

While a comparison between output and intermediate results from two different consequence models can provide insights into subsystem processes, results produced from VOLCANO are difficult to compare to results from other consequence modules; no other module abstracts disruption of waste packages by basaltic magma. However, the relative effects of igneous activity processes might be better understood in combination with the effects of other disruptive event process models (e.g., FAULTO). For instance, waste package failure data found in *wpsfail.res*, *volcano.rlt*, and *faulto.rlt* might be compared.

Additionally, single parameter importance analyses for VOLCANO can be performed by repetitively varying input parameters associated with a particular igneous process {e.g., DiameterOfVolcanicConduit[m]}. For instance, an analysis examining the relationship between the amount of waste ejected (in MTU) and the conduit diameter can be performed by

repeatedly specifying smaller ranges within the assigned distribution {e.g., 5–50 m, 10–45 m, 15–40 m [16–164 ft, 33–150 ft, 50–130 ft]} and considering the release output. (Caution should be exercised when interpreting results from simulations in which input are altered beyond their intended ranges; many complex couplings can occur between parameters that can introduce unsupportable results.) A similar sensitivity analysis has been performed in a study that considered the ability of volcanic activity to release high-level waste to the accessible environment (NRC, 2001), and conduit diameter was one of the parameters of interest. This analysis effectively showed that using a single variable approach to examine the variations in ground surface dose produced by variations in conduit diameter is a straightforward means to study dose response.

A few more possible analyses the user can employ to examine module performance follow.

- The amount of waste released by intrusive events alone can be examined by setting ExtrusiveEventFlag(extrusive=1,intrusive=0) to 0 in *tpa.inp*. Once set to intrusive, in the geometric model LengthOfVolcanicDike[m] in *tpa.inp* can be constrained to either 2 or 11 km [1.2 or 7.8 mi] to compare the effects of event size on dose.
- The amount of waste released via the airborne pathway, can be compared to the amount released via the groundwater pathway. Variations in dose can be examined simply by turning the extrusive event flag on and off [ExtrusiveEventFlag(extrusive=1,intrusive=0)] in *tpa.inp*.
- The mass of waste calculated for airborne release and delivered to either ASHPLUMO and ASHRMOVO or ASHREMOB can be compared using the geometric and the distribution models [toggle between values for the event flag VolcanoModel(1=Geometric,2=Distribution)]. The distribution model allows for alternative eruption scenarios that affect more waste packages (e.g., an offset conduit).

14.8 References

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15 IGNEOUS ACTIVITY ASH REMOBILIZATION (ASHREMOB)

The objective of this chapter is to describe an abstracted model for the Igneous Activity Ash Remobilization module (ASHREMOB)¹ in TPA Version 5.1 for estimating inhalation doses to the receptor. This abstraction assesses the redistribution of radionuclides in soil and biosphere characteristics. This abstraction uses the results from abstractions of the Igneous Disruptive Event Involving Magma module (VOLCANO)² (Chapter 14), including the entrainment of high-level waste in the eruption conduit and airborne transport of radionuclides [offline simulations of the TEPHRA Version 1.0 code (hereafter TEPHRA Version 1.0) that specify auxiliary input data]. Based on the insight that the estimated total dose for extrusive volcanism is dominated by the inhalation of resuspended volcanic ash (NRC, 2005), ASHREMOB was developed to calculate doses only for the inhalation pathway, as described in this chapter.

ASHREMOB provides improved estimates of volcanic eruption consequences by accounting for (i) wind-field variations along the height of the eruption column, which affect the initial deposition of tephra, and (ii) first-order processes affecting fluvial and eolian redistribution of tephra. Results from detailed analytical work on airborne transport of radionuclides and redistribution of radionuclides in soil are assimilated into TPA Version 5.1 as an auxiliary input data file (i.e., *remob_lut.dat*) and as *tpa.inp* parameter values. VOLCANO provides the mass of high-level waste ejected to ASHREMOB. Other inputs are described in Section 15.3 [see Eq. (15-1)]. ASHREMOB computes time histories of airborne concentrations of high-level waste and inhalation doses. Although ASHREMOB is executed in the reference-case simulations for the igneous disruptive scenario, the igneous disruptive scenario calculations are not performed for the nominal scenario. Refer to the flag settings in Section 15.4 for executing the igneous disruptive scenario.

Abstracted models for the Igneous Activity Airborne Transport module (ASHPLUMO)³ (Chapter 16), the Igneous Activity Deposition and Evolution of Ash module (ASHRMOVO)⁴ (Chapter 16), and the Dose Conversion Analysis for Ground Surface module (DCAGS)⁵ (Chapter 17) are also mentioned in this chapter. ASHPLUMO/ASHRMOVO and DCAGS describe the other abstracted models for eruptive igneous consequences, which use a single wind direction and a single wind speed for calculating the atmospheric transport of tephra contaminated with high-level radioactive waste and deposition of tephra at a point on the ground surface near the receptor.

¹The Igneous Activity Ash Remobilization module is referenced frequently throughout this chapter. The abbreviation ASHREMOB will be used.

²The Igneous Disruptive Event Involving Magma module is referenced frequently throughout this chapter. The abbreviation VOLCANO will be used.

³The Igneous Activity Airborne Transport module is referenced frequently throughout this chapter. The abbreviation ASHPLUMO will be used.

⁴The Igneous Activity Deposition and Evolution of Ash module is referenced frequently throughout this chapter. The abbreviation ASHRMOVO will be used.

⁵The Dose Conversion Analysis for Ground Surface module is referenced frequently throughout this chapter. The abbreviation DCAGS will be used.

15.1 Conceptual Model

Consequences of a low probability, extrusive volcanic event are modeled in VOLCANO and other modules for a subsurface volcanic conduit that directly intersects the potential repository at Yucca Mountain. In eruption simulations, waste package entrainment by magma flowing in the potential conduit results in the release of high-level waste as trace contamination of the erupting tephra, with subsequent atmospheric transport and deposition on the ground surface modeled using TEPHRA Version 1.0. Following initial deposition from the plume, redistribution (or remobilization) occurs through the long-term transport of tephra by wind (eolian remobilization) and surficial water drainage in Fortymile Wash (fluvial remobilization). Figure 15-1 illustrates that the direction of fluvial remobilization of contaminated tephra is toward the hypothetical receptor location south of the potential repository. Resuspension of ash particles {i.e., tephra <2 mm [0.08 in]} produces airborne concentrations of ash and associated high-level waste, referred to as the airborne mass load. The estimated total dose for extrusive volcanism, which is dominated by the inhalation of resuspended volcanic ash, is significantly influenced by the amount of ash particles in the air (NRC, 2005). Ash redistribution processes may significantly affect estimates of contaminated ash in the airborne mass load used for calculating inhalation dose to the receptor.

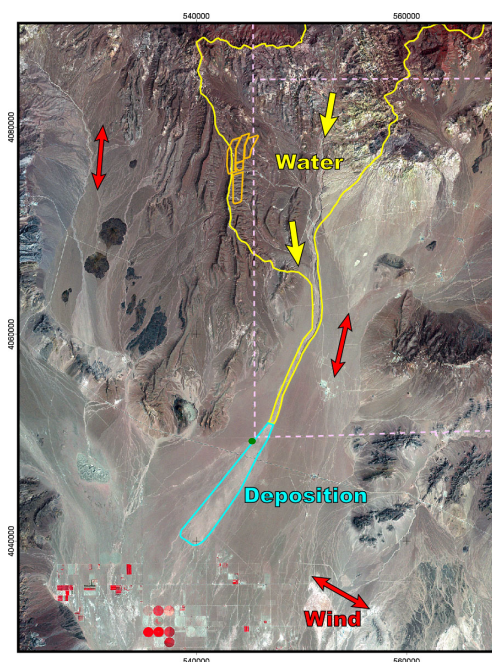


Figure 15-1. Satellite Image Showing the Fortymile Wash Catchment Basin (Yellow Line), Depositional Fan (Blue Shape), Potential Repository Site (Set of Adjacent Orange Shapes), Nevada Test Site Boundary (Dashed Magenta Line), Location for Determining Any Initial Tephra Deposit at the Receptor (Small Green Point Near the Corner of the Nevada Test Site Boundary), General Direction of Water Flow in Fortymile Wash (Yellow Arrows), and General Trends of Near-Surface Winds (Red Arrows)

A conceptual model was formulated to address the potential remobilization and redistribution of contaminated tephra in the Fortymile Wash drainage system (Hooper, 2005). A sediment budget was constructed to account for long-term fluvial redistribution processes in the Fortymile Wash drainage system (Hooper, 2005). Following a potential volcanic eruption, a submillimeter- to meter-thick layer of tephra may be deposited on the hillslopes around Yucca Mountain that are part of the Fortymile Wash watershed.

Surface processes subsequently may remobilize and redistribute the tephra deposit. Through time, potentially significant amounts of resuspendible particles containing high-level waste may be transported to the general area of the receptor. Results from the process-level conceptual model development, based on observations at actual eruptions, and detailed analyses (Hooper, 2005) were directly factored into the development of this abstracted model for TPA Version 5.1 (Benke, et al., 2006; Hooper and Benke, 2006).

ASHREMOB accounts for three components of the airborne concentration of high-level waste through time at the receptor location: (i) the contribution from any ash initially deposited at the receptor location, (ii) the contribution from the later fluvial remobilization of ash, and (iii) the contribution from the later eolian remobilization of ash. The airborne concentration of high-level waste through time at the receptor location is determined as the sum of these three contributions. Figure 15-2 shows the three components and the sum for an example eruption that deposits ash in each of the three source regions. The example shown corresponds to an eruption that deposits ash in each of the three source regions. Because modeled eruptions may not always deposit ash in all three source regions, there may be some realizations in which at least one of the three contributions is zero. The total airborne concentration of high-level waste available for inhalation by the receptor is calculated as the sum of outdoor, indoor, and offsite contributions. The remainder of this chapter describes the abstracted model for tephra redistribution and resuspension in the Yucca Mountain region (i.e., ASHREMOB, invoked when the AshEvolutionMode flag is set to 1). When ASHREMOB is invoked, ASHPLUMO, ASHRMOVO, and DCAGS are automatically not used in TPA Version 5.1 calculations. As mentioned previously, ASHREMOB is used to calculate inhalation doses only.

15.2 Model Support and Assumptions

Based on the previous insight that the estimated total dose for extrusive volcanism is dominated by the inhalation of resuspended volcanic ash (NRC, 2005), ASHREMOB accounts for only the inhalation pathway. There are no calculations for other pathways (such as external irradiation from the contaminated ground surface). Because leaching of radionuclides in soils is not expected to be a significant process (NRC, 2005, Appendix D, Section 4.3.13.1), explicit treatment for leaching is not included in ASHREMOB.

To calculate the airborne concentration of high-level waste at the receptor location, weighting factors are used to account for contributions from the three source regions (i.e., initial deposit at the receptor location, fluvial remobilization, and eolian remobilization). The weighting factors convert the airborne concentration of high-level waste above each source region to a concentration available for inhalation by the receptor. The airborne mass loading model for tephra from an initial deposit at the receptor location is similar to the model used in DCAGS described in Chapter 17. The main difference is that ASHREMOB accounts for receptor exposure from multiple sources of contamination, in contrast to a single contamination source in DCAGS.

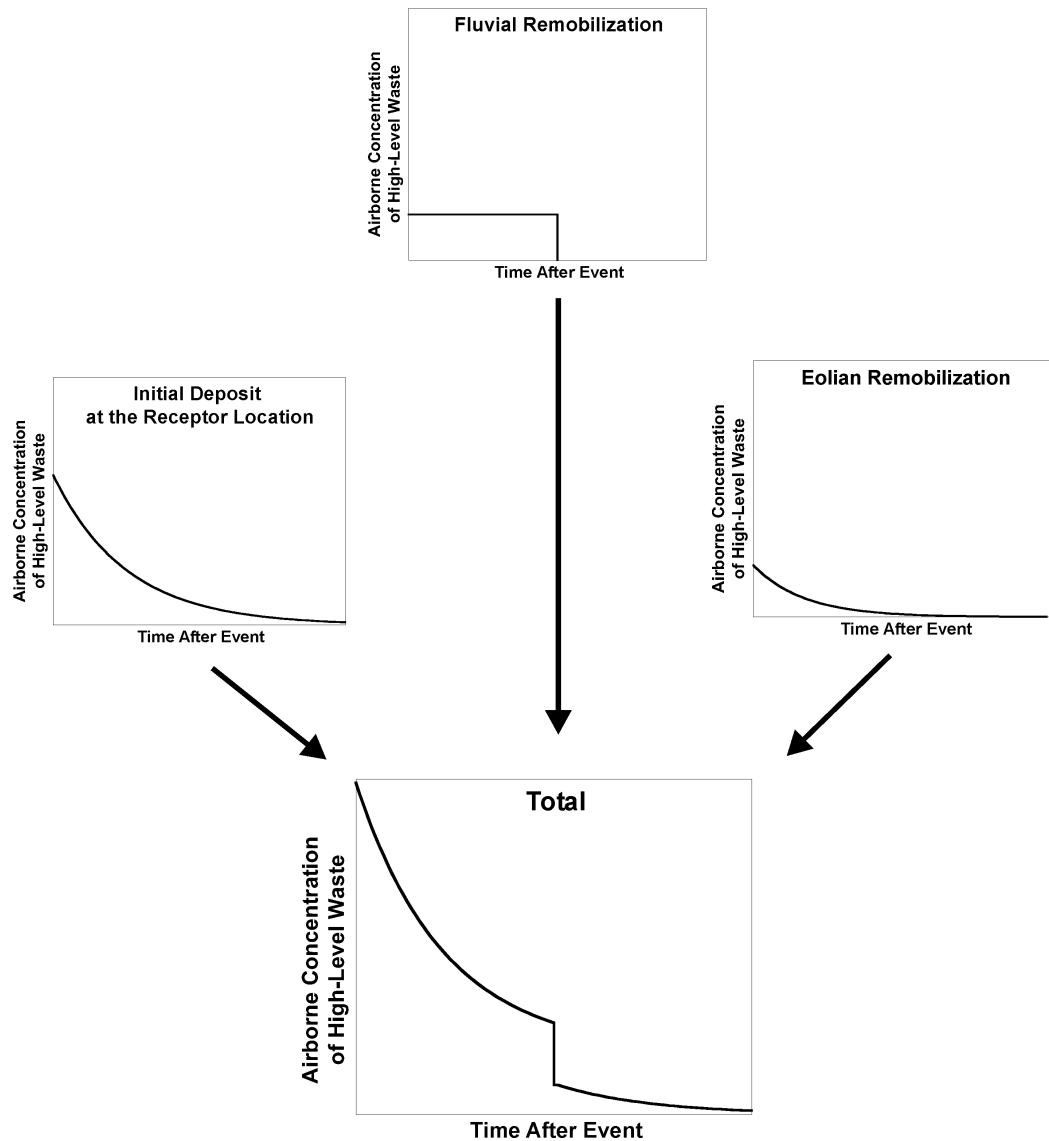


Figure 15-2. Schematic Representation of the Time Evolution of the Total Airborne Concentration of High-Level Waste at the Receptor Location Resulting From Contributions From the Initial Deposit at the Receptor Location, Fluvial Remobilization, and Eolian Remobilization

For the fluvial remobilization contribution, observations at actual eruptions suggest that fluvial remobilization events are frequent enough to periodically replenish the deposition region of Fortymile Wash with fresh sediment (Hill and Connor, 2000; Hooper, 2005). The Yucca Mountain region outside of the Fortymile Wash drainage system is generally characterized by desert pavements of coarse, interlocking clasts that effectively armor the underlying soil from wind entrainment (Middleton, 1997). Tephra deposits from the original eruption plume would be affected by geomorphologic processes and are expected to weather in place to form a stable deposit (i.e., less susceptible to airborne resuspension). Compared to stationary old tephra, fresh deposits of remobilized tephra could be more susceptible to resuspension.

The estimated mass load of ash in the Fortymile Wash catchment basin is assumed to remain approximately constant with time due to flood events that are frequent relative to the time frame for development of a desert pavement. In other words, the airborne mass load at the deposition region of Fortymile Wash is modeled as constant between the time of the eruption and $t_{\text{duration},f}$ which represents the time for fluvial remobilization to deplete the ash from the Fortymile Wash catchment basin [Eq. (15-13)]. This modeling assumption is applied to airborne mass loading estimates from fluvially remobilized tephra to account for potential increases in the susceptibility to airborne resuspension.

ASHREMOB accounts for fluvial remobilization by maintaining an elevated airborne mass load for the time period that Fortymile Wash yields contaminated sediment. Uniform mixing of remobilized ash and clean sediment is used to account for the dilution of radionuclides in fluvial deposits. The abstraction does not model individual flood events and does not calculate the thickness of fluvial sediment on the depositional area from each flood event. Time between events (e.g., the eruption or fluvial remobilization events) is not computed. The abstraction effectively assumes that each deposit of fluvial sediment has a thickness that is greater than the resuspendible layer thickness. In general, the susceptibility of fluvial sediments to airborne resuspension is expected to decrease with time. The abstraction, however, does not reduce the airborne mass load over fluvial deposits with time because older fluvial sediment would be buried by newer deposits of fresh fluvial sediment from subsequent flood events. Under certain circumstances, fresh fluvial sediment (e.g., from a small flood event) may be thinner than the resuspendible layer thickness, which represents a condition where the resuspendible layer thickness contains both fresh (more susceptible to resuspension) and old (less susceptible to resuspension) fluvial sediment. The net effect of this condition is a potential reduction to the airborne mass load. Based on the short time in between flood events (T_f ; see Table 15-1), the effect is not expected to be large. Nonetheless, the described simplifications represent some inherent conservatism because potential reductions in the airborne mass load with time are not included in the abstraction for fluvial remobilization.

Hooper (2005) presents a first-order model for fluvial remobilization of ash that describes a significant increase in posteruption sediment yield followed by a gradual decrease with time. Because the abstraction does not model individual flood events, the time dependence of posteruption sediment yield is not modeled. ASHREMOB uses an average posteruption sediment yield to compute (i) the time period that Fortymile Wash yields contaminated sediment, $t_{\text{duration},f}$ and (ii) dilution of contaminated sediment with clean sediment. Use of an average posteruption sediment yield may overestimate (i) the duration that Fortymile Wash yields contaminated sediment deposits with thicknesses greater than the resuspendible layer thickness, (ii) the period of nonzero airborne concentration of high-level waste at the receptor location from the resuspension of contaminated fluvial deposits, and (iii) the risk resulting from

long-term fluvial redistribution of tephra. At times greater than $t_{\text{duration},f}$, further fluvial remobilization in Fortymile Wash results in the deposition of noncontaminated sediment over the older contaminated sediment deposit, which represents the end of the airborne contamination contribution from the fluvial source region. To account for this transition, ASHREMOB sets the airborne particle load to zero for times greater than $t_{\text{duration},f}$ [see discussion on $S_A(t)$ in Section 15.3.1.1]. For eolian remobilization, contributions to airborne contamination are proportional to the fractional area of the source region covered by contaminated tephra. Dilution of the airborne contamination due to resuspension of clean soil underneath thin tephra deposits is based on the average thickness of tephra in tephra-covered areas [see Eq. (15-16)]. As is modeled for the initial deposit at the receptor location, a simple exponential decay function is also used for eolian remobilization to model the reduction in the particle mass load with time from an elevated value following the eruption to a constant, long-term value.

For both the primary tephra-fall deposit at the receptor location and eolian deposits in the Yucca Mountain region, the airborne mass load reduction with time following the eruption is modeled as a simple exponential decay relationship (Anspaugh, et al., 1975). Resuspension of clean underlying soil also is accounted for when the tephra thicknesses are less than the resuspendible layer thickness. Because surface layers of fluvial deposits are expected to be replenished frequently by periodic flood events, the exponential reduction of the airborne mass load with time is not applied to fluvial deposits, and the accumulated thickness of tephra and sediment on the Fortymile Wash depositional area with time is not explicitly calculated by ASHREMOB. After Fortymile Wash is depleted of contaminated tephra, the modeled fluvial component no longer contributes to the airborne concentration of high-level waste. Because it is assumed that long-term (with respect to an annual time frame) heavy surface-disturbing conditions do not apply to fluvial deposits in the Fortymile Wash depositional area, the product of the airborne ash mass load for light disturbance with a multiplicative weighting factor is used to determine the fluvial redistribution contribution. The weighting factor with the airborne mass load from resuspended fluvial deposits is used to capture the general effect of the detailed processes for fluvial remobilization.

For estimating annual-average airborne particle mass loads, resuspension from heavy surface-disturbing activities is modeled only for the initial deposit at the receptor location and not for the fluvial and eolian source regions. Large-scale heavy disturbance conditions, such as sandstorms in the fluvial and eolian source regions, are neglected because the probability of occurrence is low and the duration of exposure is short relative to the annual time frame. Small-scale heavy disturbance conditions in those regions, such as plowing fields, are neglected because the surface area affected by increased surface-disturbing activity, at any given time, is likely a small fraction of the total surface area for the source region. Additionally, localized increases in surface disturbance of the fluvial and eolian source regions are expected to have little effect on the annual-average airborne mass load at the receptor location because (i) the airborne concentration is reduced by dispersion as the resuspension plume migrates downwind and (ii) the wind blows the plume from the localized surface-disturbing activities directly toward the receptor only part of the time.

The modeling component for mass loading consists of two categories for surface-disturbing activities: heavy and light. As described by Mohanty, et al. (2005, Chapter 5), a larger number of activity categories, such as sleeping, sedentary, light work, moderate work, and hard work, could be conceptualized. However, limitation of the model to only two categories is a reasonable simplification because time spent during little or no disturbance is coupled with a

general airborne mass load for light disturbance (i.e., the model does not include a separate category for ambient airborne mass load). The abstracted modeling component for mass loading in TPA Version 5.1 was developed to account for both differences in mass loads from surface-disturbing activities and the fraction of time that the receptor spends outdoors, indoors, and offsite. The implied modeling assumption is that the number of categories for airborne mass loads (seven in Table 15-1) and occupancy fractions (five in Table 15-1) provides sufficient flexibility and transparency to estimate annual-average concentrations of airborne particulates for inhalation calculations.

Calculations of the indoor airborne concentration of high-level waste assume the same proportions from each of three source regions (i.e., initial deposit at the receptor location, fluvial remobilization, and eolian remobilization) in the calculated total outdoor airborne particle concentration. In other words, the relative amounts of the total airborne particle concentration from the three source regions are assumed to be the same indoors and outdoors as a straightforward way to account for indoor contamination that originates from multiple sources of contamination outdoors. The concentration of high-level waste in indoor ash and the resulting indoor airborne concentration of high-level waste are influenced by outdoor surface-disturbing activities.

15.3 Implementation of Conceptual Model in TPA Version 5.1

ASHREMOB calculates temporal evolutions of the airborne concentration of high-level waste at the receptor location and the resulting inhalation dose following a volcanic eruption that intersects the potential repository at Yucca Mountain. The abstracted model uses a lookup table that contains input data determined from detailed offline analyses, which calculate the three-dimensional deposition of ash with a stratified wind field (refer to Section 15.5 for additional information on the lookup table). ASHREMOB converts initial characteristics of the contaminated tephra-fall deposit within the Yucca Mountain region into a time history of annual effective dose equivalent (or annual effective dose) for the inhalation of resuspended contaminated ash by the receptor.

Previous versions of the TPA code employed a single mass quantity for high-level waste that conveniently accounted for the bulk transport of radioactive material in erupting tephra and resuspended ash. In TPA Version 5.1, the utility module INVENT (Chapter 4) calculates time-dependent radionuclide activities on a per mass basis for two types of representative waste forms. The total airborne concentration of high-level waste is combined with radionuclide activities per unit mass of high-level waste to estimate doses from each radionuclide and all radionuclides.

Figure 15-3 shows the flow of information in TPA Version 5.1 when the user selects the abstracted model for tephra remobilization following a volcanic eruption (i.e., when `AshEvolutionMode` flag is set to 1). This chapter focuses on the four modeling components highlighted in yellow in Figure 15-3. The passing of information from one module or component to the next is denoted with arrows. In addition to information transferred from other modules and

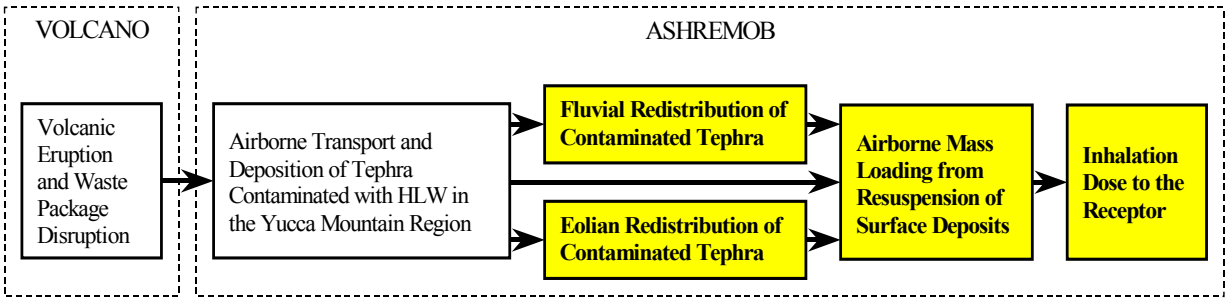


Figure 15-3. Information Flow Diagram for ASHREMOB

components, each component may have specific inputs. Inputs can be specified as parameters in *tpa.inp* or in auxiliary files of input data (e.g., *remob_lut.dat*).

During a TPA Version 5.1 simulation, when the AshEvolutionMode flag is set to a value of 1, each TPA Version 5.1 realization selects a set of parameter values from the lookup table (*remob_lut.dat*, see Section 15.5). The lookup table contains 1,024 parameter sets, which is large compared to the typical number of realizations used in a simulation. Thus, the selection is typically performed without repetition of lookup table values within the same simulation. Repetition can occur, however, if the number of realizations exceeds the number of parameter sets in the lookup table. Using the parameter values selected for each realization, ASHREMOB uses the following equations to estimate the airborne concentration of high-level waste through time at the receptor location and the resulting inhalation dose through time.

The inhalation dose per year (rem/yr) in ASHREMOB for the j^{th} radionuclide is calculated as

$$D_{inh,j}(t) = B I_j \eta_{HLW,j}(t) H_{RMEI}(t) A \quad (15-1)$$

where

$D_{inh,j}(t)$	—	time-dependent inhalation dose per year (rem/yr) for the j^{th} radionuclide
B	—	breathing rate [cm^3/s] as specified by the <i>tpa.inp</i> parameter InhalationRate5[cm^3/s] {for <i>tpa.inp</i> parameter Age&Dosimetry[1=Inf,2=Todl,3=PTeen,4=Teen,5=Adlt,6=AdltFG11] equal to 5}
I_j	—	inhalation dose coefficient per unit intake [Sv/Bq] for the j^{th} radionuclide, provided in the auxiliary data file <i>gnewdf.dat</i>
$\eta_{HLW,j}(t)$	—	time-dependent activity of the j^{th} radionuclide per gram of high-level waste [Ci/g] provided by INVENT

$H_{\text{RMEI}}(t)$	—	total airborne concentration of high-level waste available for inhalation by the receptor [g/m ³]
t	—	time following the volcanic eruption [yr]
A	—	a unit conversion factor equal to $1.167 \times 10^{14} \frac{\text{rem}}{\text{Ci}} \frac{\text{Bq}}{\text{Sv}} \frac{\text{m}^3}{\text{cm}^3} \frac{\text{s}}{\text{yr}}$

The total inhalation dose is calculated as the sum of all radionuclide inhalation doses. The total airborne concentration of high-level waste available for inhalation by the receptor is calculated as the sum of the outdoor, indoor, and offsite contributions

$$H_{\text{RMEI}}(t) = H_{\text{RMEI,outdoor}}(t) + H_{\text{RMEI,indoor}}(t) + H_{\text{RMEI,offsite}}(t) \quad (15-2)$$

where

$H_{\text{RMEI,outdoor}}(t)$	—	outdoor airborne concentration of high-level waste at the receptor location [g/m ³]
$H_{\text{RMEI,indoor}}(t)$	—	indoor airborne concentration of high-level waste available for inhalation by the receptor [g/m ³]
$H_{\text{RMEI,offsite}}(t)$	—	offsite airborne concentration of high-level waste available for inhalation by the receptor [g/m ³]

Inhalation of resuspended radioactive material is modeled for exposure outdoors, indoors, and offsite. The next sections present the mathematical relationships used to determine the airborne concentration of high-level waste for outdoor, indoor, and offsite exposure.

15.3.1 Outdoor Exposure

The outdoor airborne concentration of high-level waste [g/m³] at the receptor location is calculated as

$$H_{\text{RMEI,outdoor}}(t) = f_{\text{out-H}} H_{i-H}(t) + f_{\text{out-L}} H_{i-L}(t) + (f_{\text{out-H}} + f_{\text{out-L}}) H_f(t) + (f_{\text{out-H}} + f_{\text{out-L}}) H_e(t) \quad (15-3)$$

where

$H_{i-H}(t)$	—	airborne concentration of high-level waste from the initial ash deposit at the receptor location during heavy disturbance [g/m ³]
$H_{i-L}(t)$	—	airborne concentration of high-level waste from the initial ash deposit at the receptor location during light disturbance [g/m ³]
$H_f(t)$	—	airborne concentration of high-level waste from the fluvial remobilization of ash [g/m ³]

$H_e(t)$	—	airborne concentration of high-level waste from the eolian remobilization of ash [g/m ³]
f_{out-H}	—	fraction of time receptor spends outdoors with heavy disturbance [unitless] as specified by the <i>tpa.inp</i> parameter OccupancyFractionOutsideHeavyDisturbance[]
f_{out-L}	—	fraction of time receptor spends outdoors with light disturbance [unitless] as specified by the <i>tpa.inp</i> parameter OccupancyFractionOutsideLightDisturbance[]

For each realization, the calculated tephra deposit is partitioned into three source regions that represent (i) initial deposits (if any) at the receptor location denoted by the symbol *i*, (ii) potential deposits in the Fortymile Wash drainage system subject to fluvial redistribution denoted by the symbol *f*, and (iii) potential deposits in areas subject to eolian redistribution denoted by the symbol *e*. A discussion on each of the calculations [i.e., $H_{i-H}(t)$, $H_{f-L}(t)$, $H_f(t)$, and $H_e(t)$] follows separately. The occupancy parameters, f_{out-H} and f_{out-L} , and other input parameters for the reference case are discussed in Section 15.4.

15.3.1.1 Airborne Concentration of High-Level Waste From the Initial Deposit at the Receptor Location

The airborne concentration of high-level waste from the initial deposit addresses heavy and light disturbances separately. Both expressions depend on the thickness of the initial deposit relative to the resuspendible layer thickness. The airborne concentration from the initial deposit during heavy disturbance is calculated as

$$H_{i-H}(t) = c_i \beta(t) \left[(S_{ash,out-H} - S_{out-H}) e^{-\lambda_r t} + S_{out-H} \right] \quad (15-4)$$

where

c_i	—	concentration factor for high-level waste in ash for the initial deposit at the receptor location (grams of high-level waste per unit area/gram of ash per unit area) [g _{HLW} /g _{ash}]
$S_{ash,out-H}$	—	outdoor mass load above fresh ash with heavy disturbance [g/m ³] as specified by the <i>tpa.inp</i> parameter AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]
S_{out-H}	—	outdoor mass load above soil with heavy disturbance [g/m ³] as specified by the <i>tpa.inp</i> parameter AirborneMassLoadOutsideHeavyDisturbance[g/m3]
λ_r	—	rate of reduction of airborne mass load [1/yr] as specified by the <i>tpa.inp</i> parameter RateOfReductionOfMassLoadingFactor[1/yr]

$\beta(t)$ — fraction of resuspended mass that originates from the layer of contaminated tephra

$$\left\{ \begin{array}{ll} 1 & \text{if } \frac{c_{\text{ash},i} e^{-\lambda_b t}}{\rho_{\text{ash}} \left(10,000 \frac{\text{cm}^2}{\text{m}^2}\right)} > d_r \\ \frac{c_{\text{ash},i} e^{-\lambda_b t}}{\rho_{\text{ash}} d_r \left(10,000 \frac{\text{cm}^2}{\text{m}^2}\right)} & \text{if } \frac{c_{\text{ash},i} e^{-\lambda_b t}}{\rho_{\text{ash}} \left(10,000 \frac{\text{cm}^2}{\text{m}^2}\right)} \leq d_r \end{array} \right\}$$

d_r — resuspendible layer thickness [cm] as specified by the *tpa.inp* parameter DepthOfResuspendibleLayer[cm]

λ_b — bulk removal rate of ash from the initial deposit [1/yr] as specified by the *tpa.inp* parameter RelativeRateOfBlanketRemoval[1/yr]

$c_{\text{ash},i}$ — mass of ash per unit area for the initial deposit at the receptor location [g/m²], provided in the auxiliary data file *remob_lut.dat*

ρ_{ash} — density of ash deposited in the Fortymile Wash catchment basin and at the receptor location [g/cm³] as specified by the *tpa.inp* parameter AshBulkDensity[g/cm3]

The contribution from the initial deposit during light disturbance is calculated as

$$H_{i-L}(t) = w_i c_i \beta(t) \left[(S_{\text{ash,out-L}} - S_{\text{out-L}}) e^{-\lambda_r t} + S_{\text{out-L}} \right] \quad (15-5)$$

where

w_i — weighting factor for the contribution of the airborne mass load above the initial deposit to the total airborne particle concentration at the receptor location [unitless] as specified by the *tpa.inp* parameter WeightingFactorInitialDeposit[]

$S_{\text{ash,out-L}}$ — outdoor mass load above fresh ash with light disturbance [g/m³] as specified by the *tpa.inp* parameter AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]

$S_{\text{out-L}}$ — outdoor mass load above soil with light disturbance [g/m³] as specified by the *tpa.inp* parameter AirborneMassLoadoutsideLightDisturbance[g/m3]

Heavy disturbance activities and outdoor mass loads during heavy disturbances do not apply to the contributions from fluvial and eolian remobilizations (refer to additional discussion in Section 15.2). Because the outdoor mass load during heavy disturbances is assumed to result from surface-disturbing activities at the receptor location, a weighting factor is not included in Eq. (15-4). The concentration factor, c_i , is a value calculated from lookup table parameters (Table 15-3) and the mass of high-level waste ejected into the accessible environment, as determined by VOLCANO [see X_{ejected} in Eq. (14-1)], in the following manner

$$c_i = \frac{c_{HLW,i}}{c_{ash,i}} X_{ejected} \quad (15-6)$$

where

$c_{HLW,i}$ — mass of high-level waste per unit area for the initial deposit at the receptor location [g/m²], provided in the auxiliary data file *remob_lut.dat*

For thin ash deposits, the airborne mass load is diluted to account for resuspended contaminated ash with noncontaminated soil [see $\beta(t)$ term in Eqs. (15-4) and (15-5)]. If the ash deposit is thicker than or equal to the resuspendible layer thickness, d_r , no dilution is modeled. If the ash deposit is thinner than the resuspendible layer thickness, the dilution factor equals the ratio of the ash deposit thickness to the thickness of the resuspendible layer (<1). To account for dilution of radionuclide concentrations in resuspendible layers with time, the thickness of the contaminated ash deposit reduces exponentially with time after the eruption due to erosion effects and deposition of noncontaminated soil particles. The reduction rate, λ_b , is specified by the *tpa.inp* parameter RelativeRateOfBlanketRemoval[1/yr].

15.3.1.2 Airborne Concentration of High-Level Waste at the Receptor Location From Fluvial Remobilization

The airborne concentration of high-level waste at the receptor location from fluvial remobilization is calculated as

$$H_f(t) = w_f c_f d_f S_f(t) \quad (15-7)$$

where

W_f — weighting factor for the contribution of the airborne mass load above the sediment deposit from fluvial remobilization to the total airborne particle concentration at the receptor location [unitless] as specified by the *tpa.inp* parameter WeightingFactorFluvial[]

C_f — concentration factor for high-level waste in fluvial ash [g_{HLW}/g_{ash}]

d_f — dilution factor for mixing noncontaminated and contaminated sediments

$S_f(t)$ — airborne mass load above the sediment deposit [g/m³]

When ash remains in the Fortymile Wash catchment basin, ASHREMOB sets the airborne mass load above the sediment deposit, $S_f(t)$ equal to the value of the *tpa.inp* parameter for the outdoor airborne mass load of ash above a fresh deposit for light disturbance [$S_{ash,out-L}$, as specified by the *tpa.inp* parameter AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]]. After the ash has been depleted from the Fortymile Wash catchment basin, ASHREMOB sets $S_f(t)$ equal to zero (refer to additional discussion in Section 15.2).

The concentration factor, c_f , is a value calculated from lookup table parameters (Table 15-3) and the mass of high-level waste ejected into the accessible environment, as determined by VOLCANO [see $X_{ejected}$ in Eq. (14-1)], in the following manner

$$c_f = \frac{m_{\text{HLW},f}}{m_{\text{ash},f}} X_{\text{ejected}} \quad (15-8)$$

where

- $m_{\text{HLW},f}$ — mass of high-level waste deposited in the Fortymile Wash catchment basin from the eruption [g], provided in the auxiliary data file *remob_lut.dat*
- $m_{\text{ash},f}$ — mass of ash deposited in the Fortymile Wash catchment basin from the eruption [g], provided in the auxiliary data file *remob_lut.dat*

The dilution factor, d_f , is calculated as

$$d_f = \frac{v_{\text{ash},f}}{v_{\text{sediment},f} + v_{\text{ash},f}} \quad (15-9)$$

where

- $v_{\text{ash},f}$ — total volume of ash deposited in the Fortymile Wash catchment basin [m³]
- $v_{\text{sediment},f}$ — total volume of noncontaminated sediment yielded by the Fortymile Wash drainage system during the time period of fluvial ash remobilization [m³]

The ash volume is calculated from parameters in the lookup table (Table 15-3) and *tpa.inp* as

$$v_{\text{ash},f} = \frac{m_{\text{ash},f}}{\rho_{\text{ash}} \left(1,000,000 \frac{\text{cm}^3}{\text{m}^3} \right)} \quad (15-10)$$

where ρ_{ash} is the bulk density of volcanic ash [g/cm³] as specified by the *tpa.inp* parameter AshBulkDensity[g/cm3].

The sediment volume, $v_{\text{sediment},f}$, also is calculated from parameters in the lookup table (Table 15-3) and *tpa.inp* as

$$v_{\text{sediment},f} = Y_{\text{sediment},f} (A_{\text{basin},f} - a_{\text{ash},f}) n_{\text{deplete}} \quad (15-11)$$

where

- $Y_{\text{sediment},f}$ — preeruption sediment volume through Fortymile Wash per unit drainage basin area per discharge event [m/event] as specified by the *tpa.inp* parameter AmbientSedimentYieldVolumePerBasinAreaPerEvent[m/event]

- $A_{\text{basin},f}$ — total area of the drainage basin that discharges through Fortymile Wash [m²] as specified by the *tpa.inp* parameter AreaDrainageBasinFluvial[m2]
- $a_{\text{ash},f}$ — area of the Fortymile Wash catchment basin with an ash deposit from the eruption [m²], provided in the auxiliary data file *remob_lut.dat*
- n_{deplete} — number of significant flow events required to deplete the Fortymile Wash catchment basin of ash [unitless]

The number of significant flow events required to deplete the Fortymile Wash catchment basin of ash is determined from the following relationship

$$n_{\text{deplete}} = \frac{V_{\text{ash},f}}{Y_{\text{ash},f} a_{\text{ash},f}} \quad (15-12)$$

where $Y_{\text{ash},f}$ is the posteruption volume of fluvial remobilized ash yielded from Fortymile Wash per unit catchment basin area per discharge event [m/event] as specified by the *tpa.inp* parameter PostEruptionFluvialAshYieldVolumePerAreaPerEvent[m/event].

The duration of fluvial remobilization component, $t_{\text{duration},f}$, depends on the timing of the fluvial remobilization events and is computed as

$$t_{\text{duration},f} = n_{\text{deplete}} T_f \quad (15-13)$$

where T_f is the average time between significant flow events [yr/event] as specified by the *tpa.inp* parameter TimeBetweenFlowEvents[yr].

15.3.1.3 Airborne Concentration of High-Level Waste at the Receptor Location From Eolian Remobilization

The airborne concentration of high-level waste at the receptor location from eolian remobilization is calculated as

$$H_e(t) = w_e c_e d_e \left[(S_{\text{ash},\text{out-L}} - S_{\text{out-L}}) e^{-\lambda_r t} + S_{\text{out-L}} \right] \quad (15-14)$$

where

- w_e — weighting factor for the contribution of the airborne mass load above the initial ash deposit in the eolian source area to the total airborne particle concentration at the receptor location [unitless] as specified by the *tpa.inp* parameter WeightingFactorEolian[]
- c_e — concentration factor for high-level waste in the eolian ash deposit [$g_{\text{HLW}}/g_{\text{ash}}$]
- d_e — dilution factor for the eolian sediments [unitless]

The concentration factor, c_e , is a value calculated from lookup table parameters (Table 15-3) and the mass of high-level waste ejected into the accessible environment, as determined by VOLCANO [see X_{ejected} in Eq. (14-1)], in the following manner

$$c_e = \frac{m_{\text{HLW},e}}{m_{\text{ash},e}} X_{\text{ejected}} \quad (15-15)$$

where

- $m_{\text{HLW},e}$ — mass of high-level waste deposited in the eolian source region from the eruption [g], provided in the auxiliary data file *remob_lut.dat*
- $m_{\text{ash},e}$ — mass of ash deposited in the eolian source region from the eruption [g], provided in the auxiliary data file *remob_lut.dat*

Dilution of contributions from the eolian source region is modeled to account for the amount of tephra-free area within the source region and resuspension of clean soil underneath thin tephra deposits. The dilution factor, d_e , is calculated from values in the lookup table (Table 15-3) and *tpa.inp* parameters as

$$d_e = \frac{a_{\text{ash},e}}{A_{\text{eolian}}} \tau \quad (15-16)$$

where

- $a_{\text{ash},e}$ — area of the eolian source region with an initial ash deposit from the eruption [m^2], provided in the auxiliary data file *remob_lut.dat*
- $\rho_{\text{ash},e}$ — density of ash deposited in the eolian source region [g/m^3], primarily composed of distal locations from the volcanic vent, as specified by the *tpa.inp* parameter DensityOfDistalAsh[g/m^3]
- A_{eolian} — total area of the eolian source region [m^2] as specified by the *tpa.inp* parameter AreaEolianSourceRegion[m^2]
- τ — representative fraction of resuspended mass that originates from contaminated tephra in the eolian source region

$$\left\{ \begin{array}{ll} 1 & \text{if } \frac{m_{\text{ash},e} (100 \frac{\text{cm}}{\text{m}})}{a_{\text{ash},e} \rho_{\text{ash},e}} > d_r \\ \frac{m_{\text{ash},e} (100 \frac{\text{cm}}{\text{m}})}{a_{\text{ash},e} \rho_{\text{ash},e} d_r} & \text{if } \frac{m_{\text{ash},e} (100 \frac{\text{cm}}{\text{m}})}{a_{\text{ash},e} \rho_{\text{ash},e}} \leq d_r \end{array} \right\}$$

15.3.2 Indoor Exposure

Estimates of the total concentration of high-level waste in indoor ash account for different high-level waste concentrations from the three source regions (i.e., initial deposit at the receptor location, fluvial remobilization, and eolian remobilization). Calculations of the indoor airborne

concentration of high-level waste use the same proportions from each of three source regions in the calculated total outdoor airborne particle concentration. In other words, the proportion of the total airborne particle concentration from the three components is the same indoors and outdoors. The term proportion is used in these calculations instead of the term fraction to avoid confusion with the occupancy fractions.

During heavy disturbance outdoors, the total airborne particle concentration (g/m^3) at the receptor location is calculated as

$$P_{\text{out-H}}(t) = \left\{ \begin{array}{l} \left[(S_{\text{ash,out-H}} - S_{\text{out-H}})e^{-\lambda_r t} + S_{\text{out-H}} \right] + w_f S_f(t) + w_e \left[(S_{\text{ash,out-L}} - S_{\text{out-L}})e^{-\lambda_r t} + S_{\text{out-L}} \right] \\ \text{for realizations with an initial tephra deposit at the receptor location} \\ \text{or} \\ S_{\text{out-H}} + w_f S_f(t) + w_e \left[(S_{\text{ash,out-L}} - S_{\text{out-L}})e^{-\lambda_r t} + S_{\text{out-L}} \right] \\ \text{for realizations without an initial tephra deposit at the receptor location} \end{array} \right\} \quad (15-17)$$

As mentioned previously, heavy disturbance activities are assumed to occur only on the initial deposit at the receptor location. In other words, heavy disturbance activities and outdoor mass loads during heavy disturbance do not apply to the contributions from fluvial and eolian remobilization. For this reason, a weighting factor is not included in the first term of the right-hand side of Eq. (15-17).

The proportions of the particle concentration from the three source regions (i.e., initial deposit at the receptor location, fluvial remobilization, and eolian remobilization) when the receptor is engaged in heavy disturbance activities outdoors are

$$\begin{aligned} p_{i-H}(t) &= \frac{\left[(S_{\text{ash,out-H}} - S_{\text{out-H}})e^{-\lambda_r t} + S_{\text{out-H}} \right]}{P_{\text{out-H}}(t)} \\ p_{f-H}(t) &= \frac{w_f S_f(t)}{P_{\text{out-H}}(t)} \\ p_{e-H}(t) &= \frac{w_e \left[(S_{\text{ash,out-L}} - S_{\text{out-L}})e^{-\lambda_r t} + S_{\text{out-L}} \right]}{P_{\text{out-H}}(t)} \end{aligned} \quad (15-18)$$

Eq. (15-18) is presented for realizations with an initial tephra deposit at the receptor location. For realizations without an initial tephra deposit at the receptor location, $p_{i-H}(t)$ equals $S_{\text{out-H}}/P_{\text{out-H}}(t)$. During light disturbance outdoors, the total airborne particle concentration (g/m^3) at the receptor location is calculated as

$$P_{\text{out-L}}(t) = \left\{ \begin{array}{l} w_i \left[(S_{\text{ash,out-L}} - S_{\text{out-L}}) e^{-\lambda_r t} + S_{\text{out-L}} \right] + w_f S_f(t) + w_e \left[(S_{\text{ash,out-L}} - S_{\text{out-L}}) e^{-\lambda_r t} + S_{\text{out-L}} \right] \\ \text{for realizations with an initial tephra deposit at the receptor location} \\ \text{or} \\ w_i S_{\text{out-L}} + w_f S_f(t) + w_e \left[(S_{\text{ash,out-L}} - S_{\text{out-L}}) e^{-\lambda_r t} + S_{\text{out-L}} \right] \\ \text{for realizations without an initial tephra deposit at the receptor location} \end{array} \right\} \quad (15-19)$$

The proportions of the particle concentration from the three source regions (i.e., initial deposit at the receptor location, fluvial remobilization, and eolian remobilization) when the receptor is engaged in light disturbance activities outdoors are

$$\begin{aligned} p_{i-L}(t) &= \frac{w_i \left[(S_{\text{ash,out-L}} - S_{\text{out-L}}) e^{-\lambda_r t} + S_{\text{out-L}} \right]}{P_{\text{out-L}}(t)} \\ p_{f-L}(t) &= \frac{w_f S_f(t)}{P_{\text{out-L}}(t)} \\ p_{e-L}(t) &= \frac{w_e \left[(S_{\text{ash,out-L}} - S_{\text{out-L}}) e^{-\lambda_r t} + S_{\text{out-L}} \right]}{P_{\text{out-L}}(t)} \end{aligned} \quad (15-20)$$

for realizations with an initial tephra deposit at the receptor location. For realizations without an initial tephra deposit at the receptor location, $p_{i-L}(t)$ equals $S_{\text{out-L}}/P_{\text{out-L}}(t)$.

The final proportions for the three source regions are calculated as the weighted sum of the proportions and occupancy fractions for heavy and light disturbance divided by the total fraction of time exposed outdoors

$$\begin{aligned} p_i(t) &= \frac{p_{i-H}(t) f_{\text{out-H}} + p_{i-L}(t) f_{\text{out-L}}}{f_{\text{out-H}} + f_{\text{out-L}}} \\ p_f(t) &= \frac{p_{f-H}(t) f_{\text{out-H}} + p_{f-L}(t) f_{\text{out-L}}}{f_{\text{out-H}} + f_{\text{out-L}}} \\ p_e(t) &= \frac{p_{e-H}(t) f_{\text{out-H}} + p_{e-L}(t) f_{\text{out-L}}}{f_{\text{out-H}} + f_{\text{out-L}}} \end{aligned} \quad (15-21)$$

These proportions account for the total outdoor particle load to which the receptor is exposed outdoors and are used to calculate the airborne concentration of high-level waste indoors.

The indoor airborne concentration of high-level waste (g/m^3) available for inhalation by the receptor is calculated as

$$H_{\text{RMEI,indoor}}(t) = f_{\text{in-H}} [p_i(t)c_i f_R(t) + p_f(t)c_f d_f + p_e(t)c_e d_e] S_{\text{in-H}} + f_{\text{in-L}} [p_i(t)c_i f_R(t) + p_f(t)c_f d_f + p_e(t)c_e d_e] S_{\text{in-L}} \quad (15-22)$$

where

- $S_{\text{in-H}}$ — indoor mass load for dust with heavy disturbance (g/m^3) as specified by the *tpa.inp* parameter AirborneMassLoadInsideHeavyDisturbance[g/m^3]
- $S_{\text{in-L}}$ — indoor mass load for dust with light disturbance (g/m^3) as specified by the *tpa.inp* parameter AirborneMassLoadInsideLightDisturbance[g/m^3]
- $f_{\text{in-H}}$ — fraction of time receptor spends indoors with heavy disturbance as specified by the *tpa.inp* parameter OccupancyFractionInsideHeavyDisturbance[]
- $f_{\text{in-L}}$ — fraction of time receptor spends indoors with light disturbance as specified by the *tpa.inp* parameter OccupancyFractionInsideLightDisturbance[]
- $f_R(t)$ — time-dependent fraction of resuspended mass originating from contaminated volcanic layer (unitless) equal to

$$1 \text{ if } \frac{c_{\text{ash},i} e^{-\lambda_b t}}{\rho_{\text{ash}} \left(10,000 \frac{\text{cm}^2}{\text{m}^2}\right)} > d_r \text{ or } \frac{c_{\text{ash},j} e^{-\lambda_b t}}{\rho_{\text{ash}} d_r \left(10,000 \frac{\text{cm}^2}{\text{m}^2}\right)} \text{ if } \frac{c_{\text{ash},j} e^{-\lambda_b t}}{\rho_{\text{ash}} \left(10,000 \frac{\text{cm}^2}{\text{m}^2}\right)} \leq d_r$$

15.3.3 Offsite Exposure

The offsite occupancy fraction is included only for completeness to allow for a fraction of time the receptor may spend far away from Amargosa Valley and the Yucca Mountain region. Because offsite locations are intended to be far away from the potential repository (i.e., well beyond the eolian source region), it is assumed that the offsite locations are free of contaminated tephra. The reference-case value for the offsite airborne mass load is thus equal to zero. Although its contribution is intended to be nil, a relationship still is established for the offsite airborne concentration of high-level waste that is similar to the relationships presented previously. Because unique concentration and dilution factors are not explicitly derived for offsite locations, the concentration and dilution factors for the eolian contribution are included as proxies in the relationship for the offsite airborne concentration of high-level waste available for inhalation by the receptor

$$H_{\text{RMEI,offsite}} = f_{\text{offsite}} c_e d_e S_{\text{offsite}} \quad (15-23)$$

where

- S_{offsite} — offsite airborne mass load [g/m^3] as specified by the *tpa.inp* parameter AirborneMassLoadOffsite[g/m^3]
- f_{offsite} — fraction of time receptor spends offsite as specified by the *tpa.inp* parameter OccupancyFractionOffsite[g/m^3]

15.4 Input Parameters in *tpa.inp*

The *tpa.inp* parameter AshEvolutionMode[0=no_remob,1=ashremob] is the flag used to choose between the two abstracted modeling approaches for estimating consequences from a volcanic eruption. Allowed values of the AshEvolutionMode flag are either 1 (reference-case value), to account for a stratified wind field and estimate the effects of ash remobilization within the Yucca Mountain region, or 0, to fix the wind direction toward the receptor and neglect the effects of ash remobilization (Chapters 16 and 17). Figure 15-4 displays simplified flow charts of igneous eruption consequence modules for TPA Version 5.1 and their relationship to the AshEvolutionMode[0=no_remob,1=ashremob] flag. Figures 15-3 and 17-1 provide additional information on the general function of each consequence module. Refer to Chapter 14 for a description of VOLCANO. As indicated in Figure 15-4, VOLCANO determines the source term of erupted high-level waste and is common to both options for modeling eruptive igneous consequences.

Table 15-1 presents *tpa.inp* parameters used by ASHREMOB for estimating inhalation dose from a potential eruption. Parameters listed in the ASHREMOB input block of Table 15-1 are exclusive to ASHREMOB. The other parameters listed in Table 15-1 are used by ASHREMOB and other modules (see the first column of Table 15-1). To serve as a reference guide, Table 15-1 also presents the symbols used for each of the *tpa.inp* parameters in the equations of this chapter. Because ASHREMOB is used to model consequences from the igneous disruptive scenario (i.e., not the nominal scenario), input flags used by ASHREMOB and recommendations for flag settings are presented in Table 15-2.

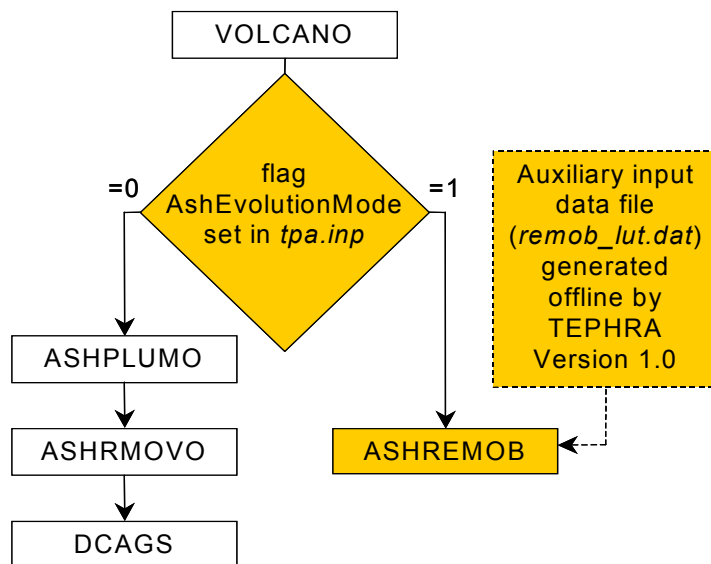


Figure 15-4. Simplified Flow Chart of Igneous Eruption Consequence Modules for TPA Version 5.1 with ASHREMOB Highlighted in Gold

Table 15-1. Reference Data for Parameters of tpa.inp Used by ASHREMOB (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	Age&Dosimetry[1=Inf,2=Todl, 3=PTeen,4=Teen,5=Adlt, 6=AdltFG11]	Flag to select the receptor age group and the internal dosimetry methodology	iconstant 5	Adult receptor is required for Yucca Mountain calculations by 10 CFR 63.312(e). Reference-case value is set to International Commission on Radiological Protection Publication 72 (International Commission on Radiological Protection, 2002, 1996) internal dosimetry and adult receptor. Federal Guidance No. 11 (U.S. Environmental Protection Agency, 1988) adult dosimetry values are a user-selectable option. If flag is set to preadult age group, user is responsible for uncommitting, entering, and justifying related age-dependent input parameters in DCAGW and DCAGS or ASHREMOB.
GENTPA	InhalationRate5[cm3/s]* *Only the input parameter for inhalation rate corresponding to the reference-case selection of receptor age and dosimetry is presented in this table.	B Inhalation rate for Adult: ICRP72 receptor age group (Only used if Age&Dosimetry flag is set to 5)	constant 270	Reference-case value is equal to the default adult chronic inhalation rate in GENII 1.485 code (Napier, et al., 1988). Magnitude of breathing rate is influenced by the level of human activity. Reference-case value is slightly higher than the value for an adult male (International Commission on Radiological Protection, 1995, Table 6).
ASHRMOVO	RelativeRateOfBlanketRemoval [1/yr]	A_b Bulk removal rate from the initial tephra deposit [1/yr]	constant 0.0007	Only traces of the tephra-fall deposit are preserved at the youngest Yucca Mountain region volcano, Lathrop Wells, which is around 100,000 years old. Recent work by Delgado-Granados, et al. (1998) at Xitle volcano, Mexico, has shown that substantial amounts of basaltic tephra-fall deposits are preserved from this 2,000-year-old eruption. The area around Xitle volcano receives around 500–700 mm [20–28 in] of annual rainfall, in contrast to the roughly 100-mm [4-in] annual rainfall in the Yucca Mountain region. Although many factors, such as topographic slope, degree of incision, and eolian sedimentation affect tephra-fall erosion, areas of greater annual rainfall should experience higher erosion rates of nonconsolidated fall deposits than areas of lower annual rainfall. Thus, tephra-fall deposits in the Yucca Mountain region likely are significantly preserved for around 10,000 years, and a removal half-life of 1,000 years is selected. Removal rate equals $1/n$ 2 divided by the half-life.

Table 15-1. Reference Data for Parameters of *tpa.inp* Used by ASHREMOB (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	AshBulkDensity[g/cm ³]	ρ_{ash} Bulk density for volcanic ash deposited in the Fortymile Wash catchment basin and at the receptor location [g/cm ³]	constant 1.2	Data based on <i>in-situ</i> measurements of tephra deposits during the 1995 Cerro Negro eruption made at 1 km [0.6 mi] from the vent (Hill, et al., 1998, p. 1,232).
DCAGS	DepthOfResuspendibleLayer[cm]	d_r Thickness of the upper soil layer that is available for resuspension [cm]	constant 0.3	Wiggs (1997) supports a 0.1–1 cm [0.04–0.4 in] range, with 1 cm [0.4 in] being for poorly sorted, coarse-grained deposits {i.e., grain size on order of 1 cm [0.4 in]}. The 0.3 cm [0.12 in] value seems reasonable, given that the tephra will likely have an average grain size on the order of 0.1 cm [0.04 in]. Because the maximum entrainable particle size is 0.01 cm [0.004 in], the 0.1–cm [0.04-in] ash will form an unentrainable lag deposit that shields finer particles from turbulent wind entrainment unless they can escape between the 0.1 cm [0.04 in] particle interstices.
DCAGS	RateOfReductionOfMassLoading Factor[1/yr]	λ_r Rate at which the airborne mass load factor decreases with time from the initial value after the eruption [1/yr]	constant 0.07	Limited reduction in airborne mass loads measured on deposits 4 years after 1995 Cerro Negro eruption (Hill, et al., 2000). Assuming exponential decay (Anspaugh, et al., 1975), this relationship indicates a half-life for reduction in mass load on the order of 10 years. Reduction rate equals $\ln 2$ divided by the half-life.

Table 15-1. Reference Data for Parameters of *tpa.inp* Used by ASHREMOB (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadAboveFreshAsh BlanketHeavyDisturbance[g/m ³]	$S_{\text{ash, out-H}}$ Outdoor airborne mass load of resuspended ash due to heavy disturbance activities [g/m ³]	uniform 1.0e-3, 1.0e-2	Outdoor mass loads over ash deposits for heavy disturbance activities have been measured within this range. Measurements were taken 4 years after the 1995 Cerro Negro eruption in Nicaragua at a height of 1.5 m [4.9 ft] above the tephra deposits located about 5 km [3.1 mi] from the vent (Hill, et al., 2000). Digging and driving over deposits resulted in airborne mass loads of $\sim 10^{-2}$ g/m ³ [$\sim 10^{-5}$ oz/ft ³], which was assigned as the maximum value. Walking over deposits resulted in airborne mass loads of $\sim 10^{-3}$ g/m ³ [$\sim 10^{-6}$ oz/ft ³], which was assigned as the minimum value. Range is supported also by posteruption measurements near Montserrat volcano by Searl, et al. (2002).
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadAboveFreshAsh BlanketLightDisturbance[g/m ³]	$S_{\text{ash, out-L}}$ Outdoor airborne mass load of resuspended ash due to light disturbance activities [g/m ³]	uniform 1.0e-4, 1.0e-3	Outdoor mass loads over ash deposits for light disturbance activities have been measured within this range. Measurements were taken 4 years after the 1995 Cerro Negro eruption in Nicaragua at a height of 1.5 m above the tephra deposits located about 5 km [3.1 mi] from the vent (Hill, et al., 2000). Walking over deposits resulted in airborne mass loads of $\sim 10^{-3}$ g/m ³ [$\sim 10^{-6}$ oz/ft ³], which was assigned as the maximum value. Airborne mass loads over undisturbed deposits were $\sim 10^{-4}$ g/m ³ [$\sim 10^{-7}$ oz/ft ³] in 4 ± 2 m/s [13 ± 7 ft/s] winds, which was assigned as the minimum value. Range is supported also by posteruption measurements near Montserrat volcano by Searl, et al. (2002).
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadOutsideHeavy Disturbance[g/m ³]	$S_{\text{out-H}}$ Outdoor airborne mass load of resuspended soil due to heavy disturbance activities [g/m ³]	constant 7.0e-4	This value corresponds to the maximum value in the range of airborne mass loads for outdoor activities assuming soil conditions (Mohanty, et al., 2005, Table 5-4).

Table 15-1. Reference Data for Parameters of *tpa.inp* Used by ASHREMOB (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadOutsideLight Disturbance[g/m ³]	S_{out-L} Outdoor airborne mass load of resuspended soil due to light disturbance activities [g/m ³]	constant 1.0e-4	This value corresponds to the minimum value in the range of airborne mass loads for outdoor activities assuming soil conditions (Mohanty, et al., 2005, Table 5-4).
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadInsideHeavy Disturbance[g/m ³]	S_{in-H} Indoor airborne mass load of resuspended soil and ash due to heavy disturbance activities [g/m ³]	triangular 1.0e-4, 5.0e-4, 1.0e-3	Screening values of indoor mass loads for building renovation and residential exposure scenarios are discussed in a literature summary by Kennedy and Streng (1992). They describe a range of 0.00005 to 0.0001 g/m ³ [5×10^{-8} to 1×10^{-7} oz/ft ³] as representing longer term average concentrations that account for airborne dust from nonradioactive sources. They further consider the range a prudently conservative estimate for radioactive dust loadings in the workplace or household. Because fine ash particles are expected to elevate normal dust loadings and this parameter is for heavy disturbance conditions, we take the recommendation of 0.0001 g/m ³ [10^{-7} oz/ft ³] as the lower end of a triangular distribution that extends to a maximum value that is equal to the low end of outdoor mass loading for fresh ash {0.001 g/m ³ [10^{-6} oz/ft ³]} described above, with the midpoint of this range {(0.0005 g/m ³) [5×10^{-7} oz/ft ³]} assumed to be a reasonably conservative mode of a triangular distribution, selected to avoid overemphasizing the extreme high and low ends of the range.

Table 15-1. Reference Data for Parameters of *tpa.inp* Used by ASHREMOB (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadInsideLight Disturbance[g/m ³]	S_{in-L} Indoor airborne mass load of resuspended soil and ash due to light disturbance activities [g/m ³]	triangular 1.0e-5, 5.0e-5, 1.0e-4	Screening values of indoor mass loads for building renovation and residential exposure scenarios are discussed in a literature summary by Kennedy and Strenge (1992). They describe a range of 0.00005 to 0.0001 g/m ³ [5×10^{-8} to 1×10^{-7} oz/ft ³] as representing longer term average concentrations that account for airborne dust from nonradioactive sources. They further consider the range a prudently conservative estimate for radioactive dust loadings in the workplace or household. Because this parameter is for light disturbance conditions that span a range of disturbance conditions (including no disturbance at all), the recommendation in Kennedy and Strenge (1992) of 0.0001 g/m ³ [10^{-7} oz/ft ³] is selected as the upper end of a triangular distribution that extends to a minimum value {(0.00001 g/m ³) [10^{-8} oz/ft ³]} encompassing a dust loading representing relatively clean air {(0.00002 g/m ³) [2×10^{-8} oz/ft ³] (Kennedy and Strenge, 1992)}, with the midpoint of this range {(0.00005 g/m ³) [5×10^{-8} oz/ft ³]} assumed to be a reasonably conservative mode of a triangular distribution, selected to avoid overemphasizing the extreme high and low ends of the range.
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadOffsite[g/m ³]	$S_{offsite}$ Offsite airborne mass load of contaminated particles [g/m ³]	constant 0.0	Offsite locations are assumed to be well beyond the eolian source region and free of contamination.
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionOutsideHeavy Disturbance[]	f_{out-H} Fraction of time receptor spends outdoors with heavy disturbance [unitless]	constant 0.125	Based on an assumption of 2.75 hr/day of moderate work and 0.25 hr/day of hard work outdoors (Mohanty, et al., 2005, Chapter 5).

Table 15-1. Reference Data for Parameters of *tpa.inp* Used by ASHREMOB (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionOutsideLightDisturbance[]	f_{out-L} Fraction of time receptor spends outdoors with light disturbance [unitless]	constant 0.084	Based on an assumption of 2 hr/day of light work outdoors (Mohanty, et al., 2005, Chapter 5).
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionInsideHeavyDisturbance[]	f_{in-H} Fraction of time receptor spends indoors with heavy disturbance [unitless]	constant 0.104	Based on an assumption of 2 hr/day of moderate work and 0.5 hr/day of hard work indoors (Mohanty, et al., 2005, Chapter 5).
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionInsideLightDisturbance[]	f_{in-L} Fraction of time receptor spends indoors with light disturbance [unitless]	constant 0.583	Based on an assumption of 8 hr/day sleeping, 3 hr/day sedentary, and 3 hr/day of light work indoors (Mohanty, et al., 2005, Chapter 5).
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionOffsite[]	$f_{offsite}$ Fraction of time receptor spends offsite [unitless]	constant 0.104	Based on an assumption of 1.25 hr/day outdoors and 1.25 hr/day indoors offsite (Mohanty, et al., 2005, Chapter 5). Offsite locations are assumed to be well beyond the eolian source region and free of contamination.
GLOBAL	AshEvolutionMode [0=no_ashremob, 1=ashremob]	User-selected flag for calculating evolution of ash at receptor location (0 implies wind direction fixed toward receptor without ash remobilization, 1 implies wind direction sampled and ash remobilization effects included)	iconstant 1	User option

Table 15-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHREMOB (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHREMOB	AshPlumeRealizationIndex[]	Index counter for sampling from the <i>remob_lut.dat</i> lookup table	iuniform 1, 1024	Produces random sampling from the 1,024 realizations of the <i>remob_lut.dat</i> lookup table for atmospheric transport and deposition of tephra in a stratified wind field (Mohanty, et al., 2005, Chapter 6).
ASHREMOB	WeightingFactorInitialDeposit[]	W_i Weighting factor for how much the airborne mass load above the initial deposit contributes to the total airborne particle concentration at the receptor location [unitless]	constant 0.3334	Value selected for near-equal contributions from each of the three components (Mohanty, et al., 2005, Chapter 6). Values for the three weighting factors are not required to sum to unity.
ASHREMOB	WeightingFactorFluvial[]	W_f Weighting factor for how much the airborne mass load above the sediment deposit from fluvial remobilization contributes to the total airborne particle concentration at the receptor location [unitless]	constant 0.3333	Value selected for near-equal contributions from each of the three components (Mohanty, et al., 2005, Chapter 6). Values for the three weighting factors are not required to sum to unity.

Table 15-1. Reference Data for Parameters of *tpa.inp* Used by ASHREMOB (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHREMOB	AmbientSedimentYieldVolumePer BasinAreaPerEvent[m/event]	$Y_{\text{sediment},f}$ Preeruption sediment volume yield per unit drainage basin area that discharges through Fortymile Wash per discharge event [m/event]	usersuppliedpwiscdf 27 values, cumulative probability 0.00001, 0 0.000012, 0.0015 0.000014, 0.0244 0.000016, 0.0747 0.000018, 0.1442 0.00002, 0.2346 0.000022, 0.3346 0.000024, 0.4375 0.000026, 0.5351 0.000028, 0.6076 0.00003, 0.6778 0.000032, 0.7377 0.000034, 0.7886 0.000036, 0.828 0.000038, 0.8616 0.00004, 0.8875 0.000042, 0.9127 0.000044, 0.9349 0.000046, 0.9521 0.000048, 0.9666 0.00005, 0.9779 0.000052, 0.9862 0.000054, 0.9928 0.000056, 0.9976 0.000058, 0.9992 0.00006, 0.9999 0.000062, 1	Derived from site-specific estimates for ranges of sediment thickness, age of sediments, and depositional area, whereby uncertainties were propagated using uniform distributions for each range {Sediment thickness = U[1,2] m; Age of sediments = U[4, 10] kyr; Depositional area = U[22,26] km ² } in Hooper and Benke (2006). The resulting distribution for ambient sediment yield in units of m ³ /m ² /yr was converted to units of m ³ /m ² /event with a multiplication by 4 yr/event (i.e., value of the parameter TimeBetweenFlowEvents[yr]). The parameter PostEruptionFluvialAshYieldVolumePerAreaPerEvent[m/event] is correlated to the sampled value of this parameter.
ASHREMOB	AreaDrainageBasinFluvial[m2]	$A_{\text{basin},f}$ Total area of the drainage basin [m ²] that discharges through Fortymile Wash	constant 8.15e8	Standard spatial attribute for the watershed area derived from geographic information system and planimetric methods (Hooper and Benke, 2006).

Table 15-1. Reference Data for Parameters of *tpa.inp* Used by ASHREMOB (continued)

(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)

Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHREMOB	TimeBetweenFlowEvents[yr]	T_f Average time between significant flow events [yr]	constant 4.0	Based on peak sediment discharge measurements at Fortymile Wash from 1969 to 1998 (Hooper and Benke, 2006).
ASHREMOB	PostEruptionFluvialAshYield VolumePerAreaPerEvent[m/event]	$Y_{ash,f}$ Posteruption volume yield of fluvial remobilized ash at the Fortymile Wash depositional region per unit drainage basin area per discharge event [m/event]	usersuppliedpwisecdf 27 values, cumulative probability 0.00002, 0 0.000024, 0.0015 0.000028, 0.0244 0.000032, 0.0747 0.000036, 0.1442 0.00004, 0.2346 0.000044, 0.3346 0.000048, 0.4375 0.000052, 0.5351 0.000056, 0.6076 0.00006, 0.6778 0.000064, 0.7377 0.000068, 0.7886 0.000072, 0.828 0.000076, 0.8616 0.00008, 0.8875 0.000084, 0.9127 0.000088, 0.9349 0.000092, 0.9521 0.000096, 0.9666 0.0001, 0.9779 0.000104, 0.9862 0.000108, 0.9928 0.000112, 0.9976 0.000116, 0.9992 0.00012, 0.9999 0.000124, 1	Correlated parameter with a value set to twice the sampled value of AmbientSedimentYield VolumePerBasinAreaPerEvent[m/event] (Hooper and Benke, 2006). Tephra is easily eroded compared to most other surface materials. Sediment yield from a tephra-covered drainage basin is greater per unit area than the sediment yield from an ambient drainage basin (Segerstrom, 1950). To account for accelerated erosion, the mean of the calculated posteruption sediment yield is two times the ambient sediment yield over the lifetime of the potential tephra deposit. This parameter affects (i) the time period that fluvial remobilization contributes contaminated airborne particulates to the inhalation dose and (ii) dilution of fluvial deposits due to mixing with clean sediment.

Table 15-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHREMOB (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHREMOB	WeightingFactorEolian[]	W_e Weighting factor for how much the particle mass load above the initial ash deposit in the eolian source area contributes to the total airborne particle concentration at the receptor location [unitless]	constant 0.3333	Value selected for near-equal contributions from each of the three components (Mohanty, et al., 2005, Chapter 6). Values for the three weighting factors are not required to sum to unity.
ASHREMOB	DensityOfDistalAsh[g/m3]	$\rho_{ash,e}$ Density [g/m ³] of the distal ash deposited in the eolian source region, which is primarily composed of distal locations from the volcanic vent	constant 8.0e5	Derived from 1995 Cerro Negro eruption (Hill, et al., 1998).
ASHREMOB	AreaEolianSourceRegion[m2]	A_{eolian} Area of the eolian source region [m ²] with an initial ash deposit from the eruption	constant 2.1e9	Generalized area surrounding the receptor location for the source of ambient airborne particulates. This parameter is used to calculate the dilution factor for eolian remobilization (Mohanty, et al., 2005, Chapter 6).

Table 15-1. Reference Data for Parameters of tpa.inp Used by ASHREMOB (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Correlated Parameters	Independent variable: AmbientSedimentYieldVolumePer BasinAreaPerEvent[m/event] Dependent variable: PostEruptionFluvialAshYield VolumePerAreaPerEvent[m/event]	Correlation between AmbientSediment YieldVolumePer BasinAreaPer Event[m/event] and PostEruption FluvialAshYield VolumePerArea PerEvent[m/event]	correlateinputs 0.99	The value of the PostEruptionFluvialAshYieldVolumePerAreaPerEvent [m/event] parameter is correlated to the sampled value of the AmbientSedimentYield VolumePerBasinAreaPerEvent[m/event] parameter. The value of 0.99 is selected because a value of 1.0 is not allowed by the Latin Hypercube Sampling routine.

Table 15-2. Input Flags Used by ASHREMOB	
Input Flag Name	Description
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	This flag, located in the GLOBAL input block in <i>tpa.inp</i> , activates the igneous disruptive scenario calculations. The flag must be set to a value of 1 to invoke ASHREMOB.
Age&Dosimetry[1=Inf,2=ToDI,3=PTeen,4=Teen,5=Adlt,6=AdltFG11]	This flag, located in the GENTPA input block in <i>tpa.inp</i> , selects the exposure parameters and dose coefficients used in the consequence calculations. For ASHREMOB, InhalationRate _n [cm ³ /s] is the key exposure input parameter, where <i>n</i> represents the selected value of the Age&Dosimetry flag.
VolcanoModel(1=Geometric,2=Distribution)	This flag, located in the VOLCANO input block in <i>tpa.inp</i> , selects the source term model in VOLCANO, which determines the amount of high-level waste erupted for use in ASHREMOB.
ExtrusiveEventFlag(extrusive=1,intrusive=0)	This flag, located in the VOLCANO input block in <i>tpa.inp</i> , allows the user to toggle between extrusive plus intrusive and intrusive only igneous activity events. Because ASHREMOB is designed specifically for modeling extrusive igneous activity events, this flag must be set to a value of 1 for ASHREMOB.
DirectReleaseOnlyFlag(yes=1,no=0)	This flag, located in the GLOBAL input block in <i>tpa.inp</i> , is used to streamline calculations and reduce execution times for TPA Version 5.1 simulations of extrusive igneous activity events. Because ASHREMOB is designed specifically for modeling extrusive igneous activity events, it is recommended that this flag be set to a value of 1 for ASHREMOB if groundwater doses from igneous intrusion are not needed.

Table 15-2. Input Flags Used by ASHREMOB (continued)	
Input Flag Name	Description
AshEvolutionMode[0=no_ashremob,1=ashremob]	This flag, located in the GLOBAL input block in <i>tpa.inp</i> , allows the user to select between the two options for igneous activity consequence modeling. This flag must be set to a value of 1 to invoke ASHREMOB.

15.5 Auxiliary Input Data and External Process Models

The modeling component for airborne transport and deposition of contaminated tephra in the Yucca Mountain region is abstracted into TPA Version 5.1 with an auxiliary data file (named *remob_lut.dat*), referred to as the “lookup table,” which is generated from offline analyses using TEPHRA Version 1.0 for airborne transport of radionuclides during a volcanic eruption. Based on the modeling approach in Connor, et al. (2001), TEPHRA Version 1.0 generates three-dimensional plots of the tephra deposit and includes modifications for a stratified wind field and for high-level waste incorporation with erupting tephra. Hooper, et al. (2006) provides additional information on modeling with TEPHRA Version 1.0.

The lookup table is generated from 1,024 realizations of TEPHRA Version 1.0 using stochastic sampling of Yucca Mountain-specific volcanic parameters. Table 15-3 describes the parameters in the lookup table. Table 15-4 shows the format for the lookup table. In TPA Version 5.1, lookup table parameters for high-level waste are based on 1 metric ton of high-level waste entrained in erupted tephra, and calculations in ASHREMOB are scaled by the total metric tons of high-level waste erupted, as determined from VOLCANO. Dose coefficients per unit intake [Sv/Bq], used to calculate whole body doses (effective dose or effective dose equivalent) for each pathway, are specified in the auxiliary data file, *gnewdf.dat*.

15.6 Intermediate Outputs and Information Passed to Other Modules

The intermediate outputs from ASHREMOB are described in Table 15-5. In general, volcanic dose refers to the estimated dose for all biosphere pathways associated with the igneous disruptive scenario where an eruption conduit intersects the repository and results in the release of high-level waste directly into the atmosphere as contaminated tephra. Because ASHREMOB only computes dose for the inhalation pathway, these output files for volcanic dose actually report inhalation doses when igneous eruptions are simulated using ASHREMOB. There are no optional intermediate output files for ASHREMOB.

No information is passed from ASHREMOB to other modules.

Table 15-3. Parameters in the ASHREMOB Auxiliary Input Data File (*remob_lut.dat*) in TPA Version 5.1, Where the Values for High-Level Waste Are Based on 1 Metric Ton of High-Level Waste Entrained in Erupted Tephra, and the Symbols *i*, *f*, and *e* Represent the Three Source Regions

Parameter	Description
$C_{HLW,i}$	Mass of high-level waste for the initial deposit at the receptor location per unit area [g/m ²]
$C_{ash,i}$	Mass of ash for the initial deposit at the receptor location per unit area [g/m ²]
$m_{HLW,f}$	Mass of high-level waste deposited in the Fortymile Wash catchment basin from the eruption [g]
$m_{ash,f}$	Mass of ash deposited in the Fortymile Wash catchment basin from the eruption [g]
$a_{ash,f}$	Area of the Fortymile Wash catchment basin with an ash deposit from the eruption [m ²]
$m_{HLW,e}$	Mass of high-level waste deposited in the eolian source region from the eruption [g]
$m_{ash,e}$	Mass of ash deposited in the eolian source region from the eruption [g]
$a_{ash,e}$	Area of the eolian source region with an initial ash deposit from the eruption [m ²]

Table 15-4. Format for *remob_lut.dat* Consisting of *n* Realizations of TEPHRA Version 1.0*

$C_{HLW,i,1}$	$C_{ash,i,1}$	$m_{HLW,f,1}$	$m_{ash,f,1}$	$a_{ash,f,1}$	$m_{HLW,e,1}$	$m_{ash,e,1}$	$a_{ash,e,1}$
$C_{HLW,i,2}$	$C_{ash,i,2}$	$m_{HLW,f,2}$	$m_{ash,f,2}$	$a_{ash,f,2}$	$m_{HLW,e,2}$	$m_{ash,e,2}$	$a_{ash,e,2}$
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$C_{HLW,i,n}$	$C_{ash,i,n}$	$m_{HLW,f,n}$	$m_{ash,f,n}$	$a_{ash,f,n}$	$m_{HLW,e,n}$	$m_{ash,e,n}$	$a_{ash,e,n}$

*Offline simulations of TEPHRA Version 1.0 are used to generate the lookup table. Each row corresponds to the results from a single realization of TEPHRA Version 1.0, denoted by the indices (1, 2, ..., *n*). A description of the lookup table parameters is provided in Table 15-3.

Table 15-5. Intermediate Output Files Created During Execution of ASHREMOB	
Output File	Contents
<i>airpkdos.res</i>	Total peak volcanic dose from all nuclides, the time of the peak volcanic dose, and the contribution to the peak volcanic dose from each radionuclide. This file is described in further detail in Chapter 19.
<i>arpkds_c.res</i>	Total peak volcanic dose from all nuclides, the time of the peak volcanic dose, and the contribution to the peak volcanic dose from each radionuclide for the first simulation period. This file is described in further detail in Chapter 19.
<i>npkdoset.res</i>	Peak dose and corresponding time of peak by radionuclide for each realization.
<i>npkdst_c.res</i>	Peak dose and corresponding time of peak by radionuclide and realization for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr].
<i>pkmndose.res</i>	Dose value for each realization at the time of peak mean dose.
<i>gsccdf.res</i>	Ground surface release complementary cumulative distribution function for the simulation period. This is a legacy file.
<i>gsccdf_c.res</i>	Ground surface release complementary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. This is a legacy file.
<i>gwccdf.res</i>	Groundwater release complementary cumulative distribution function for the simulation period. This is a legacy file.
<i>gwccdf_c.res</i>	Groundwater release complementary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. This is a legacy file.
<i>relccdf.res</i>	Total release complimentary cumulative distribution function for the simulation period.
<i>relgwgs.res</i>	Groundwater, ground surface, and total release for the simulation period; values for each realization.
<i>rlccdf_c.res</i>	Total release complimentary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr].
<i>rlgwgs_c.res</i>	Groundwater, ground surface, and total release for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]; values for each realization.
<i>totdose.res</i>	Time history of volcanic dose for the atmospheric transport pathway. This file is described in further detail in Chapter 19.
<i>totdos_c.res</i>	Time history of volcanic dose for the atmospheric transport pathway associated with the first simulation period. This file is described in further detail in Chapter 19.

Table 15-5. Intermediate Output Files Created During Execution of ASHREMOB (continued)	
Output File	Contents
<i>rgsna.tpa</i>	Time history of volcanic dose for each radionuclide averaged over all realizations.
<i>rgsnr.tpa</i>	Time history of volcanic dose for each radionuclide and realization.
<i>rgssa.tpa</i>	Time history of volcanic dose summed for all radionuclides and averaged over all realizations.
<i>rgssr.tpa</i>	Time history of volcanic dose summed for all radionuclides and for each realization.
<i>rgwgssa.tpa</i>	Time history of volcanic dose summed for all radionuclides and averaged over all realizations.
<i>ashremob.out</i>	Time histories for (i) airborne mass loads for each source region (any initial deposit at receptor location during light and heavy disturbance activities, fluvial remobilization, and eolian remobilization); (ii) airborne concentrations of high-level waste for the calculated quantities $H_{i-H}(t)$, $H_{i-L}(t)$, $H_f(t)$, $H_e(t)$, $H_{RMEI, outdoor}(t)$, $H_{RMEI, indoor}(t)$, $H_{RMEI, offsite}(t)$, and $H_{RMEI}(t)$ and (iii) total outdoor particle loads during light and heavy disturbance activities.

15.7 Techniques for Understanding Module Performance

While there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of processes modeled by ASHREMOB. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques may be useful to understand their effects on system-level performance. Furthermore, ASHREMOB uses a lookup table (i.e., auxiliary input data file named *remob_lut.dat*) to incorporate offline modeling with TEPHRA Version 1.0 for the airborne transport and deposition of contaminated tephra (see Section 15.5).

In addition, "pinch-point" techniques, wherein output or intermediate results produced from ASHREMOB can be understood in combination with output or intermediate results from other modules (e.g., VOLCANO), may help to better evaluate subsystem processes. Key outputs and intermediate results useful for these comparisons include time histories of volcanic doses in the *rgssa.tpa* and *rgssr.tpa* output files, airborne concentrations of high-level waste in the *ashremob.out* intermediate result file, and the mass of waste ejected in the *volcano.rlt* intermediate result file (see Section 14.6). In addition, the *lhs.out* intermediate result file (refer to Chapter 19 for more information) can be used to determine the sampled values of individual input parameters for each realization. In particular, the sampled value of the *tpa.inp* input parameter AshPlumeRealizationIndex[] determines the row of data used from the lookup table (*remob_lut.dat*) for that TPA Version 5.1 realization.

Toggleing between the values of the *tpa.inp* parameter flag AshEvolutionMode[0=no_ashremob,1=ashremob] allows the user to switch between the two

abstracted modeling approaches for estimating consequences from an igneous eruption (see Figure 15-4 and Section 15.4). Comparing the results from the two approaches can lead to insights on subsystem model performance. In addition to differences in airborne transport and remobilization of contaminated tephra, ASHREMOB only calculates doses for the inhalation pathway. In contrast, the alternative approach invokes DCAGS calculations for inhalation and noninhalation pathways, as described in Chapter 17.

For ASHREMOB, analysis for each of three source regions (initial deposit at receptor location, fluvial, and eolian) can be used to quantify the relative contributions of each source region to the total inhalation dose. Specifically, the three weighting factors in *tpa.inp* {WeightingFactorInitialDeposit[], WeightingFactorFluvial[], and WeightingFactorEolian[]} and the auxiliary input data in *remob_lut.dat* can be used to magnify or diminish the effects from an individual source region in ASHREMOB. For example, the contributions from an individual source region can be minimized by assigning low values to all lookup table entries for the mass of high-level waste deposited in that source region. In addition, contributions from outdoor and indoor exposure to the total inhalation dose can be assessed by minimizing values for the *tpa.inp* parameters for indoor occupancy fraction {OccupancyFractionInsideHeavyDisturbance[] and OccupancyFractionInsideLightDisturbance[]}, which will maximize contributions from outdoor exposure.

To investigate the significance of the high-level waste concentration factor in ash [i.e., mass ratio of high-level waste to ash, an intermediate quantity shown in Eqs. (15-6), (15-8), and (15-15) that is specified by *remob_lut.dat* and VOLCANO data], inhalation dose outputs (y-axis) for a set of realizations can be plotted against the values taken for the high-level concentration factor (x-axis). Alternatively, individual realizations can be sorted in order of decreasing inhalation dose so that bar charts or other comparisons can display the significance of the high-level waste concentration factor.

Further, single parameter importance analyses can be performed by repetitively varying input parameters associated with particular subsystem processes modeled by ASHREMOB and analyzing output and intermediate results from various consequence modules, as mentioned previously. Single parameter importance analyses could be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. For ASHREMOB calculations, the mean-value approach requires using a single set of auxiliary input data, which is selected based on its location in *remob_lut.dat* {i.e., selection of a value for the *tpa.inp* input parameter AshPlumeRealizationIndex[]}. This set of auxiliary input data corresponds to the results of a single realization for the airborne transport and deposition of contaminated tephra and is based on a single set of simulated volcanic eruption characteristics and atmospheric conditions in TEPHRA Version 1.0. As a result, the “mean-value” selection for the AshPlumeRealizationIndex[] input parameter does not necessarily represent mean or median values of the individual parameters in the ASHREMOB auxiliary input data file. In summary, caution should be used when interpreting ASHREMOB results from a mean-value simulation. To capture the full range of the 1,024 sets of auxiliary input data in *remob_lut.dat*, it is recommended that the user set the *tpa.inp* parameter NumberOfRealizations to a value of 1,024 when ASHREMOB is used (refer to Section 15.4 for flag settings).

Alternatively, a single parameter importance analysis could be performed by repetitively specifying smaller ranges within the parameter's original distribution in *tpa.inp*. The TPA code supports input parameters for their provided ranges. The user should exercise care in interpreting results from simulations in which input parameters are altered beyond their intended

ranges. Key input parameters and data that can influence the inhalation doses calculated by ASHREMOB include

- Airborne mass loading values (several *tpa.inp* input parameters beginning with AirborneMassLoad...; refer to Table 15-1)
- *Tpa.inp* parameters for sediment and ash yields from Fortymile Wash {AmbientSedimentYieldVolumePerBasinPerEvent[m/event] and PostEruptionFluvialAshYieldVolumePerAreaPerEvent[m/event]}
- Eight lookup table parameters from the auxiliary input data file (*remob_lut.dat*; see Table 15-3)
- Mass of waste ejected in *volcano.rlt* as determined by VOLCANO (see Section 14.6)

Several other key parameters that are specified as constants in the reference-case data set, such as the ASHREMOB weighting factors {WeightingFactorInitialDeposit[], WeightingFactorFluvial[], and WeightingFactorEolian[]} and occupancy fractions (several parameters beginning with OccupancyFraction...; refer to Table 15-1), may also influence ASHREMOB inhalation doses. As stated previously, values for the weighting factors are not required to sum to unity.

As mentioned previously, the lookup table (*remob_lut.dat*) contains high-level waste values that are normalized to 1 metric ton of waste ejected. ASHREMOB scales these values by the mass of waste ejected determined by VOLCANO. As another example, the high-level waste concentration in tephra deposits on the ground surface could be determined by scaling the deposited mass of high-level waste in *remob_lut.dat* by the mass of waste ejected in *volcano.rlt*.

15.8 References

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16 IGNEOUS ACTIVITY AIRBORNE TRANSPORT (ASHPLUMO) AND IGNEOUS ACTIVITY DEPOSITION AND EVOLUTION OF ASH (ASHRMOVO)

The objective of this chapter is to describe the Igneous Activity Airborne Transport module (ASHPLUMO)¹ and the Igneous Activity Deposition and Evolution of Ash module (ASHRMOVO)² that are implemented in the igneous disruptive event scenario. ASHPLUMO estimates the deposition of both tephra (i.e., ash) and incorporated spent fuel in mass per unit area at the receptor location after an extrusive volcanic event has penetrated the potential repository. ASHRMOVO calculates areal radionuclide densities at the receptor location after a volcanic event has deposited a contaminated tephra deposit.

The igneous disruptive scenario is not executed for the nominal scenario. The user can specify the igneous disruptive scenario by setting the *tpa.inp* flag VolcanicDisruptiveScenarioFlag(yes=1,no=0) to 1. Following the Igneous Disruptive Event Involving Magma module (VOLCANO)³ (Chapter 14), the Igneous Activity Ash Remobilization module (ASHREMOB)⁴ (Chapter 15) executes in the reference case for the igneous disruptive scenario. An alternative ash evolution mode can be used (i.e., ASHPLUMO and ASHRMOVO). Following VOLCANO, where the *tpa.inp* input flag AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0, ASHPLUMO estimates airborne transport of volcanic ash, ASHRMOVO models soil processes affecting concentration of contaminants in the deposited ground surface tephra layer, and the Dose Conversion Analysis for Ground Surface module (DCAGS)⁵ (Chapter 17) calculates pathway and dose calculations (Figure 16-1).

16.1 Conceptual Model

Basaltic volcanism encompasses a variety of eruption styles depending on the eruption energy. The energy of basaltic eruptions ranges from effusive activity, where the predominant products are lava flows, to explosive activity, resulting in fragmentation of the magma into scoria fragments and transport of scoria into the atmosphere as pyroclasts. This latter style of activity generally results in the formation of scoria cones such as those found in the Yucca Mountain region and is the focus of the volcanism described in this module. Explosive volcanic activity of this kind could effect dispersal of contaminated ash from the potential repository location to the dose receptor location. Key processes such as entrainment of spent fuel in the subvolcanic

¹The Igneous Activity Airborne Transport module is referenced frequently throughout this chapter. The abbreviation ASHPLUMO will be used.

²The Igneous Activity Deposition and Evolution of Ash module is referenced frequently throughout this chapter. The abbreviation ASHRMOVO will be used.

³The Igneous Disruptive Event Involving Magma module is referenced frequently throughout this chapter. The abbreviation VOLCANO will be used.

⁴The Igneous Activity Ash Remobilization module is referenced frequently throughout this chapter. The abbreviation ASHREMOB will be used.

⁵The Dose Conversion Analysis for Ground Surface module is referenced frequently throughout this chapter. The abbreviation DCAGS will be used.

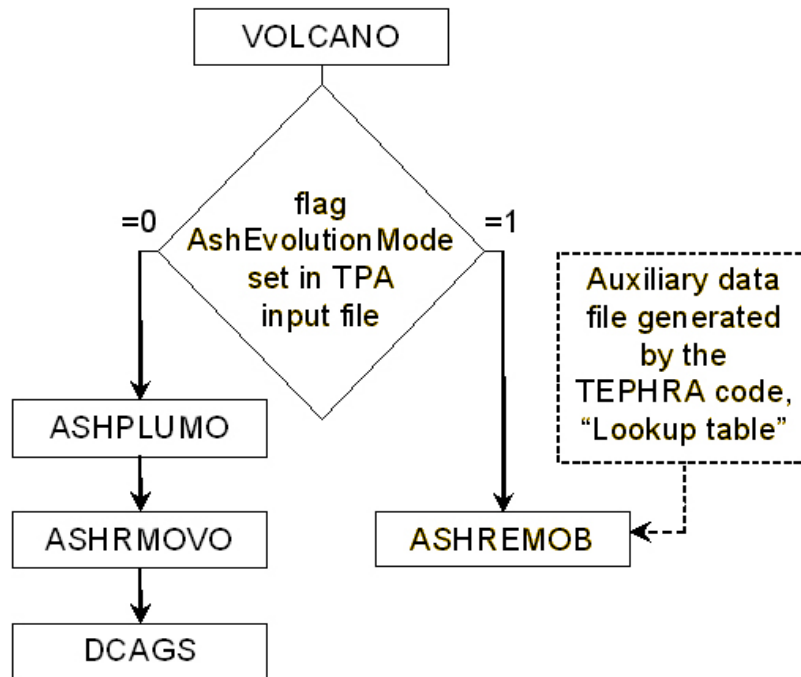


Figure 16-1. Information Diagram for Flow Chart of Volcanic Eruption Consequence Modules

conduit, dispersal of contaminated ash, and airborne transport and deposition of radionuclides are included in the conceptual model. Dispersal of volcanic ejecta (a mix of ash, cinders, bombs, and blocks collectively referred to as tephra) is modeled according to such factors as height of the eruption column, particle-size distribution, and structure of the winds aloft. Ash specifically refers to particles less than 2 mm [0.08 in] in diameter, although for simplicity in this chapter, it also refers to slightly larger volcanic particles.

Figure 16-2 shows the igneous eruption scenario. The release, transport, and exposure scenario considers four subprocesses: (i) magma enters the potential repository and becomes contaminated with spent fuel particles, (ii) tephra forms from the magma and spent fuel is incorporated into the tephra (Jarzemba and LaPlante, 1996), (iii) an eruption column and radioactively contaminated ash plume form and produce fallout at various distances downwind from the volcano (Suzuki, 1983; Jarzemba, 1997), and (iv) radionuclide contamination causes doses at the receptor (Jarzemba and LaPlante, 1996; LaPlante and Poor, 1997). Specifically, VOLCANO (Chapter 14) considers subprocess (i), ASHPLUMO addresses subprocesses (ii) and (iii), ASHRMOVO considers the ash evolution in the biosphere portion of subprocess (iv), and DCAGS addresses the dose to the receptor portion of subprocess (iv).

16.1.1 Igneous Activity Airborne Transport (ASHPLUMO)

To assess the potential radiation doses that could occur after a basaltic eruption, the deposition of spent fuel (and hence radionuclides) in the biosphere after such an event needs to be estimated. Tephra or volcanic particles ejected from the volcano are assumed to carry the

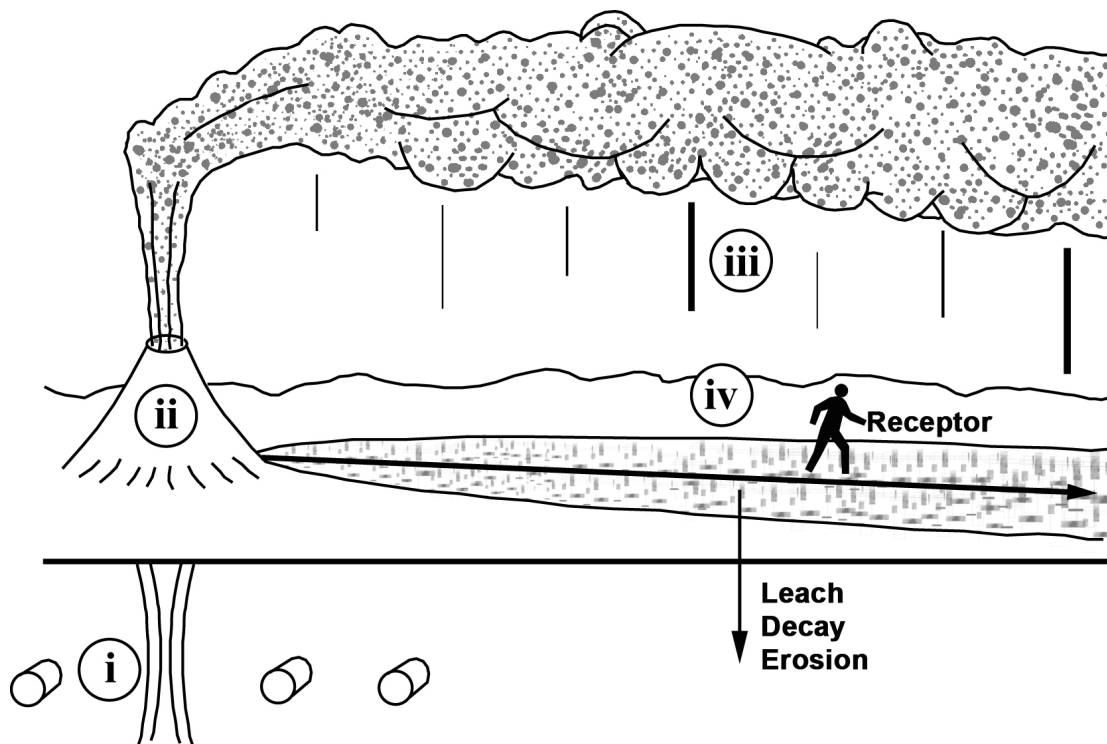


Figure 16-2. The Igneous Eruption Scenario Displaying Release, Transport, and Exposure Subprocesses

spent fuel fragments. ASHPLUMO is an abstraction of the airborne transport of volcanic ash (i.e., tephra) including any incorporated spent fuel particulate from the potential repository to points located downwind from the eruptive event. The main processes that ASHPLUMO considers for the transport of ash are (i) spent fuel particulate incorporation into the ash, (ii) dispersion in the eruption column and plume, (iii) wind blowing ash downwind from the event, and (iv) deposition of ash and radionuclides from the air to the ground surface at the receptor location.

16.1.2 Igneous Activity Deposition and Evolution of Ash (ASHRMOVO)

ASHRMOVO is an abstraction of the leaching and removal of radionuclides from a contaminated surface layer after an extrusive volcanic event has deposited radionuclides on the Earth's surface. The main processes modeled by ASHRMOVO are removal of radionuclides from the contaminated ash deposit by (i) dissolution and leaching by infiltrating water, (ii) radioactive decay, and (iii) erosion of the ash deposit.

Infiltrating water can dissolve radionuclides in the ash deposit (also called a blanket) and transport them to deeper layers. Because the spatial domain of the exposure pathway for dose modeling (Chapter 17) is limited to the upper surface layer of soil (where crop roots can intercept contaminants), this transport to deeper layers removes leached radionuclides from the biosphere.

Radioactive decay of nuclides in the ash deposit is accounted for in this model. Any radioactive progeny formed from decay is also considered.

Deposit erosion is accounted for in the model as a first order process. The blanket erosion term is considered as net erosion (deposition to the receptor location from ash eroded from areas outside the receptor location minus that eroded from the receptor). Mechanical redistribution of tephra is not modeled in ASHRMOVO.

16.2 Model Support and Assumptions

16.2.1 Airborne Transport and Deposition of Ash

ASHPLUMO executes the standalone code ASHPLUME (Jarzemba, et al., 1997) in a deterministic mode using input from other modules (e.g., VOLCANO) that describe characteristics of the eruption, such as volcanic power and duration together with the size distribution of the ash particles. The standalone code ASHPLUME uses the model described in Suzuki (1983) that relates eruption magnitude to ash transport and deposition and is modified to relate eruption magnitude to spent fuel transport and deposition for Yucca Mountain based on a few simple assumptions (Jarzemba, et al., 1997).

16.2.1.1 Incorporation of Fuel Into Ash

The model in the standalone code ASHPLUME for spent fuel incorporation in ash is detailed in Jarzemba, et al. (1997) and assumes that all spent fuel particles are eventually incorporated into larger tephra or ash particles. The mathematical formulation for this approach makes the simplifying assumption that all waste particles with diameters less than a certain fraction of the diameter of ash particles, determined by the incorporation ratio, are attached to ash particles for transport. Motivation for this approach is to bound the particle-size and density distribution for estimating the dispersion of contaminated waste. To illustrate the application of the model, Jarzemba, et al. (1997) arbitrarily chose an incorporation ratio corresponding to a maximum fuel particle size equal to half the diameter of the ash particle. For example, a 1-cm [0.4-in] fuel particle cannot be incorporated into a 0.5-cm [0.2-in] volcanic ash particle. Fuel particles larger than half the ash particle diameter cannot be incorporated into an ash particle and therefore cannot be transported downwind. It is likely that only a percentage of the spent fuel particles are incorporated in this fashion, and some of the spent fuel is transported as bare particles.

16.2.2 Transport Model and Particle Size

The transport model in the standalone code ASHPLUME uses a dispersion-advection transfer-function-type solution, which is empirical (e.g., eddy diffusivity constant and column shape parameter). Because the solution uses empirical constants based on observations at analogous volcanoes, the application of this model to Yucca Mountain assumes that future eruptions that occur at the potential repository site are similar to those observed at the present time at other locations.

The model developed by Suzuki (1983) is appropriate for particles of a mean diameter greater than about 15–30 μm [6×10^{-4} – 1.2×10^{-3} in]. This cutoff is generally accepted to be the lower limit for the importance of gravitational settling of particles (Cember, 1983; Heffter and Stunder, 1993). For particle sizes less than about 15 μm [6×10^{-4} in], atmospheric turbulence is great

enough to keep the particle aloft for a longer time than is predicted by the model. Because the typical mean diameter of ash particles after an eruption is generally much larger than 15 μm [6×10^{-4} in] (Suzuki, 1983), this model is useful for calculating the distribution for the vast majority of ash and, hence, incorporated radionuclides.

In contrast to a Gaussian model, the standalone code ASHPLUME provides an improved approach that treats the erupting column as a line source reaching some maximum height governed by the energy and mass flow of the eruption. A linear decrease in the upward velocity of particles is assumed, resulting in segregation of ash or ash and waste particles in the ascending column by settling velocity, which is a function of grain size, shape, and density. A Gaussian plume model does not accurately account for the effects of gravitational settling of volcanic particles with large diameters (i.e., centimeters). Ash and high-level waste particles are removed from the column based on the settling velocity, the decrease in the upward velocity of the column as a function of height, and a probability density function that attempts to capture particle diffusion out of the column where vertical lift is provided. The dispersion of the ash and high-level waste diffused out of the column is modeled for a uniform wind field and is governed by the diffusion-advection equation with vertical settling. Jarzemba and LaPlante (1996), Jarzemba (1997), and Jarzemba, et al. (1997) contain more complete descriptions of the derivation, structure, and use of the standalone code ASHPLUME and its algorithms. The model has been benchmarked against actual eruptions with good agreement (Hill, et al., 1998; Connor, et al., 2001).

16.2.3 Wind Data

The transport model in the standalone code ASHPLUME as implemented by ASHPLUMO in TPA Version 5.1 assumes the wind speed and direction do not vary during the course of the event. Variations in wind velocity and direction during the event could lead to a wider distribution of spent fuel than those predicted with a single velocity and direction. TPA Version 5.1 has the capability, within ASHREMOB, to evaluate the importance of these variable wind assumptions.

16.3 Implementation of Conceptual Model in TPA Version 5.1

16.3.1 Igneous Activity Airborne Transport (ASHPLUMO)

16.3.1.1 Incorporation of Spent Fuel Into Ash

Currently, the fuel fraction model developed by Jarzemba, et al. (1997) is used to abstract the complex process of high-level waste incorporation and transport. Waste particles are assumed to be incorporated into erupting pyroclasts following the rule

$$\rho_c = \log \left[\frac{d_{min}^a}{d^f} \right] \quad (16-1)$$

where

ρ_c — incorporation ratio [unitless] as specified by the *tpa.inp* parameter
IncorporationRatio

d^f — diameter of the waste particle to be incorporated [cm]

d_{min}^a — minimum diameter of a pyroclast required to transport this particle [cm]

The model uses the power and duration of the eruption, along with other properties of the ash particulates, and develops a spent fuel distribution from those sampled parameters. The spent fuel distribution can then be transported and deposited to the ground surface at the receptor location as mass and translated into radioactivity that can then be used to model human dose.

Tephra released from the eruption that penetrates the potential repository settles on the ground surface. The mass of spent fuel per unit area at the receptor location is needed to calculate dose. A model for spent fuel incorporation into ash was created to calculate the mass of spent fuel per unit area at the receptor. This model requires introducing a function to determine the mass of fuel per unit mass of volcanic ash as a function of the logdiameter of the ash after it has been contaminated with spent fuel, $FF(\rho^a)$. The ash mass is assumed to be distributed lognormally with respect to particle size

$$f(\rho^a) = \frac{1}{\sqrt{2\pi}\sigma_d} \exp\left(-\frac{(\rho^a - \rho_{mean}^a)^2}{2\sigma_d^2}\right) \quad (16-2)$$

where

- $f(\rho^a)$ — normalized (per unit mass) probability distribution of ash mass as a function of ρ^a
- σ_d — standard deviation of the logparticle size [cm] as specified by the *tpa.inp* parameter AshParticleSizeDistributionStandardDeviation
- ρ^a — logdiameter of ash particle size [cm]
- ρ_{mean}^a — mean of the logdiameter of ash particle size [cm] as specified by the *tpa.inp* parameter AshMeanParticleLogDiameter[d_in_cm]

To determine $FF(\rho^a)$, the fuel fraction (ratio of fuel mass to ash mass) as a function of ρ^a , one must consider that all fuel particles of a size smaller than $(\rho^a - \rho_c)$ can simultaneously be incorporated into ash particles of size ρ^a or larger, where ρ_c is the incorporation ratio. The fuel fraction as a function of ρ^a is determined by summing all the incremental contributions of fuel mass to the ash mass from fuel sizes smaller than $(\rho^a - \rho_c)$.

An expression for the fuel fraction is given as

$$FF(\rho^a) = \frac{U}{Q} \int_{\rho=\rho^a-\rho_c}^{\rho^a} \frac{m(\rho - \rho_c)}{1 - F(\rho)} d\rho \quad (16-3)$$

where

- $FF(\rho^a)$ — fuel fraction as a function of particle size [unitless]
- Q — total mass of ash ejected in the event [g]
- U — total mass of fuel ejected in the event [g]
- ρ — common logarithm of ash particle diameter d [cm]

- $F(\rho)$ — cumulative distribution of ash mass with ρ
- $m(\rho - \rho_c)$ — normalized probability distribution of fuel mass with $(\rho - \rho_c)$

This equation assumes the resulting contaminated particles follow the same size distribution as the original volcanic ash particles. For each simulation, Eq. (16-3) is numerically integrated to calculate the distribution of tephra on the Earth's surface resulting from a basaltic eruption assumed to disrupt the potential repository.

16.3.1.2 Transport Model and Particle Size

The tephra dispersal model described in Suzuki (1983) can be summarized by the equation that describes the areal density of accumulated ash on the Earth's surface after an eruption

$$X(x,y) = \int_{\rho=\rho_{\min}}^{\rho_{\max}} \int_{z=0}^H \frac{5QP(z)f(\rho)}{8\pi C(t+t_s)^{5/2}} \exp\left[-\frac{5\{(x-ut)^2+y^2\}}{8C(t+t_s)^{5/2}}\right] dz d\rho \quad (16-4)$$

where

- $X(x,y)$ — mass of ash per unit area accumulated at location (x,y) [g/cm²]
- ρ — common logarithm of ash particle diameter d [cm]
- $\rho_{\min}$ — minimum value of ρ
- $\rho_{\max}$ — maximum value of ρ
- H — height of the eruption column above the vent [km]
- z — vertical distance from the ground surface [km]
- Q — total quantity of erupted material [g]
- $P(z)$ — function for particle diffusion at height within dz about z [unitless]
- $f(\rho)$ — distribution function for particles with a logdiameter within $d\rho$ about ρ normalized per unit mass [unitless]
- C — constant relating the eddy diffusivity and the particle fall time [cm²/s^{5/2}] as specified by the *tpa.inp* parameter
ConstantRelatingFallTimetoEddyDiffusivity[cm2/s5/2]
- t — particle fall time [s]
- t_s — particle diffusion time in the eruption column [s]
- x — x-coordinate on the surface of the Earth [cm]; coordinate oriented in the same direction as the prevailing wind
- u — wind speed [cm/s] as specified by the *tpa.inp* parameter WindSpeed[cm/s]
- y — y-coordinate on the surface of the Earth [cm]; coordinate oriented perpendicular to the direction of the prevailing wind

The integrand of Eq. (16-4) is multiplied by $FF(\rho^a)$ and then recalculated to find the spent fuel density at location (x,y) . The derivation of Eq. (16-4) assumes the following, which are reiterated here from Suzuki (1983):

- The erupted material consists of a finite quantity of volcanic particles.
- The distribution of the diameter of these particles has a single mode.
- All particles fall at the terminal velocity and finally accumulate on the ground.

Two additional assumptions are made for the treatment of spent fuel:

- The distribution of spent fuel particle diameters is well described by a logtriangular distribution.
- The size distribution of contaminated ash particles is unaffected by the incorporation of spent fuel particles.

The probability density distribution function for particle diffusion out of the eruption column $P(z)$ is given by (Suzuki, 1983)

$$P(z) = \frac{\beta W_0 Y \exp(-Y)}{V_0 H [1 - (1 + Y_0) \exp(-Y_0)]} \quad (16-5)$$

where

- $P(z)$ — function for particle diffusion at height within the eruption column [km]
- Y — $\frac{\beta W(z)}{V_0}$ [unitless]
- Y_0 — $\frac{\beta W_0}{V_0}$ [unitless]
- β — constant controlling the diffusion of particles out of the eruption column [unitless] as specified by the *tpa.inp* parameter VolcanicColumnConstantBeta
- W_0 — volcanic eruption velocity at the vent exit [cm/s]
- $W(z)$ — particle velocity as a function of height equal to $W_0(1 - z / H)$ [cm/s]
- V_0 — particle terminal velocity at sea level [cm/s]
- H — height of eruption column above vent [km]

The terms Y and Y_0 have been modified from Suzuki (1983) where they were equal to $\beta(W(z) - V_0) / V_0$ and $\beta(W_0 - V_0) / V_0$ because with the former definition of Y , $P(z)$ has a negative value at heights approaching the top of the column. The definition of Y_0 has been altered to maintain identity as the value of $Y(z)$ at $z = 0$.

16.3.1.3 Wind Field

Wind speed and wind direction are important parameters for predicting the distribution of ash after a volcanic eruption. Wind speed is sampled from the distribution by the *tpa.inp* parameter

WindSpeed[cm/s]. Wind direction, as specified by the *tpa.inp* parameter WindDirection[degrees], is set 90° clockwise from east (i.e., south) to ensure that the wind blows directly toward the receptor to compensate for not modeling the posteruption movement or remobilization of contaminated ash. ASHPLUMO provides an abstraction of the transport of contaminated ash (i.e., tephra) from the potential repository to points located downwind from the event.

16.3.2 Igneous Activity Deposition and Evolution of Ash (ASHRMOVO)

ASHRMOVO uses generalized analytical solutions to calculate dynamic serial radioactive decay, including nonradioactive decay losses by leaching or erosion. For the volcanic exposure scenario, ASHRMOVO calculates the time history of radionuclide surficial contamination following the event by using analytical solutions to the following differential equations contained in the INVENT utility module (Section 4.6)

$$\begin{aligned}\frac{dN_i(t)}{dt} &= \lambda_{i-1}^p N_{i-1}(t) - \lambda_i^p N_i(t) - \lambda_i^l N_i(t) - \lambda^B N_i(t) \\ &= \lambda_{i-1}^p N_{i-1}(t) - \lambda_i^T N_i(t)\end{aligned}\quad (16-6)$$

where

- $N_i(t)$ — time-dependent areal density of radionuclide i [mol/m²]
- $N_{i-1}(t)$ — time-dependent areal radionuclide density of the parent [mol/m²]
- λ_i^p — removal (or generation) of a contaminant through radioactive decay [1/yr]
- λ_i^l — relative leach rate of radionuclide i from the ash blanket [1/yr]
- λ^B — bulk removal of the blanket through surface erosion [1/yr], as specified by the *tpa.inp* parameter RelativeRateOfBlanketRemoval[1/yr]
- λ_i^T — total loss rate of radionuclide i from physical decay, leaching, and surface erosion [1/yr] and equals $\lambda_i^p + \lambda_i^l + \lambda^B$

The initial conditions for the system of equations are the areal densities of the radionuclides at the time of the event. These densities are estimated by the standalone code ASHPLUME.

The relative leach rate of radionuclide i is based on a model equation in Baes and Sharp (1983). The relative leach rate has an upper limit, λ_i^{Lmax} , dependent on the solubility limit of the radionuclide and the amount of radionuclide present. When the leach processes are leach-rate limited, the relative leach rate of radionuclide i is given by

$$\lambda_i^l = \lambda_i^{Lmax} \quad N_i < \frac{S_i R_a}{\lambda_i^{Lmax}} \quad (16-7)$$

and when the leach processes are solubility limited, it is given by

$$\lambda_i^l = \frac{S_i R_a}{N_i} \equiv \frac{S_i R_a}{N_i} \quad N_i < \frac{S_i R_a}{\lambda_i^{Lmax}} \quad (16-8)$$

where

- S_i — solubility limit of radionuclide i [mol/m³]
- R_a — areal recharge of water [m³/(m² yr)]
- N_i — average radionuclide areal density over the timestep [mol/m²]

The quantity λ_i^{Lmax} is a combination of more basic parameters and is given by

$$\lambda_i^{Lmax} = \frac{P(1 - f_e^P)f_{sat}^P + I(1 - f_e^I)f_{sat}^I}{d\theta(1 + (\rho_d / \theta)K_{d_i})} \quad (16-9)$$

where

- P — annual precipitation rate as specified by the *tpa.inp* parameter AnnualPrecipitation[m/yr]
- f_e^P — fraction of precipitation water lost to evapotranspiration as specified by the *tpa.inp* parameter FractionOfPrecipitationLostToEvapotranspiration
- f_{sat}^P — fraction of year blanket is saturated because of precipitation as specified by the *tpa.inp* parameter FractionOfYearSoillsSaturatedDueToPrecipitation
- I — annual irrigation rate as specified by the *tpa.inp* parameter AnnualIrrigation[m/yr]
- f_e^I — fraction of irrigation water lost to evapotranspiration as specified by the *tpa.inp* parameter FractionOfIrrigationLostToEvapotranspiration
- f_{sat}^I — fraction of year soil is saturated because of irrigation as specified in the *tpa.inp* parameter FractionOfYearSoillsSaturatedDueToIrrigation
- d — depth of the rooting zone as specified by the *tpa.inp* parameter DepthOfTheRootingZone[m]
- ρ_d — ash bulk density [g/cm³] as specified by the *tpa.inp* parameter AshBulkDensity[g/cm3]
- θ — volumetric fraction of moisture in volcanic ash at saturation as specified by the *tpa.inp* parameter AshVolumetricMoistureFractionAtSaturation
- K_{d_i} — distribution coefficient [cm³/g] for radionuclide i as specified by the *tpa.inp* parameter KdOfElementInVolcanicAsh[cm3/g] where Element is variable and represents names of different elements

A complete demonstration of the model in ASHRMOVO, including plots of time-dependent radionuclide areal densities for an example case, is given in Jarzempa and Manteufel (1997).

16.4 Input Parameters in *tpa.inp*

Table 16-1 lists the input parameter values to ASHPLUMO and ASHRMOVO, respectively, from *tpa.inp* that are included in the reference data set for TPA Version 5.1. Other input parameters that are needed to use ASHPLUMO and ASHRMOVO are also listed in Table 16-1.

Table 16-1. Reference Data for Parameters of tpa.inp Used by ASHPLUMO and ASHRMOVO <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Disruptive Scenario Flags	VolcanismDisruptiveScenario Flag[1=yes,0=no]	Activates the igneous activity disruptive scenario calculations	iflag 1	This flag must be set to 1 for igneous disruptive events to occur; the reference case does not include disruptive scenarios.
ASHREMOB	AshEvolutionModel[0=no_ashremob,1=ashremob]	User-selected mode for calculating evolution of ash at receptor (0 implies wind direction fixed toward receptor without ash remobilization, 1 implies wind direction sampled and ash remobilization effects included)	iconstant 0	The reference case for the volcanism disruptive scenario uses ASHREMOB. To use ASHPLUMO and ASHRMOVO, this flag must be set to 1.
ASHPLUMO	DensityOfAirAtSTP[g/cm3]	Air density at standard temperature and pressure [g/cm ³]	constant 0.00129	Well-known parameter; value calculated using Lide (1994).
ASHPLUMO	ViscosityOfAirAtSTP[g/cm/s]	Air viscosity [g/cm/s]	constant 0.00017	Well-known parameter; value calculated using Lide (1994) and an authoritative empirical equation (Fox and McDonald, 1992).
ASHPLUMO	ConstantRelatingFallTimeToEddyDiffusivity[cm2/s5/2]	C Constant relating eddy diffusion to particle fall time [cm ² /s ^{5/2}]	constant 400.0	Within the Suzuki (1983) model for dispersion of tephra, eddy diffusivity is treated as a function of the fall time of tephra particles. Eddy diffusivity is determined empirically through scaling and proportionality analyses.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHPLUMO	MaximumParticleDiameterForParticleTransport[cm]	Maximum particle diameter for transport [cm]	constant 10.0	Constant describes an upper limit, drawing from studies by Pyle (1989), Hill and Connor (1995), and Hill, et al. (1998).
ASHPLUMO	MinimumFuelParticulateSize[cm]	Minimum fuel particle diameter [cm]	constant 0.0001	Minimum diameter for a logtriangular distribution is assumed to be one log unit less than the median diameter for disrupted spent nuclear fuel (NRC, 1999).
ASHPLUMO	ModeFuelParticulateSize[cm]	Median fuel particle diameter [cm]	constant 0.001	Initial grain-average diameters of spent fuel is on the order of hundreds of μm (DOE, 1988b); crush-impact studies (NRC, 1988) indicate an average diameter on the order of 100 μm . Thermal, mechanical, and chemical loads of a basaltic volcanic eruption clearly exceed those imposed by a falling ceiling panel and will thus likely fragment high-level waste further, supporting the basic assumption of a 10- μm median diameter for high-level waste transported by a basaltic volcanic eruption (NRC, 1999).
ASHPLUMO	MaximumFuelParticulateSize[cm]	Maximum fuel particle diameter [cm]	constant 0.01	Maximum diameter for a logtriangular distribution is assumed to be one log unit greater than the median diameter for disrupted spent nuclear fuel (NRC, 1999).
ASHPLUMO	MinimumAshDensityforVariationWithSize[g/cm3]	Minimum tephra density [g/cm ³]	constant 0.8	Assumed lower bound; compare with basaltic tephra deposits 20 km from the vent with densities of 0.6 g/cm ³ (Hill, et al., 1998); distal deposit porosity is about 20 percent (Walker, et al., 1984).
ASHPLUMO	MaximumAshDensityforVariationWithSize[g/cm3]	Maximum tephra density [g/cm ³]	constant 1.6	Assumed upper bound; compare with basaltic tephra deposits 1 km from the vent with densities of 1.2 g/cm ³ (Hill, et al., 1998); proximal deposit porosity is about 25 percent (Walker, et al., 1984).
ASHPLUMO	MinimumAshLogdiameterForDensityVariation[cm]	Minimum value of logarithm of ash diameter [cm]	constant -2.0	Jarzamba and LaPlante (1996) concluded that a range of one log unit in average grain size effectively encompasses the range in size-dependent density variations commonly observed in basaltic tephra-fall deposits (Hill and Trapp, 1997; Walker, et al., 1984).

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHPLUMO	MaximumAshLogdiameterForDensityVariation[cm]	Maximum value of logarithm of ash diameter [cm]	constant - 1.0	Jarzempa and LaPlante (1996) concluded that a range of one log unit in average grain size effectively encompasses the range in size-dependent density variations commonly observed in basaltic tephra-fall deposits (Hill and Trapp, 1997; Walker, et al., 1984).
ASHPLUMO	ParticleShapeParameter	Ash particle shape parameter. The shape of irregular particles with axial lengths a, b, and c can be described as $[b+c]/2a$, where a is greater than b or c	constant 0.5	Hill, et al. (1996) and Jarzempa, et al. (1997) concluded shape parameters between 0.5 and 0.25 describe irregularly shaped basaltic tephra and that variations within this range do not affect transport properties in the standalone code ASHPLUME (Suzuki, 1983).
ASHPLUMO	IncorporationRatio	ρ_c Spent fuel incorporation ratio	constant 0.3	Assumed value taken from Jarzempa and LaPlante (1996). Hill and Trapp (1997) found that a uniform distribution of uranium [0.1, 1.0] did not significantly affect dose for the reference case high-level waste grain-size characteristics (Jarzempa, et al., 1997).
ASHPLUMO	WindDirection[degrees]	Wind direction relative to due east in the counterclockwise direction [degrees]	constant -90.0	Wind direction is set 90° clockwise from east (i.e., south) to ensure that the wind blows directly toward the receptor location. Thus, when the AshEvolutionMode flag is set to implement ASHPLUMO and ASHRMOVO, the wind direction is fixed toward the receptor location to compensate for not modeling the posteruptive movement or remobilization of contaminated ash. Scoping analyses presented in Hill and Trapp (1997), Hill and Connor (2000), and Mohanty, et al. (2005) evaluate this approach.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHPLUMO	WindSpeed[cm/s]	U Wind speed [cm/s]	lognormal 103, 8110	Data at 2–7 km altitudes from Desert Rock airstrip, located about 50 km southeast of Yucca Mountain, collected by the National Climatic Data Center and reported in National Oceanic and Atmospheric Administration (1996). Average direction is relatively constant (within about 10 percent) at 2–7 km altitudes. Lognormal distribution derived from 3–4 km above ground level data because the average modeled eruption column height is approximately 3.7 km. Only used for fixed wind direction calculations.
ASHPLUMO	VolcanicEventDuration[s]	Duration of the tephra-forming eruption [s]	loguniform 8.64e4, 2.59e5	Current implementation of Suzuki (1983) in Jarzempa, et al. (1997) samples eruption power and duration to calculate particle velocity and tephra volume. Estimated Yucca Mountain region volcano tephra volumes are $1e6 \text{ m}^3$ to $1e8 \text{ m}^3$ (Hill and Connor, 2000). Using this distribution of eruption duration with power of $9.0e9$ – $5.0e11$ watts and relationships in Jarzempa, et al. (1997) gives appropriate Yucca Mountain region tephra volume distribution along with reasonable column heights of 2–7 km.
ASHPLUMO	VolcanicEventPower[W]	Volcanic event power [W]	loguniform $9.0e9$, $5.0e11$	Current implementation of Suzuki (1983) in Jarzempa, et al. (1997) samples eruption power and duration to calculate particle velocity and tephra volume. Estimated Yucca Mountain region volcano tephra volumes are $1e6 \text{ m}^3$ to $1e8 \text{ m}^3$ (Hill and Connor, 2000). Using this distribution of eruption power with durations of $8.64e4$ – $2.59e5$ seconds and relationships in Jarzempa, et al. (1997) gives appropriate Yucca Mountain region tephra volume distribution along with reasonable column heights of 2–7 km.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHPLUMO	VolcanicColumnConstantBeta	β Constant controlling the mass diffusion of volcanic particles out of the eruption column	constant 10.0	This parameter indicates the relative source strength as a function of elevation within the volcanic column. Constant value because this parameter is relatively insensitive and the value specified is sufficient for modeling Yucca Mountain region-type basaltic eruptions using the standalone code ASHPLUME (Hill and Trapp, 1997); supported by sensitivity studies conducted by Hill, et al. (1998) on the 1995 Cerro Negro eruption deposits.
ASHPLUMO	AshMeanParticleLogDiameter [d_in_cm]	ρ_{mean}^a Mean ash particle size [d_in_cm]	logtriangular 0.01, 0.1, 1.0	Based on analogous studies documented by Hill and Trapp (1997) and Walker and Croasdale (1972). Note: These values are NOT the log of mean ash diameter; they are the three points for logtriangular probability distribution function and are centimeters in diameter.
ASHPLUMO	AshParticleSizeDistribution StandardDeviation	σ_d Ash particle size distribution standard deviation	constant 1.0	Constant value recommended by Hill and Trapp (1997) with support from the modeling study by Hill, et al. (1996).
ASHRMOVO	KdOfUraniumInVolcanicAsh [cm3/g]	Uranium (U) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 13 0.17, 0.0 0.27, 0.067 0.71, 0.115 1.86, 0.184 4.85, 0.274 12.7, 0.382 33.1, 0.500 86.5, 0.618 225.9, 0.726 589.9, 0.816 1540.7, 0.885 4023.9, 0.933 6000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) sandy soil type with minimum and maximum set at the distribution 5-percent and 95-percent values.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfCuriumInVolcanicAsh[cm3/g]	Curium (Cm) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 11 7666.0, 0.0 7785.4, 0.115 9604.6, 0.184 11849.0, 0.274 14617.9, 0.382 18033.7, 0.500 22247.8, 0.618 27446.7, 0.726 33860.4, 0.816 41772.8, 0.885 44260.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam values.
ASHRMOVO	KdOfPlutoniumInVolcanicAsh [cm3/g]	Plutonium (Pu) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 12 316.0, 0.0 395.4, 0.115 742.5, 0.184 1394.1, 0.274 2617.6, 0.382 4914.8, 0.500 9228.0, 0.618 17326.6, 0.726 32532.7, 0.816 61083.7, 0.885 114691.4, 0.933 190000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using clay soil.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfAmericiumInVolcanicAsh [cm ³ /g]	Americium (Am) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 12 100.0, 0.0 192.5, 0.184 419.9, 0.274 916.0, 0.382 1998.2, 0.500 4359.0, 0.618 9509.1, 0.726 20743.7, 0.816 45251.9, 0.885 98715.8, 0.933 215345.7, 0.964 300000.0, 1.0	Cumulative distribution function developed using values from Sheppard and Thibault (1990) and Bechtel SAIC Company, LLC (2003a,b). Minimum set by minimum DOE unsaturated zone K_D value. Maximum set by measured value from Sheppard and Thibault (1990) with mean and standard deviation also from Sheppard and Thibault (1990).
ASHRMOVO	KdOfThoriumInVolcanicAsh [cm ³ /g]	Thorium (Th) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 9 1700.0, 0.0 2981.0, 0.500 5597.1, 0.618 10509.1, 0.726 19732.1, 0.816 37049.1, 0.885 69563.8, 0.933 130613.8, 0.964 170000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using sandy soil. Minimum and maximum constrained by measured K_D values from EPA (1999).
ASHRMOVO	KdOfRadiumInVolcanicAsh [cm ³ /g]	Radium (Ra) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 8 1262.0, 0.0 2230.5, 0.184 5653.3, 0.274 14328.4, 0.382 36315.50, 0.500 92042.0, 0.618 233281.2, 0.726 530000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfLeadInVolcanicAsh[cm3/g]	Lead (Pb) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 8 800.0, 0.0 955.0, 0.274 2187.8, 0.382 5011.9, 0.500 11481.5, 0.618 26302.7, 0.726 60256.0, 0.816 100000.0, 1.0	Cumulative distribution function developed using values from Allison and Allison (2005) except minimum constrained by EPA (1999) data.
ASHRMOVO	KdOfProtactiniumInVolcanicAsh [cm3/g]	Protactinium (Pa) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 13 110.0, 0.0 141.2, 0.067 235.1, 0.115 391.5, 0.184 652.0, 0.274 1085.7, 0.382 1808.0, 0.500 3010.9, 0.618 5014.1, 0.726 8349.9, 0.816 13904.9, 0.885 23155.8, 0.933 29000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam with minimum and maximum set at the distribution 5-percent and 95-percent values.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfActiniumInVolcanicAsh [cm3/g]	Actinium (Ac) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 12 100.0, 0.0 192.5, 0.115 320.5, 0.184 533.8, 0.274 888.9, 0.382 1480.3, 0.500 2465.1, 0.618 4105.2, 0.726 6836.3, 0.816 11384.4, 0.885 18958.4, 0.933 24300.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam. However, minimum set by measured americium K_d for devitrified tuff (Bechtel SAIC Company, LLC, 2003a,b) and maximum set at the distribution 95-percent value. Therefore, americium serves as an analog for actinium.
ASHRMOVO	KdOfNeptuniumInVolcanicAsh [cm3/g]	Neptunium (Np) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 13 1.30, 0.0 1.92, 0.067 3.19, 0.115 5.31, 0.184 8.85, 0.274 14.7, 0.382 24.5, 0.500 40.9, 0.618 68.0, 0.726 113.3, 0.816 188.7, 0.885 314.2, 0.933 400.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam. Standard deviation and maximum values modified to reflect data from Bertetti and Werling (2005).
ASHRMOVO	KdOfSamariumInVolcanicAsh [cm3/g]	Samarium (Sm) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 5 14000.0, 0.0 22925.4, 0.382 38177.4, 0.500 63576.6, 0.618 104000.0, 1.0	Cumulative distribution function developed using values from Zavarin, et al. (2002), except standard deviation from Sheppard and Thibault (1990) loam.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfCesiumInVolcanicAsh [cm3/g]	Cesium (Cs) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 12 1000.0, 0.0 1380.2, 0.184 2038.6, 0.274 3010.9, 0.382 4447.1, 0.500 6568.2, 0.618 9701.2, 0.726 14328.4, 0.816 21162.8, 0.885 31257.0, 0.933 46166.1, 0.964 61287.0, 1.0	Cumulative distribution function developed using values from Sheppard and Thibault (1990) for loam. Minimum set by data from Zavarin, et al. (2002) and maximum set by measured K _p value from Sheppard and Thibault (1990).
ASHRMOVO	KdOfIodineInVolcanicAsh[cm3/g]	Iodine (I) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 12 0.1, 0.0 0.12, 0.036 0.22, 0.067 0.41, 0.115 0.74, 0.184 1.35, 0.274 2.46, 0.382 4.48, 0.500 8.17, 0.618 14.88, 0.726 27.11, 0.816 43.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfTinInVolcanicAsh[cm ³ /g]	Tin (Sn) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 11 125.9, 0.0 190.5, 0.274 309.0, 0.382 501.2, 0.500 812.8, 0.618 1318.3, 0.726 2138.0, 0.816 3467.4, 0.885 5623.4, 0.933 9120.1, 0.964 10000.0, 1.0	Cumulative distribution function developed using data from Allison and Allison (2005).
ASHRMOVO	KdOfSilverInVolcanicAsh[cm ³ /g]	Silver (Ag) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 16 10.0, 0.0 14.5, 0.036 25.1, 0.067 43.7, 0.115 75.9, 0.184 131.8, 0.274 229.1, 0.382 398.1, 0.500 691.8, 0.618 1202.3, 0.726 2089.3, 0.816 3630.8, 0.885 6309.6, 0.933 10964.8, 0.964 19054.6, 0.982 31622.8, 1.0	Cumulative distribution function developed using data from Allison and Allison (2005).

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfPaladiumInVolcanicAsh [cm3/g]	Paladium (Pd) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 13 11.0, 0.0 14.2, 0.067 23.6, 0.115 39.3, 0.184 65.4, 0.274 108.9, 0.382 181.3, 0.500 301.9, 0.618 502.7, 0.726 837.1, 0.816 1394.1, 0.885 2321.6, 0.933 2850.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam with minimum and maximum set at the distribution 5-percent and 95-percent values.
ASHRMOVO	KdOfTechnetiumInVolcanicAsh [cm3/g]	Technetium (Tc) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 15 0.01, 0.0 0.016, 0.115 0.027, 0.184 0.046, 0.274 0.079, 0.382 0.135, 0.500 0.232, 0.618 0.399, 0.726 0.684, 0.816 1.174, 0.885 2.014, 0.933 3.456, 0.964 5.930, 0.982 10.176, 0.992 16.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using sandy soil with minimum and maximum constrained by measured K_d values.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfMolybdenumInVolcanicAsh [cm ³ /g]	Molybdenum (Mo) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 13 7.4, 0.0 9.5, 0.067 15.8, 0.115 26.3, 0.184 43.8, 0.274 73.0, 0.382 121.5, 0.500 202.4, 0.618 337.0, 0.726 561.2, 0.816 934.5, 0.885 1556.2, 0.933 2000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam with minimum and maximum constrained by the distribution 5-percent and 95-percent values.
ASHRMOVO	KdOfNiobiumInVolcanicAsh [cm ³ /g]	Niobium (Nb) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 13 33.0, 0.0 42.5, 0.067 70.8, 0.115 117.9, 0.184 196.4, 0.274 327.0, 0.382 544.6, 0.500 906.9, 0.618 1510.2, 0.726 2514.9, 0.816 4188.1, 0.885 6974.4, 0.933 8500.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam with minimum and maximum constrained by the distribution 5-percent and 95-percent values.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfZirconiumInVolcanicAsh [cm ³ /g]	Zirconium (Zr) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 13 135.0, 0.0 172.4, 0.067 287.1, 0.115 478.2, 0.184 796.3, 0.274 1326.1, 0.382 2208.3, 0.500 3677.5, 0.618 6124.2, 0.726 10198.5, 0.816 16983.5, 0.885 28282.5, 0.933 34550.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam with minimum and maximum constrained by the distribution 5-percent and 95-percent values.
ASHRMOVO	KdOfStrontiumInVolcanicAsh [cm ³ /g]	Strontium (Sr) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 13 3.0, 0.0 4.1, 0.067 6.8, 0.115 11.2, 0.184 18.7, 0.274 31.2, 0.382 51.9, 0.500 86.5, 0.618 144.0, 0.726 239.8, 0.816 399.4, 0.885 665.1, 0.933 900.0, 1.0	Cumulative distribution function developed using data from Zavarin, et al. (2002), except standard deviation taken from Sheppard and Thibault (1990) loam values.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfSeleniumInVolcanicAsh [cm ³ /g]	Selenium (Se) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 11 36.0, 0.0 38.1, 0.184 42.9, 0.274 48.4, 0.382 54.6, 0.500 61.6, 0.618 69.4, 0.726 78.3, 0.816 88.2, 0.885 99.5, 0.933 100.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using sandy soil, except maximum constrained by data from Allison and Allison (2005).
ASHRMOVO	KdOfNickelInVolcanicAsh[cm ³ /g]	Nickel (Ni) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwisecdf 14 60.0, 0.0 100.0, 0.036 141.3, 0.067 199.5, 0.115 281.8, 0.184 398.1, 0.274 562.3, 0.382 794.3, 0.500 1122.0, 0.618 1584.9, 0.726 2238.7, 0.816 3162.3, 0.885 4466.8, 0.933 6309.6, 1.0	Cumulative distribution function developed using data from Allison and Allison (2005), except minimum set by measured K_d from Sheppard and Thibault (1990) sandy soil.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	KdOfChlorineInVolcanicAsh [cm ³ /g]	Chlorine (Cl) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 14 0.0, 0.0 0.010, 0.018 0.014, 0.036 0.019, 0.067 0.027, 0.115 0.037, 0.184 0.052, 0.274 0.072, 0.382 0.100, 0.500 0.139, 0.618 0.194, 0.726 0.270, 0.816 0.375, 0.885 0.4, 1.0	No data for chlorine; used technetium cumulative distribution function values from Sheppard and Thibault (1990) loam soil.
ASHRMOVO	KdOfCarbonInVolcanicAsh[cm ³ /g]	Carbon (C) distribution coefficient in volcanic ash [cm ³ /g]	usersuppliedpwiscdf 13 1.12, 0.0 1.42, 0.067 2.36, 0.115 3.94, 0.184 6.6, 0.274 10.9, 0.382 18.2, 0.500 30.3, 0.618 50.4, 0.726 83.9, 0.816 139.8, 0.885 232.8, 0.933 299.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) using loam with minimum and maximum constrained by the distribution 5-percent and 95-percent values.
ASHRMOVO	SolubilityOfUraniumInVolcanicAsh [moles/liter]	Uranium (U) solubility [moles/liter]	constant 3.2e-5	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfCuriumInVolcanicAsh [moles/liter]	Curium (Cm) solubility [moles/liter]	constant 1.0e-6	Data from Kerrisk (1985). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	SolubilityOfPlutoniumInVolcanicAsh[moles/liter]	Plutonium (Pu) solubility [moles/liter]	constant 1.0e-7	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfAmericiumInVolcanicAsh[moles/liter]	Americium (Am) solubility [moles/liter]	constant 1.0e-7	Data from Kerrisk (1985). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfThoriumInVolcanicAsh [moles/liter]	Thorium (Th) solubility [moles/liter]	constant 3.2e-9	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfRadiumInVolcanicAsh [moles/liter]	Radium (Ra) solubility [moles/liter]	constant 1.0e-7	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfLeadInVolcanicAsh [moles/liter]	Lead (Pb) solubility [moles/liter]	constant 3.2e-7	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfProtactiniumInVolcanicAsh [moles/liter]	Protactinium (Pa) solubility [moles/liter]	constant 3.2e-8	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfActiniumInVolcanicAsh [moles/liter]	Actinium (Ac) solubility [moles/liter]	constant 1.0e-10	Data are from Wilson, et al. (1994). All solubilities, except for actinium, represent the mean of the distribution in logarithmic space. The minimum value from uniform distribution is used for actinium.
ASHRMOVO	SolubilityOfNeptuniumInVolcanicAsh [moles/liter]	Neptunium (Np) solubility [moles/liter]	constant 1.0e-4	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfSamariumInVolcanicAsh [moles/liter]	Samarium (Sm) solubility [moles/liter]	constant 5.1e-8	Data from Kerrisk (1985). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfCesiumInVolcanicAsh [moles/liter]	Cesium (Cs) solubility [moles/liter]	constant 1.0	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfIodineInVolcanicAsh [moles/liter]	Iodine (I) solubility [moles/liter]	constant 1.0	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	SolubilityOfTinInVolcanicAsh [moles/liter]	Tin (Sn) solubility [moles/liter]	constant 5.0e-8	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfSilverInVolcanicAsh [moles/liter]	Silver (Ag) solubility [moles/liter]	constant 3.2e-7	Best estimate. Because of a lack of data, silver is assigned the same solubility as lead (a chemically similar element).
ASHRMOVO	SolubilityOfPalladiumInVolcanicAsh [moles/liter]	Palladium (Pd) solubility [moles/liter]	constant 9.5e-4	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfTechnetiumInVolcanicAsh [moles/liter]	Technetium (Tc) solubility [moles/liter]	constant 1.0	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfMolybdenumInVolcanicAsh [moles/liter]	Molybdenum (Mo) solubility [moles/liter]	constant 3.2e-7	Best estimate. Because of a lack of data, molybdenum is assigned the same solubility as lead (a chemically similar element).
ASHRMOVO	SolubilityOfNiobiumInVolcanicAsh [moles/liter]	Niobium (Nb) solubility [moles/liter]	constant 1.0e-8	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfZirconiumInVolcanicAsh [moles/liter]	Zirconium (Zr) solubility [moles/liter]	constant 3.2e-10	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfStrontiumInVolcanicAsh [moles/liter]	Strontium (Sr) solubility [moles/liter]	constant 1.0e-4	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfSeleniumInVolcanicAsh [moles/liter]	Selenium (Se) solubility [moles/liter]	constant 1.0	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfNickelInVolcanicAsh [moles/liter]	Nickel (Ni) solubility [moles/liter]	constant 1.8e-3	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	SolubilityOfChlorineInVolcanicAsh [moles/liter]	Chlorine (Cl) solubility [moles/liter]	constant 1.0	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	SolubilityOfCarbonInVolcanicAsh [moles/liter]	Carbon (C) solubility [moles/liter]	constant 1.0	Data from Wilson, et al. (1994). See SolubilityOfActiniumInVolcanicAsh [moles/liter] for additional information.
ASHRMOVO	FractionOfPrecipitationLostToEvapotranspiration	f_e^p Fraction of precipitation lost to evapotranspiration	constant 0.68	Based on the converse of the fraction of precipitation that can reach the deep soil, drawing from Jarzempa and Manteufel (1997).
ASHRMOVO	FractionOfIrrigationLostToEvapotranspiration	f_e^i Fraction of irrigation water lost to evapotranspiration	constant 0.5	Data taken from Jarzempa and Manteufel (1997). Using all ranges as uniform and 10,000 realizations gives the attached distribution.
ASHRMOVO	FractionOfYearSoilsSaturatedDueToPrecipitation	f_{sat}^p Fraction of year blanket saturated due to precipitation	constant 0.0054	Fraction of year saturated due to precipitation (0.0054) is equivalent to about 2 days per year, signifying 1–2 storm events per year (Jarzempa and Manteufel, 1997).
ASHRMOVO	FractionOfYearSoilsSaturatedDueToIrrigation	f_{sat}^i Fraction of year blanket saturated due to irrigation	constant 0.2	Data taken from LaPlante, et al. (1995) and based on average growing time for a wide range of crops from Chambers and Mays (1994).
ASHRMOVO	AshVolumetricMoistureFractionAtSaturation	θ Volumetric fraction of moisture in volcanic ash at saturation	constant 0.4	Constant value based on current assumption that uncertainties are insignificant; data taken from Hill, et al. (1998) and Lipman and Mullineaux (1981).
ASHRMOVO	DepthOfTheRootingZone[m]	d Depth of rooting zone [m]	constant 0.15	Data from Napier, et al. (1988). TPA Version 5.1 modeling assumes that all roots are contained within the top 15 cm of soil.
ASHRMOVO	AshBulkDensity[g/cm3]	ρ_d Bulk density for volcanic ash [g/cm ³]	constant 1.2	Data based on <i>in-situ</i> measurements of tephra deposits during the 1995 Cerro Negro eruption made at 1 km from the vent (Hill, et al., 1998).

Table 16-1. Reference Data for Parameters of <i>tpa.inp</i> Used by ASHPLUMO and ASHRMOVO (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block In <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
ASHRMOVO	RelativeRateOfBlanketRemoval [1/yr]	λ^B Bulk removal rate from blanket [1/yr]	constant 0.0007	Only traces of the tephra-fall deposit are preserved at the youngest Yucca Mountain region volcano, Lathrop Wells, which is around 100,000 years old. Recent work by Delgado-Granados, et al. (1998) at Xitle volcano, Mexico, has shown that substantial amounts of basaltic tephra-fall deposits are preserved from this 2,000-year-old eruption. The area around Xitle volcano receives around 500–700 mm of annual rainfall, in contrast to the roughly 100-mm annual rainfall in the Yucca Mountain region. Although many factors, such as topographic slope, degree of incision, and eolian sedimentation, affect tephra-fall erosion, areas of greater annual rainfall are expected to experience higher erosion rates of nonconsolidated fall deposits than areas of lower annual rainfall. Thus, tephra-fall deposits in the Yucca Mountain region likely are significantly preserved for around 10,000 years. Therefore, use a removal half-life of 1,000 years.
GENTPA	AnnualPrecipitation[m/yr]	Annual precipitation rate [m/yr]	constant 0.102	Annual precipitation in Amargosa Valley determined from data reported in the Bechtel SAIC Company, LLC (2004, Table 4.1-2).
GENTPA	AnnualIrrigation[m/yr]	Annual irrigation rate [m/yr]	constant 1.12	Irrigation rate data are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004) showing irrigation rates for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods. For TPA Version 5.1 use, these crop-specific rates were used to derive representative values for crop categories consistent with the model inputs. The crop category-specific rates were averaged to derive the annual irrigation rate listed here (1.12 m/yr).

16.5 Auxiliary Input Data and External Process Models

ASHPLUMO and ASHRMOVO utilize no auxiliary input data or external process models, but ASHPLUMO uses the ASHPLUME standalone code.

16.6 Intermediate Outputs and Information Passed to Other Modules

ASHPLUMO receives the mass of spent fuel extruded in the volcanic event from VOLCANO and a set of sampled parameters from *tpa.inp* as input. For all ground surface radionuclides, ASHRMOVO transfers the areal radionuclide density in activity per unit area as a function of time at the receptor to DCAGS for dose calculation. Activity per mass of ash is also passed from ASHRMOVO to DCAGS for inhalation dose calculations.

ASHPLUMO generates intermediate input and output data transfer files while executing the ASHPLUME standalone code (Table 16-2). These files contain information only for the final realization available at the end of TPA Version 5.1 execution. ASHPLUMO intermediate input data transfer is *ashplume.in*. ASHPLUMO parameters specified in *tpa.inp* are accessed through *ashplume.in*. The intermediate output data transfer from ASHPLUMO includes *ashplume.out*. ASHPLUMO outputs for the ash and spent fuel areal densities are available in the output file, *ashplume.out*.

Output files vary depending on TPA Version 5.1 run options selected. For example, the ASHPLUMO intermediate outputs are provided in *ashout.res*. All intermediate output files (those with *.res* file names) are provided in Table 16-3. For all realizations, the contents of *ashout.res* include the time of the volcanic event, the number of waste packages exhumed, areal ash and spent fuel density, column height, ash mass, and vent exit velocity. The *ashout.res* file is further described in Chapter 19.

In addition to *ashout.res* described above, the user can specify that calculated information passed to and from ASHPLUMO and ASHRMOVO be saved as optional intermediate output for specific realizations. Tables 16-3 and 16-4 list and describe these optional intermediate output files. To specify the optional intermediate output files, the user can set *tpa.inp* parameter OutputMode(0=None,1=All,2=UserDefined) to a value of 1 or 2. When set to 1, all optional intermediate output for ASPLUMO and ASHRMOVO are saved for all realizations. When set to 2, optional intermediate output selected will be saved for realizations starting from *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by *tpa.inp* parameter UserDefinedUpperRealizationAppended. The user can select ASHPLUMO optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter SelectAppendFiles to 11 for *ashplumo.ech* and *ashplumo.rlt* or 14 for *ashplume.cum*. The user can select ASHRMOVO optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter SelectAppendFiles to 12 for *ashrmovo.ech* and *ashrmovo.rlt*.

These optional intermediate files can grow very large, and caution should be used to assure there is sufficient disk space to store the complete set of output files. To minimize the storage issues, the user can select just one module-specific set of optional intermediate output files rather than generating the full set. There currently is no mechanism to permit the selection of two or more module-specific sets other than the selection of the full set for all modules. If this is

Table 16-2. Description of Input and Output Files of the Standalone Code ASHPLUME	
File	Description
<i>infile.ash</i>	ASHPLUMO utilizes the parameters specified in the ASHPLUMO section of <i>tpa.inp</i> to write <i>infile.ash</i> . The <i>infile.ash</i> file is overwritten every time ASHPLUMO executes the standalone code ASHPLUME. Consequently, values in <i>infile.ash</i> are from the final realization.
<i>ashplume.out</i>	realization number wind speed [cm/s] wind direction [deg] mean ash particle diameter [cm] ash particle size distribution standard deviation eruption column height [km] event duration [s] ash mass [g] event power [W] volcanic column constant beta vent exit velocity [cm/s] particle shape parameter air density [gm/cm ³] air viscosity [g/cm-s] eddy diffusivity constant [cm ² /s ^{5/2}] maximum particle diameter for particle transport [cm] incorporation ratio fuel particle minimum logdiameter fuel particle median logdiameter fuel particle maximum logdiameter total fuel mass available [g]
<i>ashplume.in</i>	Intermediate file generated by the execution of the ASHPLUME standalone code. This file is a part of the stochastic sampling routine.
<i>ashcmd.out</i>	File that summarizes the input for the ASHPLUME standalone code.

Table 16-3. Output Files Created During Execution of ASHPLUMO	
File	Description
<i>gsccdf.res</i>	Ground surface release complementary cumulative distribution function for the simulation period. This is a legacy file.
<i>gsccdf_c.res</i>	Ground surface release complementary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. This is a legacy file.
<i>relccdf.res</i>	Total release complimentary cumulative distribution function for the simulation period.

Table 16-3. Output Files Created During Execution of ASHPLUMO (continued)	
File	Description
<i>rlccdf_c.res</i>	Total release complimentary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr].
<i>rlgwgs_c.res</i>	Groundwater, ground surface, and total release for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]; values for each realization.
<i>rlgwgs_c.res</i>	Groundwater, ground surface, and total release for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]; values for each realization.
<i>ashout.res</i>	Provides output data from ASHPLUMO only when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> . Data include time of volcanic event, number of waste packages exhumed, areal ash and spent fuel density, column height, ash mass, and vent exit velocity.
<i>ashplumo.rlt</i>	Output from <i>ashplumo.f</i> including ash and spent fuel areal densities.
<i>ashplumo.ech</i>	Input to <i>ashplumo.f</i> including metric tonnes of uranium ejected.
<i>ashplume.cum</i>	Cumulative output of <i>ashplume.out</i> over all realizations.

Table 16-4. Output Files Created During Execution of ASHRMOVO	
File	Description
<i>ashrmovo.rlt</i>	Output from <i>ashrmovo.f</i> including ground surface release by time and by nuclide.
<i>ashrmovo.ech</i>	Input to <i>ashrmovo.f</i> including timestep and surface areal spent fuel density.

desired, and if disk space is more limited than processing time, consider executing two or more simulations with different modules selected for optional intermediate output in each simulation.

16.7 Techniques for Understanding Module Performance

Two types of output files can be created during execution of the ASHPLUME standalone code. The first type, *ashplume.out* (Table 16-2), lists the input parameters for each individual volcano generated and the ash and fuel deposition densities for each location specified by the grid defined in *ashplume.in*. The second type of output file is created when requested by the user and consists of particle size distribution information (Tables 16-2 and 16-3). A separate file of this type is created for each location for ash and for spent fuel, for each event.

While there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of processes modeled by ASHPLUMO or ASHRMOVO. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques (e.g., Mohanty, et al., 2004) may be useful to understand their effects on system-level performance.

In addition, “pinch-point” techniques, wherein output or intermediate results produced from ASHPLUMO or ASHRMOVO can be understood in combination with output or intermediate results from other modules (e.g., VOLCANO, DCAGS), may help to better evaluate subsystem processes. Key output files and intermediate result files useful for these comparisons include *ashout.res*, *ashplumo.rlt*, and *ashrmovo.rlt*.

Furthermore, single parameter importance analyses can be performed by repetitively varying input parameters associated with particular subsystem processes modeled by ASHPLUMO or ASHRMOVO and analyzing output and intermediate results from various consequence modules, as mentioned previously. Single parameter importance analyses could be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, a single parameter importance analysis could be performed by repetitively specifying smaller ranges within the parameter’s original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges. The user should exercise care in interpreting results from simulations in which input are altered beyond their intended ranges. Key input parameters and data that can influence pathway and dose calculations include ash K_d values in *tpa.inp*, which control the retention and loss of radionuclides in the ash blanket and thereby influence the amount of radioactive contamination that can transfer to crops.

16.8 References

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17 BIOSPHERE PATHWAYS FOR CURRENT AND PLUVIAL CLIMATE CONDITIONS (DCAGW/DCAGS)

The Dose Conversion Analysis for Groundwater module (DCAGW)¹ and Dose Conversion Analysis for Ground Surface module (DCAGS)² execute exposure pathway (e.g., ingestion and inhalation) and dose conversion calculations depending on which environmental media are contaminated. The main functions of these modules are to: (i) receive climate data from the Climate and Infiltration module (UZFLOW)³ (Chapter 5) and groundwater radionuclide flux from the Saturated Zone Flow and Transport module (SZFT)⁴ (Chapter 12) or ground surface radionuclide concentrations from the Igneous Activity Deposition and Evolution of Ash module (ASHRMOVO)⁵ (Chapter 16); (ii) create input files and execute the GENTPA Version 1.0 code, which is based on the models of GENII Version 1.485 pathway modeling code (Napier, et al., 1988), to calculate human intakes of radioactivity from all pathways in the biosphere model for a given source of radioactivity; (iii) convert human intakes to doses using dose coefficients; and (iv) report time-dependent all pathway doses. Pathway and dose calculations in DCAGW and DCAGS share many similarities. Most of the information presented in this chapter applies to both modules, however, unique differences are noted where applicable.

User input selections determine which modules and subroutines are executed. Figure 17-1 shows the applicable routines based on specific input selections. DCAGW is executed for all subareas at the end of each TPA Version 5.1 realization for the reference case. If the *tpa.inp* parameter `VolcanismDisruptiveScenarioFlag(yes=1,no=0)` is set to 1, TPA Version 5.1 uses the Igneous Activity Ash Remobilization module (ASHREMOB)⁶ (Chapter 15) to conduct transport, ash remobilization, and inhalation-only pathway dose calculations. If the *tpa.inp* parameter `VolcanismDisruptiveScenarioFlag(yes=1,no=0)` is set to 1 and `AshEvolutionMode` is set to 0, the Igneous Activity Airborne Transport module (ASHPLUMO)⁷ (Chapter 16) is executed for air transport, ASHRMOVO for modeling soil processes affecting concentration of contaminants in the deposited ground surface ash layer, and DCAGS for pathway and dose calculations.

¹The Dose Conversion Analysis for Groundwater module is referenced frequently throughout this chapter. The abbreviation DCAGW will be used.

²The Dose Conversion Analysis for Ground Service module is referenced frequently throughout this chapter. The abbreviation DCAGS will be used.

³The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

⁴The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

⁵The Igneous Activity Deposition and Evolution of Ash module is referenced frequently throughout this chapter. The abbreviation ASHRMOVO will be used.

⁶The Igneous Activity Ash Remobilization module is used frequently throughout this chapter. The abbreviation ASHREMOB will be used.

⁷The Igneous Activity Airborne Transport module is referenced frequently throughout this chapter. The abbreviation ASHPLUMO will be used.

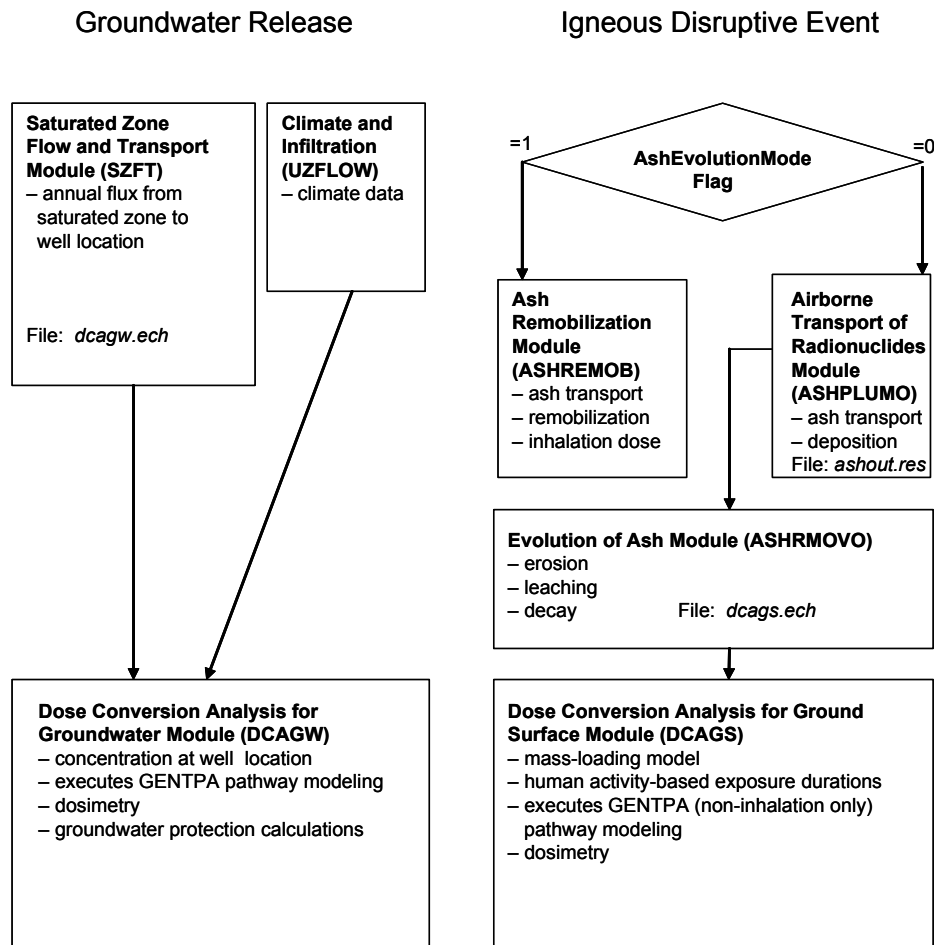


Figure 17-1. Modules Related to Pathway and Dose Calculations

17.1 Conceptual Model

The conceptual model for the biosphere pathway calculations is a hypothetical adult (the receptor) located at the receptor location in an environment (the biosphere) that is consistent with the characteristics of the Yucca Mountain region. The biosphere model considers transport of contaminants in water and soil through biosphere pathways that allow the contamination to reach the receptor. In the model, the source of contaminated water is groundwater used for drinking and irrigation of crops and livestock. Irrigation water contaminates crops eaten directly by the receptor or eaten by animals that produce food for the receptor, including meat, poultry, eggs, and milk. Irrigation water also contaminates surface soil inhaled and ingested by the receptor. Contamination ingested or inhaled by the receptor produces an internal dose to the receptor. Contaminated soil also produces an external dose to the receptor.

Four receptor activity categories are modeled that affect the amount of contaminated soil that the receptor inhales: outdoor active, outdoor inactive, indoor active, and indoor inactive

(sleeping). These categories affect the magnitude of surface-disturbing activities that can resuspend contaminated soil to air, the amount of time the receptor is exposed, and the receptor proximity to contaminated soil and air. Numerous input parameters are supplied to the model to estimate how much contamination reaches the receptor as a result of the various receptor activities that are modeled. Some examples of the types of parameters required by the model include crop-interception fractions, soil K_d values, and transfer factors for plants and animals. The magnitude of these parameters can vary by radionuclide, soil type crop variety, and livestock.

The biosphere pathway model is implemented by transporting a unit concentration of contamination through all of the biosphere pathways and calculating a dose to the receptor (i.e., a dose conversion factor). The dose conversion factor is then multiplied by the groundwater concentration provided by SZFT to calculate the dose to the receptor.

The biosphere model can also calculate the dose to the receptor from an igneous event (i.e., a volcano that erupts through the potential repository). In this scenario, the contaminated ash is deposited directly on the ground surface at the receptor location. Contaminants in soil at the receptor location are transported through the biosphere in much the same manner as contaminated water, and the dose conversion factors are calculated per unit soil concentration. The dose conversion factor is then multiplied by the soil concentration to determine the dose to the receptor.

17.1.1 Biosphere Pathways

The biosphere pathway and dose calculations are consistent with the characteristics of the physical environment surrounding Yucca Mountain and the characteristics of the receptor that could be exposed to releases from the potential repository. Regulations in 10 CFR 63.312 define specific characteristics of the receptor (i.e., the reasonably maximally exposed individual), and 10 CFR 63.305 addresses the surrounding environment of the receptor (reference biosphere). These characteristics help define the exposure scenario for TPA Version 5.1 calculations.

An exposure scenario describes the combinations of features and processes at the receptor location by which the receptor can be exposed to potential releases of contaminants. The exposure scenario modeled in TPA Version 5.1 evaluates dose to an individual adult member of a rural residential farming community located south of the potential repository site in an arid or semiarid climate zone. This scenario is consistent with the applicable characteristics of the Yucca Mountain region (LaPlante and Poor, 1997).

Pathway calculations are implemented in TPA Version 5.1 by executing GENTPA, which is based on the models of the GENII Version 1.485 pathway modeling code (Napier, et al., 1988). GENTPA is executable software within DCAGW and DCAGS that calculates human intakes of radioactivity from all pathways in the biosphere for a given source of radioactivity. DCAGW and DCAGS then use dose coefficients to convert the intakes to dose. Additional discussion of GENTPA is provided in Sections 17.3.2 and 17.3.4. Exposure pathways modeled in TPA Version 5.1 are depicted in Figure 17-2.

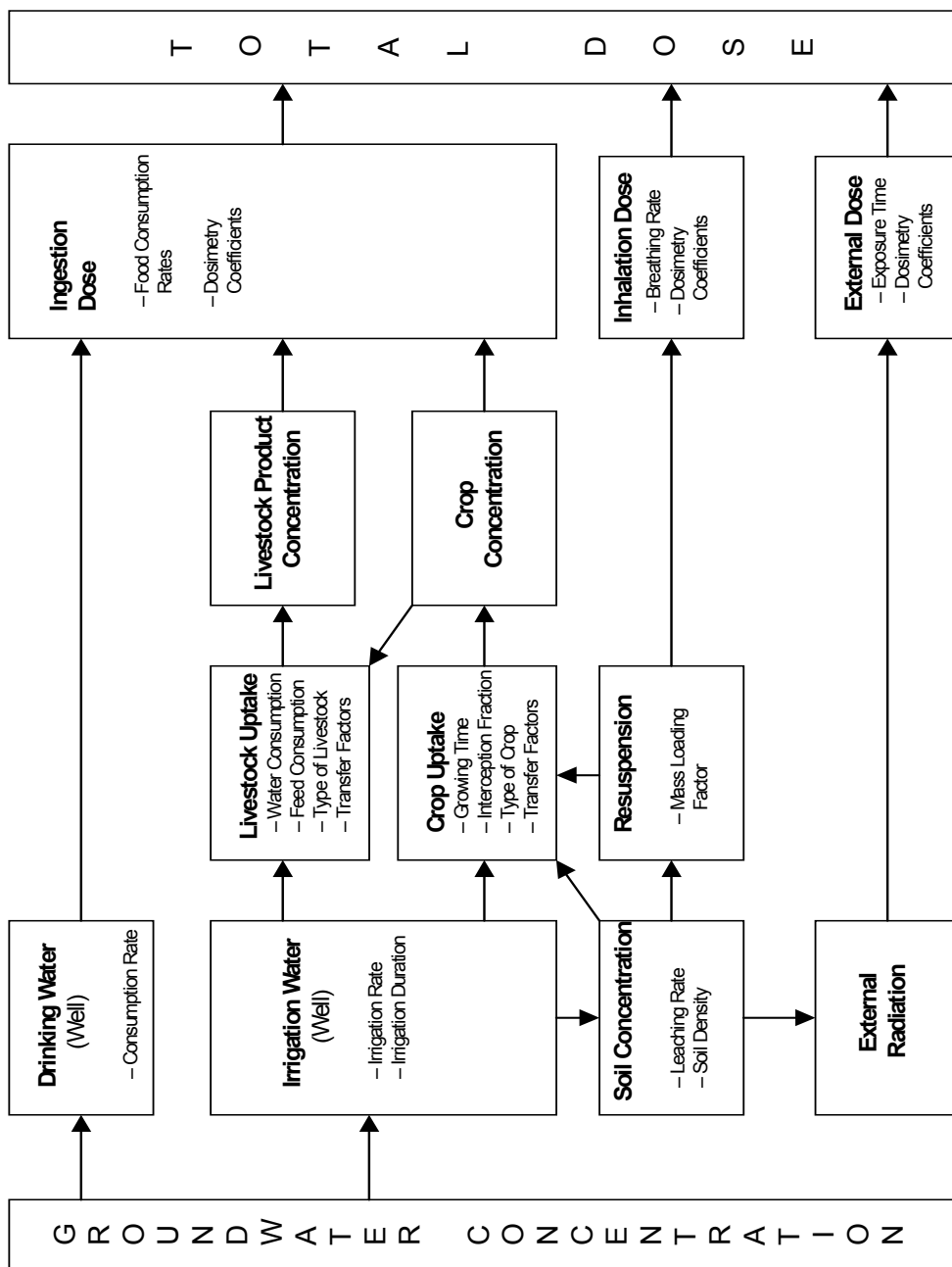


Figure 17-2. Exposure Pathways in TPA Version 5.1

When groundwater is the source of contaminants entering the biosphere, the potential exposure pathways are assumed to be those resulting from pumping and agricultural use of water consistent with present farming practices in the rural communities south of Yucca Mountain. These pathways include ingestion (contaminated drinking water, crops, animal products, and soil), inhalation of resuspended soil, and direct exposure to deposited radioactive materials.

When deposition of airborne contaminants on the ground surface from an estimated igneous disruptive event release is the source of contaminants, the modeled exposure pathways are those shown in Figure 17-2 that result from soil concentration (i.e., no groundwater concentration pathways). As previously mentioned, these pathways also include ingestion (crops, animal products, soil) and direct exposure to deposited radioactive materials.

Regional practices considered in the exposure scenarios include agricultural activities that produce food products for local consumption. Applicable food products for human consumption include vegetables (leafy and other), fruits, grains, milk, beef, poultry, and eggs. Livestock feed involves alfalfa grazing for beef and milk cows and grain feed consumption for avian livestock (chickens and egg-laying hens). Additional details of regional practices and characteristics have been previously documented by LaPlante and Poor (1997).

Groundwater protection calculations involve a different set of computed endpoints as directed by the regulations in 10 CFR 63.331. Concentration and dose limits apply to specified categories of radionuclides. Applicable computations are included in DCAGW. Here, groundwater concentrations for Ra-226, gross alpha activity including Ra-226 but excluding radon and uranium, and combined beta- and photon-emitting radionuclides are computed in the same manner as used for individual protection computations (i.e., annual saturated zone radionuclide flux divided by the representative volume, where the representative volume is specified in 10 CFR 63.332). The individual radionuclides included in each of the aforementioned categories are specified in *nuclides.dat*. Groundwater concentrations for gross alpha (including Ra-226 but excluding radon and uranium) and Ra-226 are reported directly as output. For combined beta- and photon-emitting radionuclides, the groundwater concentration is converted to whole body and organ doses as directed by the regulations in 10 CFR 63.331.

17.1.2 Human Dosimetry

For the purpose of radiation protection, dosimetry calculations estimate annual human doses from radioactivity that is inhaled, ingested, or deposited on the ground surface. Dosimetry calculations are implemented following exposure pathway calculations to convert the radionuclide intakes and external exposure time-weighted ground surface concentrations to annual human dose rates. Because dosimetry calculations are specialized, complex, and are subject to regulatory constraints, TPA Version 5.1 implements dosimetry calculations by using user-selectable sets of precalculated dose coefficients (compiled in auxiliary data files). Details of the dosimetry options and data in TPA Version 5.1 are provided in Section 17.5.1.

17.2 Model Support and Assumptions

GENTPA is based on environmental pathway models and software included in GENII Version 1.485 (Napier, et al., 1988). GENII Version 1.485 was developed by Pacific Northwest Laboratories under quality assurance plans based on the American National Standards Institute standard NQA-1 (American Society of Mechanical Engineers, 1986). GENII 1.485 was

included in a major international validation exercise (i.e., Validation of Model Predictions) organized by the International Atomic Energy Agency (1995). The Validation of Model Predictions effort compared model results with measured environmental data and concluded that results from GENII were comparable to, although slightly higher than, results of other participating models. Other published code comparisons show general agreement in results among codes with noted differences in some comparisons attributed to differences in inputs and mathematical models used for specific pathway calculations (Maheras, et al., 1994, Faillace, et al., 1994).

The following section summarizes the key assumptions that are inherent in the biosphere model. Important assumptions related to input parameters are included in the documentation of inputs in Section 17.4.

- Consumption of crops in GENTPA pathway calculations does not account for washing fruits and vegetables prior to consumption.
- Soil concentration calculations in GENTPA are based on the annual irrigation rate and annual loss from leaching. These calculations are not influenced by the growing period or irrigation time-input parameters.
- Input parameters associated with receptor behavioral characteristics are constants based on mean values, consistent with the requirements in 10 CFR 63.312(b). Food consumption rates for the receptor are based on a survey of Amargosa Valley residents (CRWMS M&O, 2000a). The survey provides the best available information on local food consumption practices. The consumption rates are representative of average consumption practices of the population that eats locally produced food.
- Irrigation for a specified time period prior to computing the dose calculation is accounted for in GENTPA. Sorption characteristics of the soil and radionuclides in the groundwater determine the degree to which buildup or washout occurs during the period of prior irrigation.
- Leaching from soil represents a loss route for contaminants in the biosphere. Secondary pathways below the soil layer are not accounted for in GENTPA.
- Modeling plant uptake using a general model involving groups of crops requires a method to be applied to derive representative plant transfer factors from available crop-specific information. For this modeling, representative crops were considered, and mean or expected values of the applicable plant uptake factors were used. Because GENTPA applies the leafy vegetable plant transfer factor to fresh forage (beef, milk), a plant transfer factor that was representative for both hay and leafy vegetable crops was selected.
- For human dosimetry modeling, the receptor is assumed to be an adult based on requirements in 10 CFR 63.312(e).
- Resuspension of contaminated soil in GENTPA applies to crop deposition, inhalation (DCAGW only), and external dose modeling.

- DCAGW and DCAGS use ground surface external dose coefficients directly from Federal Guidance Report No. 12 (EPA, 1993). The original GENII Version 1.485 divides the dose coefficients read from *grdf.dat* by 0.15 m [0.49 ft] (the depth of the contaminated soil layer) for use with volume-based external dose coefficients (Napier, et al., 1988). The external dose coefficients in Federal Guidance Report No. 12 (EPA, 1993) used in TPA Version 5.1 are area based (i.e., ground surface). Therefore, the 0.15-m [0.49-ft] value was removed from the calculations as part of GENTPA development. This was the only change made to GENII Version 1.485 algorithms for the development of GENTPA.
- Doses calculated by DCAGW and DCAGS are annual doses to an individual receptor, consistent with the requirements in 10 CFR 63.311.

17.3 Implementation of Conceptual Model in TPA Version 5.1

17.3.1 Dose Conversion Calculation Overview

The primary dose calculation approach in DCAGW and DCAGS multiplies time-dependent groundwater or ground surface radionuclide concentrations (provided by other modules) by pathway-specific biosphere dose conversion factors (i.e., calculated annual all-pathway individual dose per unit radionuclide concentration) to calculate all-pathway receptor doses. The pathway-specific biosphere dose conversion factors are the product of (i) calculated pathway-specific radionuclide human intakes (for internal exposures) or (ii) exposure time-weighted ground surface concentrations (for external exposures) and the appropriate dosimetry coefficients. User input options provide the flexibility to select which sources of dose coefficients are used (Sections 17.1.2 and 17.4). The overall dose calculation is represented by the following set of equations applicable to a groundwater release and transport scenario. For transparency, units are presented as they exist in TPA Version 5.1 input, output, and data sources.

The annual dose for exposure pathway p and radionuclide i at timestep t is calculated as

$$D_{p,i}(t) = C_i(t) E_{p,i} D_p U_{conv} \quad (17-1)$$

where

$D_{p,i}(t)$ — time-dependent annual dose for exposure pathway p and the i^{th} radionuclide [rem/yr]

$C_i(t)$ — time-dependent activity of the i^{th} radionuclide per unit volume of pumped groundwater [Ci/m³]. Computed by DCAGW as the product of annual radionuclide flux to the receptor well location (passed from SZFT) and the *tpa.inp* parameter UserDefinedPlumeCaptureFraction, divided by the annual water demand specified by the *tpa.inp* parameters UserDefinedPresentDayDilutionVolume[gal/day] and UserDefinedPluvialDilutionVolume[gal/day]

- $E_{p,i}$ — total activity of the i^{th} radionuclide per unit groundwater concentration inhaled or ingested annually by the receptor for each exposure pathway p ; computed by GENTPA [mCi/yr per mCi/L in groundwater]. For external dose calculations, this term represents the exposure time-weighted ground surface concentration for radionuclide i at the receptor location [mCi-yr/m² per mCi/L]; computed by GENTPA
- $D_{p,i}$ — dose coefficient applicable to exposure pathway p for the i^{th} radionuclide. For inhalation and ingestion dose calculations, values are in units of dose per unit intake [Sv/Bq] and provided in the auxiliary data file, *gnewdf.dat*. For external dose calculations, values represent the time-integrated dose for the i^{th} radionuclide [Sv-m²/Bq-yr] provided in the auxiliary data file, *ggrdf.dat*
- U_{conv} — factor used to implement unit conversions

The all-pathway annual dose is then calculated as the sum of the dose contributions from all radionuclides and exposure pathways

$$D_{\text{tot}}(t) = \sum_p \sum_i D_{p,i}(t) \quad (17-2)$$

The calculation of the human intake and ground surface concentration term in Eq. (17-1) ($E_{p,i}$) involves execution of biosphere pathway models in GENTPA. This code, and the models therein, are discussed in Section 17.3.2.

Calculations performed for the ground surface release scenario in DCAGS are similar, except the groundwater concentration term [$C_i(t)$] is replaced by the ground surface concentration (passed by ASHRMOVO, when selected), the intake terms [$E_{p,i}$] are different (per unit soil concentration), and the inhalation pathway modeling is not computed by GENTPA (Section 17.3.3).

17.3.2 Mathematical Models in GENTPA

Biosphere pathway calculations involve executing a series of models that evaluate initial concentrations in water, ground surface (soil), and partition contaminants to subsequent down gradient human exposure pathways in the environment. The GENII Version 1.485 software (Napier, et al., 1988) includes pathway models that are consistent with the features and processes applicable to the region surrounding Yucca Mountain. To address the biosphere pathway modeling needs of TPA Version 5.1, the pathway models in GENII Version 1.485 were recompiled to execute in the TPA Version 5.1 operating environment, and the resulting software was named GENTPA. The dosimetry modeling functions of the original GENII Version 1.485 software are not used because these computations are addressed with greater flexibility by TPA Version 5.1 using the approach described in Section 17.1.2.

Detailed descriptions of the environmental pathway models included and algorithms in GENTPA can be found in the GENII Version 1.485 user's guide (Napier, et al., 1988). Additional discussion of the models in GENTPA is provided in a detailed model abstraction description report (LaPlante, 2006). Key features and processes addressed by GENTPA include radionuclide deposition to ground surface from irrigation; surface soil processes (e.g., leaching,

sorption) affecting contaminant concentration; the calculation of crop, feed, and livestock concentrations; modeling of air concentrations from resuspended contamination; and modeling of receptor characteristics that affect exposure.

17.3.3 Mathematical Models for Mass Loading and Inhalation Dose for Ground Surface (DCAGS)

If the volcanic disruptive scenario is run (VolcanismDisruptiveScenarioFlag=1) and *tpa.inp* input parameter AshEvolutionMode=0, DCAGS is executed for pathway and dose calculations. These calculations include a specialized inhalation dose model developed to account for variations in human surface-disturbing activities that resuspend fine particulates and contribute to the inhalation dose. A similar model is executed in ASHREMOB (Chapter 15) when the ash remobilization option is selected (*tpa.inp* parameter AshEvolutionMode=1). DCAGS and ASHREMOB share a number of input parameters from *tpa.inp*.

In DCAGS, the inhalation dose per year (rem/yr) for the j^{th} radionuclide is calculated as

$$D_{\text{inh},j}(t) = B I_j \eta_j(t) f_R(t) U_{\text{conv}} [C_1 e^{-\lambda_r t} + C_2] \quad (17-3)$$

with

$$C_1 = f_{\text{out-H}} (S_{\text{ash,out-H}} - S_{\text{out-H}}) + f_{\text{out-L}} (S_{\text{ash,out-L}} - S_{\text{out-L}}) + f_{\text{in-H}} S_{\text{in-H}} + f_{\text{in-L}} S_{\text{in-L}} + f_{\text{offsite}} S_{\text{offsite}} \quad (17-4)$$

and

$$C_2 = f_{\text{out-H}} S_{\text{out-H}} + f_{\text{out-L}} S_{\text{out-L}} \quad (17-5)$$

where

- B — breathing rate [cm^3/s] as specified by the *tpa.inp* parameter InhalationRate#[cm^3/s] where # represents dosimetry selection specified by *tpa.inp* parameter Age&Dosimetry[1=Inf,2=ToDI,3=PTeen,4=Teen,5=Adlt,6=AdltFG11]
- I_j — inhalation dose coefficient per unit intake [Sv/Bq] for the j^{th} radionuclide provided in the auxiliary input data file, *gnewdf.dat*
- $\eta_j(t)$ — time-dependent activity of the j^{th} radionuclide per gram of ash near the receptor location [Ci/g] computed by DCAGS (Eq. 17-6)
- $f_R(t)$ — fraction of airborne particulate mass resuspended from the contaminated volcanic ash layer [unitless] computed by DCAGS (Eq. 17-7)
- λ_r — rate of reduction of airborne mass load [$1/\text{yr}$] as specified by the *tpa.inp* parameter RateOfReductionOfMassLoadingFactor[$1/\text{yr}$]
- $f_{\text{out-H}}$ — fraction of time receptor spends outdoors with heavy disturbance [unitless] as specified by the *tpa.inp* parameter OccupancyFractionOutsideHeavyDisturbance[]

- $S_{ash,out-H}$ — outdoor mass load above fresh ash with heavy disturbance [g/m^3] as specified by the *tpa.inp* parameter
AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]
- S_{out-H} — outdoor mass load above soil with heavy disturbance [g/m^3] as specified by the *tpa.inp* parameter
AirborneMassLoadOutsideHeavyDisturbance[g/m3]
- f_{out-L} — fraction of time receptor spends outdoors with light disturbance [unitless] as specified by the *tpa.inp* parameter
OccupancyFractionOutsideLightDisturbance[]
- $S_{ash,out-L}$ — outdoor mass load above fresh ash with light disturbance [g/m^3] as specified by the *tpa.inp* parameter
AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]
- S_{out-L} — outdoor mass load above soil with light disturbance [g/m^3] as specified by the *tpa.inp* parameter
AirborneMassLoadoutsideLightDisturbance[g/m3]
- f_{in-H} — fraction of time receptor spends indoors with heavy disturbance as specified by the *tpa.inp* parameter
OccupancyFractionInsideHeavyDisturbance[]
- S_{in-H} — indoor mass load for dust with heavy disturbance [g/m^3] as specified by the *tpa.inp* parameter
AirborneMassLoadInsideHeavyDisturbance[g/m3]
- f_{in-L} — fraction of time receptor spends indoors with light disturbance as specified by the *tpa.inp* parameter
OccupancyFractionInsideLightDisturbance[]
- S_{in-L} — indoor mass load for dust with light disturbance [g/m^3] as specified by the *tpa.inp* parameter
AirborneMassLoadInsideLightDisturbance[g/m3]
- $f_{offsite}$ — fraction of time receptor spends offsite as specified by the *tpa.inp* parameter
OccupancyFractionOffsite[]
- $S_{offsite}$ — offsite airborne mass load [g/m^3] as specified by the *tpa.inp* parameter
AirborneMassLoadOffsite[g/m3]
- U_{conv} — factor used to implement unit conversions

and

$$\eta_j(t) = \left(\frac{m^2}{10^4 \text{ cm}^2} \right) \frac{R_j(t)}{X} \quad (17-6)$$

where

- $R_j(t)$ — time-dependent activity of the j^{th} radionuclide per unit area deposited at a point location near the receptor (Ci/m^2) as computed by ASHRMOVO (Chapter 16)
- X — mass of ash per unit area initially deposited at a location near the receptor (g/cm^2) as computed by ASHPLUMO (Chapter 16)

and

$$f_R(t) = \begin{cases} \frac{X}{\rho_{ash} d_r} e^{-\lambda_b t} & \text{if } \frac{X}{\rho_{ash} d_r} e^{-\lambda_b t} < 1 \\ 1 & \text{if } \frac{X}{\rho_{ash} d_r} e^{-\lambda_b t} \geq 1 \end{cases} \quad (17-7)$$

where

- X — mass of ash per unit area initially deposited at a location near the receptor (g/cm^2) as computed by ASHPLUMO (Chapter 16)
- ρ_{ash} — density of ash [g/cm^3] as specified by *tpa.inp* parameter AshBulkDensity[g/cm^3]
- d_r — resuspendible layer thickness [cm] as specified by *tpa.inp* parameter DepthOfResuspendibleLayer[cm]
- λ_b — bulk removal rate of ash from the initial deposit [1/yr] as specified by the *tpa.inp* parameter RelativeRateOfBlanketRemoval[1/yr]
- t — time following the volcanic eruption [yr]

For details on the modeling of leaching, erosion, and radioactive decay in DCAGS, refer to Jarzempa and Manteufel (1997). The total inhalation dose is calculated as the sum of all radionuclide inhalation doses.

17.3.4 Execution of Pathway and Dose Calculations in TPA Version 5.1

The execution approach for TPA Version 5.1 pathway dose calculations (implemented by DCAGW and DCAGS) is shown in Figure 17-3. DCAGW and DCAGS read the appropriate input parameter values from *tpa.inp* and write these values to the applicable input or data files necessary for GENTPA execution. Other inputs to GENTPA are provided in fixed data files, and additional input processing steps are necessary to generate a complete set of GENTPA input files prior to execution. This is accomplished by labeling GENTPA input and data files that accept inputs from *tpa.inp* with a unique *.def extension. These files contain a full set of reference case input values, and upon execution, TPA Version 5.1 overwrites parameter information for the subset of parameters included as input in *tpa.inp*. The overwritten *.def file is then renamed with a *.inp extension, which GENTPA uses as an input file upon execution.

Any values included in GENTPA input files (*.def or *.dat) that are not listed in *tpa.inp* are effectively constant values that are not changed during TPA Version 5.1 execution. Most of the input parameters for GENTPA are included in the text file *ggenii.def* (*ggeniis.def* for DCAGS); however, additional inputs of interest are included in *gdefault.def* (*gdefaults.def* for DCAGS) and the data file *gftrans.def* (*gftranss.def* for DCAGS). Additional details of the files used to execute GENTPA are provided in Section 17.5.

Because there are multiple GENTPA code executions for each TPA Version 5.1 realization (i.e., separate sets of biosphere dose conversion factors are produced for each source of

contamination, climate state, receptor type/location), the append flag (Chapter 3) in *tpa.inp* (which provides selected input and output for each execution in *.*cum*) must be selected to generate all the input and output for each GENTPA execution in a single or multiple realization TPA Version 5.1 simulation. Therefore, the user should be aware that *.*inp* files represent only the last set of input to GENTPA that was executed in a series of executions.

Some input parameters for GENTPA are calculated from, or modified by, input provided in *tpa.inp*. Soil leaching factors, for example, are computed based on a collection of input parameters (i.e., rainfall, evapotranspiration, soil density, K_d) provided in *tpa.inp* and a leaching factor equation provided in Baes and Sharp (1983). The resulting leaching factors are written to *gftrans.def*, which is renamed to *gftrans.inp* prior to execution of GENTPA. In another example, plant and animal transfer factor values in *gftrans.def* and *gftransss.def* are read and weighted by the applicable sampled value of the PlantUptakeScaleFactor or AnimalUptakeScaleFactor input parameters from *tpa.inp*. The result is then written to *gftrans.inp*. This scaling approach allows variation to be propagated to transfer factors that are input as fixed constants in the auxiliary data file.

Following execution of GENTPA, a series of intermediate output files is produced (Section 17.6). The *genv.out* file is the primary output from GENTPA used by TPA Version 5.1. TPA Version 5.1 multiplies the values in *genv.out* by the appropriate dose coefficients in *gnewdf.dat* to generate pathway and radionuclide-specific unit (biosphere) dose conversion factors (e.g., rem/yr per Ci/m³ in groundwater) provided in a series of intermediate output files (Section 17.6) for specific combinations of source media, climate, and receptor (i.e., *gw_cb_ad.dat*, *gw_pb_ad.dat*, *gw_cb_ci.dat*, *gw_pb_ci.dat*, *gs_cb_ad.dat*, *gs_pb_ad.dat*, *gs_cb_ci.dat*, and *gs_pb_ci.dat*). Once the dose conversion factor files are generated, they are multiplied by ground surface or groundwater concentrations to compute the all-pathway doses reported in output files.

17.4 Input Parameters in *tpa.inp*

A subset of input parameters for DCAGW, DCAGS, and GENTPA execution are included in *tpa.inp* in sections labeled for these modules. This subset of parameters was selected to include inputs either found to be important in initial stochastic biosphere calculations based on prior sensitivity analyses (LaPlante and Poor, 1997) of Yucca Mountain-specific GENII-S code (Leigh, et al., 1993) runs or inputs that required a user input capability (i.e., option to sample or modify). Details regarding the input parameter values in *tpa.inp* and their justifications are provided in Table 17-1.

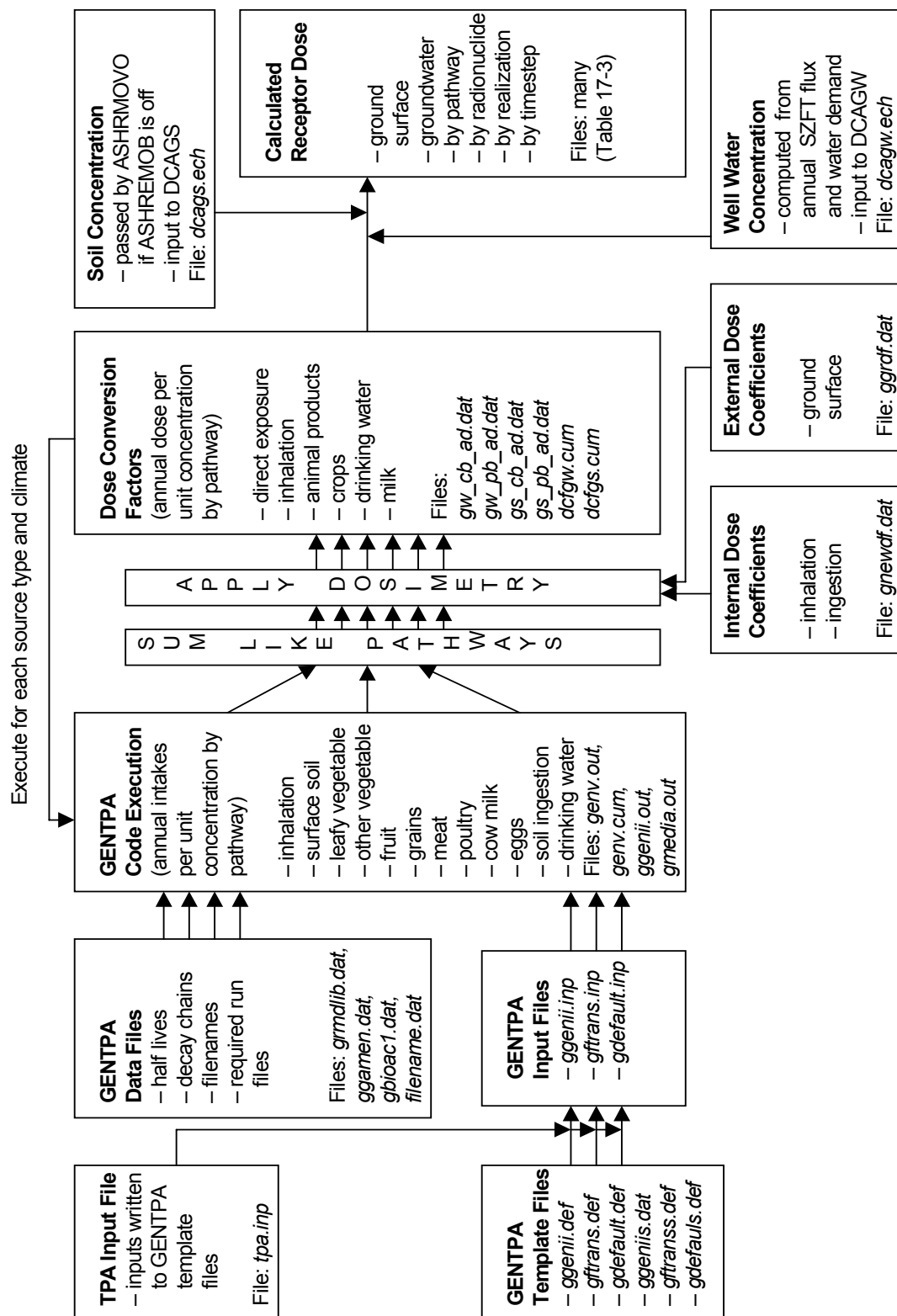


Figure 17-3. Information Flow Diagram for GENTPA Pathway and Dose Calculations in DCAGW and DCAGS

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
Groundwater Protection	GroundwaterProtectionCalc(yes=1,no=0)	Flag that controls whether groundwater protection calculations are conducted	iflag 1	Reference case value is 1. Groundwater protection calculations are conducted as part of the reference case.
Groundwater Protection	WellPumpingRateGroundwaterProtection[gal/day]	Well pumping rate for the receptor group [gal/day] that is used for groundwater protection calculations [3,000 acre-feet per year = 2676394.0 gal/day]	constant 2676394.0	Value is based on the representative volume specified in 10 CFR 63.332.
Groundwater Protection	FractionPlumeCaptureGroundwaterProtection	Fraction of the plume mass captured by pumping when the Groundwater ProtectionCalc(yes=1,no=0) is set to 1	constant 1.0	Value is consistent with the reference case assumption that all of the plume that enters the accessible environment annually is captured by the receptor's community water well. For consistency, the parameter UserDefinedPlumeCaptureFraction should be set to the same value.
DCAGW	ReceptorGroup(1=Farming, 2=Residential)	Receptor (1=member of farming community, 2=residential)	iconstant 1	A farming community receptor is consistent with 10 CFR 63.312(b) which refers to a diet and living style representative of the people who now reside in the town of Amargosa Valley, Nevada.
DCAGW	DistanceToReceptorGroup[km]	Distance to receptor [km]	constant 18	The receptor is located in the accessible environment [10 CFR 63.312(a)]. The accessible environment includes any point south of 36° 40' 13.6661" north altitude, in the predominant direction of groundwater flow (10 CFR 63.302), which is approximately 18 km [11.2 mi] (NRC, 2001).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DCAGW	PlumeCaptureModel(1=User Defined,2=Calculated)	Flag to allow the user to specify the fraction of the plume captured, instead of performing calculations; when 1 is selected, as is done for the reference case, the value specified by the parameter UserDefinedPlumeCaptureFraction is used	constant 1	Reference case value is 1 allowing the UserDefinedPlumeCaptureFraction of 1.0 to be used. The capture fraction of 1.0 is consistent with the reference case assumption that all of the plume that enters the accessible environment annually is captured by the receptor's community water well.
DCAGW	UserDefinedPlumeCapture Fraction	Fraction of the plume mass captured by pumping when the PlumeCapture Model flag = 1	constant 1	Value is consistent with the reference case assumption that all of the plume that enters the accessible environment annually is captured by the receptor's community water well. For consistency, the parameter FractionPlumeCaptureGroundwaterProtection should be set to the same value.
DCAGW	PlumeThickness[m]	Thickness of plume at receptor location; used for plume capture fraction calculations when PlumeCapture Model(1=User Defined,2=Calculated) is set to 2	uniform 10.0, 300.0	This parameter is a legacy option and not used for the reference case because the plume capture fraction is specified at a value of 1.0 (see UserDefinedPlumeCaptureFraction).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>					
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks	
DCAGW	AquiferThickness[m]	Aquifer thickness at receptor location; used for plume capture fraction calculations when PlumeCapture Model(1=User Defined,2=Calculated) is set to 2	uniform 300.0, 700.0	This parameter is a legacy option and not used for the reference case because the plume capture fraction is specified at a value of 1.0.	
DCAGW	MixingZoneThickness[m]	Mixing zone thickness at receptor location; used to calculate well pumping volume when PresentDayDilution Model(0,1,2,3,4) is set to 0 or 4	uniform 50.0, 200.0	This parameter is a legacy option and not used for the reference case because the volume of water pumped by the receptor's community is set equal to the annual water demand specified by 10 CFR 63.312(c).	
DCAGW	PresentDayDilutionModel (0,1,2,3,4)	PresentDayDilution Model(0=Calc,1=User,2=Pumped,3=UZq,4=Plume); the current configuration of TPA Version 5.1 requires the use of this switch to affect both present day and pluvial dilution models	iconstant 1	Value is set to 1 allowing the annual water demand specified in 10 CFR 63.312(c) to be used [see UserDefinedPresentDayDilutionVolume[gal/day] and UserDefinedPluvialDilutionVolume[gal/day]]. Other selections are legacy options.	

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DCAGW	UserDefinedPresentDayDilution Volume[gal/day]	Dilution volume used when the DilutionModel flag = 1; (3000 acre-feet per year = 2676394.0 gal/day)	constant 2676394.0	Value is based on the representative volume specified in 10 CFR 63.332.
DCAGW	WellPumpingRateAtReceptor Group[gal/day]	Well pumping rate for receptor group (gal/day); used to compute the dilution volume only when the PresentDayDilution Model(0,1,2,3,4) flag is set to 0 or 2	uniform 4.5e6, 1.3e7	This parameter is a legacy option because the reference case PresentDayDilutionModel(0,1,2,3,4) selection is set to 1 to allow the annual water demand specified in 10 CFR 63.312(c) to be used {see UserDefinedPresentDayDilutionVolume[gal/day] and UserDefinedPluvialDilutionVolume[gal/day]}.
DCAGW	PluvialSwitchTime[yr]	Time to switch from nonpluvial (current) biosphere climate conditions to pluvial (cooler and wetter) [yr]	constant 2000	The pluvial switch time of 2,000 years is consistent with the timestep in <i>climate2.dat</i> (Chapter 5) where mean annual precipitation and temperature have evolved to 50 percent of the variance between current climate values and glacial maximum values. This translates to a mean annual precipitation estimate, computed by UZFLOW, that represents an approximate doubling of current Amargosa Desert annual rainfall and a small decrease in mean annual temperature. The 2,000 year pluvial switch time is also consistent with the start of the glacial transition climate period described in (Bechtel SAIC Company, LLC, 2004a) that forms the basis for glacial transition crop irrigation rates and durations computed in (Bechtel SAIC Company, LLC, 2004b) which are used for pluvial period irrigation rates and durations in TPA Version 5.1 (see remarks for *.IrrigationRatePB[in/yr] and *.IrrigationTimePB[mo/yr] where * represents various crop types).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	Age&Dosimetry(1=Inf,2=ToDI, 3=PTeen,4=Teen,5=Adlt, 6=AdltFG11)	Flag to select the receptor age group and the internal dosimetry methodology	iconstant 5	Adult receptor is required for Yucca Mountain calculations by 10 CFR 63.312(e). Reference-case value is set to International Commission on Radiological Protection Publication 72 (International Commission on Radiological Protection, 2002, 1996) internal dosimetry and adult receptor. Federal Guidance No. 11 (EPA, 1988) adult dosimetry values are a user-selectable option. If flag is set to preadult age group, user is responsible for uncommitting, entering, and justifying related age-dependent input parameters in DCAGW and DCAGS or ASHREMOB.
GENTPA	InterceptionFraction/Irrigate	Irrigation interception fraction [unitless]	triangular 0.06, 0.4, 0.8	Based on review of the literature summary by Anspaugh (1987). The range encompasses the results applicable to irrigated forage crops. The mode of the distribution is the recommended value of 0.4.
GENTPA	DepthOfSurfaceSoil[cm]	Depth of surface soil [cm]	constant 15	Default value from Napier, et al. (1988). Parameter represents plow depth that is used in the model to differentiate between two soil layers (surface and deep). The surface layer is contaminated and the deep layer is clean. TPA Version 5.1 implementation assumes all roots are in surface soil layer.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	YearsOfIrrigationPriorToIntake Period[yr]	Years of irrigation water deposition prior to the intake period [yr]	constant 15	Assumption based on transient nature of farming in Amargosa Valley (insights gained from visiting with local residents). The irrigation time significantly affects soil buildup for elements such as Am, Cs, Ni, Pa, Pu, Ra, Sr, Th, and U (CRWMS M&O, 2000b), but not the key contributors to dose for the groundwater irrigation-based exposure scenario (i.e., Tc-99, I-129, Np-237). Thus, uncertainty in the parameter is not expected to be significant for the reference case results. For the igneous scenario, there is no irrigation buildup of radionuclides, and the radionuclides that dominate that scenario dose are not prone to leaching, so any "washout" effect from irrigation would be small.
GENTPA	LeafyVegetableIrrigationRatePB [in/yr]	Leafy vegetable irrigation rate for pluvial biosphere [in/yr]	triangular 15, 21, 25	Average annual irrigation rates for an upper bound glacial transition climate are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of estimated future Yucca Mountain region climate change conditions (i.e., semiarid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	OtherVegetableIrrigationRatePB [in/yr]	Other vegetable irrigation rate for pluvial biosphere [in/yr]	triangular 7, 17, 28	Average annual irrigation rates for an upper bound glacial transition climate are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of estimated future Yucca Mountain region climate change conditions (i.e., semiarid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.
GENTPA	FruitIrrigationRatePB[in/yr]	Fruit irrigation rate for pluvial biosphere [in/yr]	triangular 6, 17, 29	Average annual irrigation rates for an upper bound glacial transition climate are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of estimated future Yucca Mountain region climate change conditions (i.e., semiarid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	GrainIrrigationRatePB[in/yr]	Grain irrigation rate for pluvial biosphere [in/yr]	triangular 12, 22, 29	Average annual irrigation rates for an upper bound glacial transition climate are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of estimated future Yucca Mountain region climate change conditions (i.e., semiarid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.
GENTPA	HomeIrrigationRatePB[in/yr]	Residential irrigation rate for pluvial biosphere [in/yr]	constant 33	Average annual irrigation rates for an upper bound glacial transition climate are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of estimated future Yucca Mountain region climate change conditions (i.e., semiarid).
GENTPA	PoultryFeedIrrigationRatePB[in/yr]	Poultry feed irrigation rate for pluvial biosphere [in/yr]	triangular 12, 22, 29	Average annual irrigation rates for an upper bound glacial transition climate are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of estimated future Yucca Mountain region climate change conditions (i.e., semiarid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	HenFeedIrrigationRatePB[in/yr]	Egg-laying hen feed irrigation rate for pluvial biosphere [in/yr]	triangular 12, 22, 29	Average annual irrigation rates for an upper bound glacial transition climate are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of estimated future Yucca Mountain region climate change conditions (i.e., semiarid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.
GENTPA	LeafyVegetableIrrigationTimePB [mo/yr]	Leafy vegetable irrigation time for pluvial biosphere [mo/yr]	constant 5	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC, 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates (e.g., LeafyVegetableIrrigationRatePB[in/yr] was derived using the same growing season information).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	OtherVegetableIrrigationTimePB [mo/yr]	Other vegetable irrigation time for pluvial biosphere [mo/yr]	constant 7	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC, 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates (e.g., OtherVegetableIrrigationRatePB[in/yr] was derived using the same growing season information).
GENTPA	FruitIrrigationTimePB[mo/yr]	Fruit irrigation time for pluvial biosphere [in/yr]	constant 4	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC, 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates (e.g., FruitIrrigationRatePB[in/yr] was derived using the same growing season information).
GENTPA	GrainIrrigationTimePB[mo/yr]	Grain irrigation time for pluvial biosphere [mo/yr]	constant 6	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC, 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates (e.g., GrainIrrigationRatePB[in/yr] was derived using the same growing season information).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	HomeIrrigationTimePB[mo/yr]	Residential irrigation time for pluvial biosphere [mo/yr]	constant 12	Based on the assumption that the receptor cares for a lawn for the entire year. This assumption was informed by a pamphlet provided by a local agricultural extension office (Mills, 1993) as discussed by LaPlante and Poor (1997). Selected value is consistent with growing period used for irrigation rate (HomeIrrigationRatePB[in/yr]) derived from Bechtel SAIC Company, LLC (2004b).
GENTPA	PoultryFeedIrrigationTimePB[mo/yr]	Poultry feed irrigation time for pluvial biosphere [mo/yr]	constant 6	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC, 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates (e.g., PoultryFeedIrrigationRatePB[in/yr] was derived using the same growing season information).
GENTPA	HenFeedIrrigationTimePB[mo/yr]	Egg-laying hen feed irrigation time for pluvial biosphere [mo/yr]	constant 6	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC, 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates (e.g., HenFeedIrrigationRatePB[in/yr] was derived using the same growing season information).

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	LeafyVegetableIrrigationRateCB [in/yr]	Leafy vegetable irrigation rate for current biosphere [in/yr]	triangular 20, 34, 59	Average annual irrigation rates for current climate conditions are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of current Yucca Mountain region climate and agricultural conditions (i.e., arid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.
GENTPA	OtherVegetableIrrigationRateCB [in/yr]	Other vegetable irrigation rate for current biosphere [in/yr]	triangular 16, 31, 52	Average annual irrigation rates for current climate conditions are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of current Yucca Mountain region climate and agricultural conditions (i.e., arid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	FruitIrrigationRateCB[in/yr]	Fruit irrigation rate for current biosphere [in/yr]	triangular 27, 45, 60	Average annual irrigation rates for current climate conditions are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of current Yucca Mountain region climate and agricultural conditions (i.e., arid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category; except upper limit was truncated to maintain consistency with local permitted maximum water use as reported in LaPlante and Poor (1997).
GENTPA	GrainIrrigationRateCB[in/yr]	Grain irrigation rate for current biosphere [in/yr]	triangular 22, 35, 47	Average annual irrigation rates for current climate conditions are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of current Yucca Mountain region climate and agricultural conditions (i.e., arid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.
GENTPA	HomeIrrigationRateCB[in/yr]	Residential irrigation rate for current biosphere [in/yr]	constant 63	Average annual irrigation rates for current climate conditions are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of current Yucca Mountain region climate and agricultural conditions (i.e., arid).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	PoultryFeedIrrigationRateCB [in/yr]	Poultry feed irrigation rate for current biosphere [in/yr]	triangular 22, 35, 47	Average annual irrigation rates for current climate conditions are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of current Yucca Mountain region climate and agricultural conditions (i.e., arid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.
GENTPA	HenFeedIrrigationRateCB[in/yr]	Egg-laying hen feed irrigation rate for current biosphere [in/yr]	triangular 22, 35, 47	Average annual irrigation rates for current climate conditions are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods that are expected to be representative of current Yucca Mountain region climate and agricultural conditions (i.e., arid). The input parameter distribution represents the variation in the average annual irrigation rates for those crops included in the specified category.
GENTPA	LeafyVegetableIrrigationTimeCB [mo/yr]	Leafy vegetable irrigation time for current biosphere [mo/yr]	constant 5	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The selected value is within the range of climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., LeafyVegetableIrrigationRateCB[in/yr] was derived using the same growing season information}.

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	OtherVegetableIrrigationTimeCB [mo/yr]	Other vegetable irrigation time for current biosphere [mo/yr]	constant 5	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The selected value is within the range of climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., OtherVegetableIrrigationRateCB[in/yr] was derived using the same growing season information}.
GENTPA	FruitIrrigationTimeCB[mo/yr]	Fruit irrigation time for current biosphere [mo/yr]	constant 5	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., FruitIrrigationRateCB[in/yr] was derived using the same growing season information}. Note that a value outside the previously derived range in LaPlante and Poor (1997) is due to the inclusion of additional crops in the fruit crop category used to compute the current value.
GENTPA	GrainIrrigationTimeCB[mo/yr]	Grain irrigation time for current biosphere [mo/yr]	constant 7	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The selected value is within the range of climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., GrainIrrigationRateCB[in/yr] was derived using the same growing season information}.

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	HomeIrrigationTimeCB[mo/yr]	Residential irrigation time for current biosphere [mo/yr]	constant 12	Based on the assumption that the receptor cares for a lawn for the entire year. This assumption was informed by a pamphlet provided by a local agricultural extension office (Mills, 1993) as discussed by LaPlante and Poor (1997). Selected value is consistent with growing period used for irrigation rate (HomeIrrigationRateCB[in/yr]) derived from Bechtel SAIC Company, LLC (2004b).
GENTPA	PoultryFeedIrrigationTimeCB [mo/yr]	Poultry feed irrigation time for current biosphere [mo/yr]	constant 7.0	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The selected value is within the range of climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., PoultryFeedIrrigationRateCB[in/yr] was derived using the same growing season information}.
GENTPA	HenFeedIrrigationTimeCB[mo/yr]	Egg-laying hen feed irrigation time for current biosphere [mo/yr]	constant 7.0	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The selected value is within the range of climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., HenFeedIrrigationRateCB[in/yr] was derived using the same growing season information}.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	PoultryFeedGrowTime[day]	Poultry feed growing time [day]	constant 200	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The selected value is within the range of climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., PoultryFeedIrrigationRateCB[in/yr] was derived using the same growing season information}.
GENTPA	HenFeedGrowTime[day]	Egg-laying hen feed growing time [day]	constant 200	Crop-specific growing season lengths applicable to the current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC (2004b, Table 6.4-1). The selected value is within the range of climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., HenFeedIrrigationRateCB[in/yr] was derived using the same growing season information}.
GENTPA	BeefFreshForageDietFraction	Beef cattle fresh forage diet fraction [unitless]	normal 0.12, 0.98	Values are from a Nevada test site pathways study by Breshears, et al. (1992) and are relevant to southern Nevada livestock husbandry.
GENTPA	MilkFreshForageDietFraction	Dairy cattle fresh forage diet fraction [unitless]	normal 0.12, 0.98	Values are from a Nevada test site pathways study by Breshears, et al. (1992) and are relevant to southern Nevada livestock husbandry.
GENTPA	BeefFreshForageGrowTime[day]	Beef cattle fresh forage growing time [day]	uniform 30.0, 62.0	The values are derived from available information on alfalfa discussed by Stichler (1991) and Kennedy and Strenge (1992) as discussed by LaPlante and Poor (1997). Range encompasses value used to derive BeefFreshForageIrrigationTimeCB[mo/yr] and BeefFreshForageIrrigationRateCB[in/yr].

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	MilkFreshForageGrowTime[day]	Dairy cattle fresh forage growing time [day]	uniform 30.0, 62.0	The values are derived from available information on alfalfa discussed by Stichler (1991) and Kennedy and Strenge (1992) as discussed by LaPlante and Poor (1997). Range encompasses value used to derive BeefFreshForageIrrigationTimeCB[mo/yr] and BeefFreshForageIrrigationRateCB[in/yr].
GENTPA	BeefFreshForageIrrigationRatePB[in/yr]	Beef cattle fresh forage irrigation rate for pluvial biosphere [in/yr]	constant 33	Same data source as for LeafyVegetableIrrigationRatePB[in/yr], except a constant value is used because alfalfa is assumed to be the primary feed crop as described in LaPlante and Poor (1997).
GENTPA	MilkFreshForageIrrigationRatePB[in/yr]	Milk fresh forage irrigation rate for pluvial biosphere [in/yr]	constant 33	Same data source as for LeafyVegetableIrrigationRatePB[in/yr], except a constant value is used because alfalfa is assumed to be the primary feed crop as described in LaPlante and Poor (1997).
GENTPA	BeefFreshForageIrrigationTimePB[mo/yr]	Beef cattle fresh forage irrigation time for pluvial biosphere [mo/yr]	constant 7	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., BeefFreshForageIrrigationRatePB[in/yr] was derived using the same growing season information}.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	MilkFreshForageIrrigationTimePB[mo/yr]	Dairy cattle fresh forage irrigation time for pluvial biosphere [mo/yr]	constant 7	Crop-specific growing season lengths for eastern Washington State were documented as an analog for future upper bound glacial transition climate agricultural conditions in the Yucca Mountain region (Bechtel SAIC Company, LLC 2004b, Table 6.4-1). The selected value is within the range of potential future climate and agricultural conditions discussed in LaPlante and Poor (1997); however, the specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., MilkFreshForageIrrigationRatePB[in/yr] was derived using the same growing season information}.
GENTPA	BeefFreshForageIrrigationRateCB[in/yr]	Beef cattle fresh forage irrigation rate for current biosphere [in/yr]	constant 60	Same data source as for LeafyVegetableIrrigationRateCB[in/yr], except a constant value is used because alfalfa is assumed to be the primary feed crop (as described in LaPlante and Poor, 1997), and the current value was truncated to maintain consistency with local permitted maximum water use as reported in LaPlante and Poor (1997).
GENTPA	MilkFreshForageIrrigationRateCB[in/yr]	Dairy cattle fresh forage irrigation rate for current biosphere [in/yr]	constant 60	Same data source as for LeafyVegetableIrrigationRateCB[in/yr], except a constant value is used because alfalfa is assumed to be the primary feed crop (as described in LaPlante and Poor, 1997), and the current value was truncated to maintain consistency with local permitted maximum water use as reported in LaPlante and Poor (1997).

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	BeefFreshForageIrrigationTimeCB[mo/yr]	Beef cattle fresh forage irrigation time for current biosphere [mo/yr]	constant 9	Crop-specific growing season lengths applicable to current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC 2004b, Table 6.4-1. The specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., BeefFreshForageIrrigationRateCB [in/yr] was derived using the same growing season information}. Note that a slightly higher value is used than was considered in LaPlante and Poor (1997) and this value was also truncated from the reported value in the current reference (11 months) to maintain consistency with the corresponding irrigation rate {BeefFreshForageIrrigationRateCB[in/yr]} which was truncated to avoid exceeding the local permitted maximum water use.
GENTPA	MilkFreshForageIrrigationTimeCB[mo/yr]	Dairy cattle fresh forage irrigation time for current biosphere [mo/yr]	constant 9	Crop-specific growing season lengths applicable to current climate and agricultural conditions in the Yucca Mountain region are provided in Bechtel SAIC Company, LLC 2004b, Table 6.4-1. The specific point estimate is preferred to maintain consistency with the annual average irrigation rates {e.g., MilkFreshForageIrrigationRateCB[in/yr] was derived using the same growing season information}. Note that a slightly higher value is used than was considered in LaPlante and Poor (1997) and the value was also truncated from the reported value in the current reference (11 months) to maintain consistency with the corresponding irrigation rate {MilkFreshForageIrrigationRateCB[in/yr]} which was truncated to avoid exceeding the local permitted maximum water use.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	DrinkingWaterConsumptionRate5[L/yr]	Drinking water consumption rate for adult: ICRP72 [L/yr]	constant 730	Specified in the Nuclear Regulatory Commission regulation 10 CFR 63.312(d) that the reasonably maximally exposed individual drinks 2 liters [0.53 gal] of water per day. That value equals 730 liters per year.
GENTPA	LeafyVegetableConsumptionRate5[kg/yr]	Leafy vegetable consumption rate for adult: ICRP72 [kg/yr]	constant 15	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced leafy vegetables, based on a survey of local residents (CRWMS M&O, 2000a).
GENTPA	OtherVegetableConsumptionRate5[kg/yr]	Other vegetable consumption rate for adult: ICRP72 [kg/yr]	constant 7.8	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced root vegetables, based on a survey of local residents (CRWMS M&O, 2000a).
GENTPA	FruitConsumptionRate5[kg/yr]	Fruit consumption rate for adult: ICRP72 [kg/yr]	constant 16	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced fruit, based on a survey of local residents (CRWMS M&O, 2000a).
GENTPA	GrainConsumptionRate5[kg/yr]	Grain consumption rate for adult: ICRP72 [kg/yr]	constant 0.48	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced grain, based on a survey of local residents (CRWMS M&O, 2000a).
GENTPA	BeefConsumptionRate5[kg/yr]	Beef consumption rate for adult: ICRP72 [kg/yr]	constant 2.9	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced meat, based on a survey of local residents (CRWMS M&O, 2000a).
GENTPA	PoultryConsumptionRate5[kg/yr]	Poultry consumption rate for adult: ICRP72 [kg/yr]	constant 0.8	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced poultry, based on a survey of local residents (CRWMS M&O, 2000a).
GENTPA	MilkConsumptionRate5[kg/yr]	Milk consumption rate for adult: ICRP72 [kg/yr]	constant 4.1	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced milk, based on a survey of local residents (CRWMS M&O, 2000a).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	EggConsumptionRate5[kg/yr]	Egg consumption rate for adult: ICRP72 [kg/yr]	constant 6.7	This is the mean annual consumption rate of an adult population in Amargosa Valley that consumes locally produced eggs, based on a survey of local residents (CRWMS M&O, 2000a).
GENTPA	InhalationExposureTime5[hr]	Inhalation exposure time for adult: ICRP72 [hr/yr]	constant 4843	Based on information in Mohanty, et al. (2005, Chapter 5) and Kennedy and Strenge (1992), including a 0.5 indoor exposure factor; 6,022 hr/yr indoors; 1,832 hr/yr outdoors; (i.e., 6,022 × 0.5 + 1,832 = 4,843). About 17 hours per week are assumed to be spent outside of the area for employment.
GENTPA	InhalationRate5[cm ³ /s]	<i>B</i> Inhalation rate for adult: ICRP72 receptor age group [cm ³ /s]	constant 270	Reference case value is equal to the default adult chronic inhalation rate in GENII 1,485 (Napier, et al., 1988). Magnitude of breathing rate is influenced by the level of human activity. Reference-case value is slightly higher than the value for an adult male (International Commission on Radiological Protection, 1995, Table 6).
GENTPA	SoilContaminationExposureTime5[hr]	Soil contamination exposure time adult: ICRP72 [hr/yr]; only used for DCAGW external dose calculations; DCAGS computes the comparable input parameter (see IndoorShielding Factor)	constant 1832	Based on same assumptions for outdoor activity as for InhalationExposureTime5[hr].

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	PlantUptakeScaleFactor	Plant uptake scaling factor used to scale plant transfer factors in <i>gfrans.dat</i>	lognormal 0.10, 9.8	The range for this parameter is the 0.1- to 99.9-percent interval using distribution statistics from International Union of Radioecologists (1989). For Yucca Mountain relevant crop types and elements, an uncertainty factor of four generally bounded the data (LaPlante and Poor, 1997). Assuming the data are lognormally distributed and the uncertainty factor used in the reference was for a 95-percent confidence interval, the applicable geometric standard deviation is 2. Applying this geometric standard deviation to a 0.1- and 99.9-percentile interval using lognormal distribution statistics results in the range of 0.1 to 9.8. This scale factor is multiplied by the tabulated plant uptake factors to induce variation in the fixed (tabulated) values.
GENTPA	AnimalUptakeScaleFactor	Animal uptake scaling factor used to scale animal transfer factors in <i>gfrans.dat</i>	lognormal 0.10, 9.8	Information quantifying uncertainty in animal uptake factors equivalent to that available for plants was not provided in the source documentation, but the scale factor distribution applied to plant uptake (based on a geometric standard deviation of 2) generally encompassed the variation reported for the animal uptake factors in International Atomic Energy Agency (1994). (See remarks for PlantUptakeScaleFactor.)

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_Cm[cm3/g]	Soil K_d for Curium [cm ³ /g]	usersuppliedpwisecdf 11 7666.0, 0.0 7785.4, 0.115 9604.6, 0.184 11849.0, 0.274 14617.9, 0.382 18033.7, 0.500 22247.8, 0.618 27446.7, 0.726 33860.4, 0.816 41772.8, 0.885 44260.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam values.
GENTPA	KD_Soil_Pu[cm3/g]	Soil K_d for Plutonium [cm ³ /g]	usersuppliedpwisecdf 12 316.0, 0.0 395.4, 0.115 742.5, 0.184 1394.1, 0.274 2617.6, 0.382 4914.8, 0.500 9228.0, 0.618 17326.6, 0.726 32532.7, 0.816 61083.7, 0.885 114691.4, 0.933 190000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) clay soil values.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_U[cm3/g]	Soil K_d for Uranium [cm ³ /g]	usersuppliedpwiseCDF 13 0.17, 0.0 0.27, 0.067 0.71, 0.115 1.86, 0.184 4.85, 0.274 12.7, 0.382 33.1, 0.500 86.5, 0.618 225.9, 0.726 589.9, 0.816 1540.7, 0.885 4023.9, 0.933 6000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) sandy soil values. Minimum and maximum set at the distribution 5- and 95-percent values.
GENTPA	KD_Soil_Am[cm3/g]	Soil K_d for Americium [cm ³ /g]	usersuppliedpwiseCDF 12 100.0, 0.0 192.5, 0.184 419.9, 0.274 916.0, 0.382 1998.2, 0.500 4359.0, 0.618 9509.1, 0.726 20743.7, 0.816 45251.9, 0.885 98715.8, 0.933 215345.7, 0.964 300000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) and Bechtel SAIC Company, LLC (2003a,b). Minimum set by minimum unsaturated zone K_d value (Bechtel SAIC Company, LLC, 2003a,b). Maximum is measured value from Sheppard and Thibault (1990) with mean and standard deviation from same.

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_Np[cm3/g]	Soil K_d for Neptunium [cm ³ /g]	usersuppliedpwiseCDF 13 1.30, 0.0 1.92, 0.067 3.19, 0.115 5.31, 0.184 8.85, 0.274 14.7, 0.382 24.5, 0.500 40.9, 0.618 68.0, 0.726 113.3, 0.816 188.7, 0.885 314.2, 0.933 400.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam soil values. Standard deviation and maximum values modified to reflect data from Bertetti and Werling (2005).
GENTPA	KD_Soil_Ra[cm3/g]	Soil K_d for Radium [cm ³ /g]	usersuppliedpwiseCDF 8 1262.0, 0.0 2230.5, 0.184 5653.3, 0.274 14328.4, 0.382 36315.5, 0.500 92042.0, 0.618 233281.2, 0.726 530000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam soil values.
GENTPA	KD_Soil_Pb[cm3/g]	Soil K_d for Lead [cm ³ /g]	usersuppliedpwiseCDF 8 800.0, 0.0 955.0, 0.274 2187.8, 0.382 5011.9, 0.500 11481.5, 0.618 26302.7, 0.726 60256.0, 0.816 100000.0, 1.0	Cumulative distribution function developed using values from Allison and Allison (2005) except minimum constrained by EPA (1999) data.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_Cs[cm3/g]	Soil K_d for Cesium [cm ³ /g]	usersuppliedpwiscdf 12 1000.0, 0.0 1380.2, 0.184 2038.6, 0.274 3010.9, 0.382 4447.1, 0.500 6568.2, 0.618 9701.2, 0.726 14328.4, 0.816 21162.8, 0.885 31257.0, 0.933 46166.1, 0.964 61287.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam soil values. Minimum set by data from Zavarin, et al. (2002) and maximum set by measured K_d values from Sheppard and Thibault (1990).
GENTPA	KD_Soil_Th[cm3/g]	Soil K_d for Thorium [cm ³ /g]	usersuppliedpwiscdf 9 1700.0, 0.0 2981.0, 0.500 5597.1, 0.618 10509.1, 0.726 19732.1, 0.816 37049.1, 0.885 69563.8, 0.933 130613.8, 0.964 170000.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) sandy soil values. Minimum and maximum constrained by measured K_d values from EPA (1999).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_I[cm ³ /g]	Soil K _p for Iodine [cm ³ /g]	usersuppliedpwiseCDF 12	Cumulative distribution function developed from Sheppard and Thibault (1990) loam soil values.
			0.1, 0.0 0.12, 0.036 0.22, 0.067 0.41, 0.115 0.74, 0.184 1.35, 0.274 2.46, 0.382 4.48, 0.500 8.17, 0.618 14.88, 0.726 27.11, 0.816 43.0, 1.0	
GENTPA	KD_Soil_Tc[cm ³ /g]	Soil K _p for Technetium [cm ³ /g]	usersuppliedpwiseCDF 15	Cumulative distribution function developed from Sheppard and Thibault (1990) sandy soil values.
			0.01, 0.0 0.016, 0.115 0.027, 0.184 0.046, 0.274 0.079, 0.382 0.135, 0.500 0.232, 0.618 0.399, 0.726 0.684, 0.816 1.174, 0.885 2.014, 0.933 3.456, 0.964 5.930, 0.982 10.176, 0.992 16.0, 1.0	

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_Ni[cm3/g]	Soil K_p for Nickel [cm ³ /g]	usersuppliedpwiscdf 14 60.0, 0.0 100.0, 0.036 141.3, 0.067 199.5, 0.115 281.8, 0.184 398.1, 0.274 562.3, 0.382 794.3, 0.500 1122.0, 0.618 1584.9, 0.726 2238.7, 0.816 3162.3, 0.885 4466.8, 0.933 6309.6, 1.0	Cumulative distribution function developed from data in Allison and Allison (2005) with minimum set by measured values from Sheppard and Thibault (1990) for sandy soil.
GENTPA	KD_Soil_Cl[cm3/g]	Soil K_p for Chlorine [cm ³ /g]	usersuppliedpwiscdf 14 0.0, 0.0 0.010, 0.018 0.014, 0.036 0.019, 0.067 0.027, 0.115 0.037, 0.184 0.052, 0.274 0.072, 0.382 0.100, 0.500 0.139, 0.618 0.194, 0.726 0.270, 0.816 0.375, 0.885 0.4, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam soil values.

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_C[cm3/g]	Soil K_d for Carbon [cm ³ /g]	usersuppliedpwiseCDF 13 1.12, 0.0 1.42, 0.067 2.36, 0.115 3.94, 0.184 6.6, 0.274 10.9, 0.382 18.2, 0.500 30.3, 0.618 50.4, 0.726 83.9, 0.816 139.8, 0.885 232.8, 0.933 299.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam soil values. Minimum and maximum constrained by the distribution 5- and 95-percent values.
GENTPA	KD_Soil_Se[cm3/g]	Soil K_d for Selenium [cm ³ /g]	usersuppliedpwiseCDF 11 36.0, 0.0 38.1, 0.184 42.9, 0.274 48.4, 0.382 54.6, 0.500 61.6, 0.618 69.4, 0.726 78.3, 0.816 88.2, 0.885 99.5, 0.933 100.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) sandy soil values. Maximum constrained by data from Allison and Allison (2005).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	KD_Soil_Nb[cm3/g]	Soil K_d for Niobium [cm ³ /g]	usersuppliedpwiseCDF 13 33.0, 0.0 42.5, 0.067 70.8, 0.115 117.9, 0.184 196.4, 0.274 327.0, 0.382 544.6, 0.500 906.9, 0.618 1510.2, 0.726 2514.9, 0.816 4188.1, 0.885 6974.4, 0.933 8500.0, 1.0	Cumulative distribution function developed from Sheppard and Thibault (1990) loam soil values. Minimum and maximum constrained by the distribution 5- and 95-percent values.
GENTPA	AnnualPrecipitation[m/yr]	Annual precipitation rate [m/yr]	constant 0.102	Annual precipitation in Amargosa Valley determined from data reported in the Bechtel SAIC Company, LLC (2004b, Table 4.1-2).
GENTPA	AnnualIrrigation[m/yr]	Annual irrigation rate [m/yr]	constant 1.12	Irrigation rate data are tabulated in Table 6.5-2 of Bechtel SAIC Company, LLC (2004b) showing irrigation rates for various crops applicable to the Yucca Mountain region. These rates were calculated using established agricultural formulas that incorporate data on local climate, soil, crops, and irrigation methods. For TPA Version 5.1 use, these crop-specific rates were used to derive representative values for crop categories consistent with the model inputs. The crop category-specific rates were averaged to derive the annual irrigation rate listed here (1.12 m/yr).
GENTPA	SoilBulkDensity[g/cm3]	Soil bulk density [g/cm ³]	constant 1.5	Based on LaPlante and Poor (1997).
GENTPA	SoilVolumetricWaterContent	Soil volumetric water content [ml/cm ³]	constant 0.35	Data from Tanner (1991) for soils similar to Amargosa Valley farming soils.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
GENTPA	TotalAnnualEvapotranspiration [m/yr]	Total annual evapotranspiration [m/yr]	constant 1.14	Using data in Bechtel SAIC Company, LLC (2004b), the average irrigation rate for all crop groups (see description of the Annual Irrigation rate of 1.12 m/yr) and the annual precipitation in Amargosa Valley from data reported in the Bechtel SAIC Company, LLC (2004b, Table 4.1-2) (0.102 m/yr) were summed, and the mean over watering rate for all crops reported in Table 6.9-1 (0.079 m/yr) was subtracted from this sum to estimate the evapotranspiration (because precipitation + irrigation – evapotranspiration = overwatering). The resulting evapotranspiration is 1.14 m/yr. This value was checked against U.S. Geological Survey estimates of deep percolation for farming locations in Amargosa Valley (U.S. Geological Survey, 2003) for additional confidence. U.S. Geological Survey concludes that 8 to 16 percent of irrigation water becomes deep percolation. Applying the low estimate to the average irrigation rate used to calculate evapotranspiration ($1.12 \text{ m/yr} \times 0.08$) results in a deep percolation estimate of 0.090 m/yr. This value compares with the aforementioned 0.079 value for over watering reported by Bechtel SAIC Company, LLC (2004b).
DCAGS	DepthOfResuspendibleLayer [cm]	d_r Thickness of the upper soil layer that is available for resuspension [cm]	constant 0.3	Wiggs (1997) supports a 0.1–1 cm range, with 1 cm being for poorly sorted, coarse-grained deposits (i.e., grain size on order of 1 cm). The 0.3-cm value seems reasonable, given that the tephra will likely have an average grain size on the order of 0.1 cm. Because the maximum entrainable particle size is 0.01 cm, the 0.1 cm-size ash will form an unentrainable lag deposit that shields finer particles from turbulent wind entrainment unless they can escape between the 0.1-cm particle interstices.

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) (Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DCAGS	RateOfReductionOfMassLoading Factor[1/yr]	λ_r Rate at which the airborne mass load factor decreases with time from the initial value after the eruption [1/yr]	constant 0.07	Limited reduction in airborne mass loads measured on deposits 4 years after 1995 Cerro Negro eruption (Hill, et al., 2000). Assuming exponential decay (e.g., Anspaugh, et al., 1975), this relationship indicates a half-life for reduction in mass load on the order of 10 years.
ASHRMOVO	RelativeRateOfBlanketRemoval [1/yr]	λ_b Bulk removal rate from the initial tephra deposit [1/yr]	constant 0.0007	Only traces of the tephra-fall deposit are preserved at the youngest Yucca Mountain region volcano, Lathrop Wells, which is around 100,000 years old. Recent work by Delgado-Granados, et al. (1998) at Xitle volcano, Mexico, has shown that substantial amounts of basaltic tephra-fall deposits are preserved from this 2,000-year-old eruption. The area around Xitle volcano receives around 500–700 mm [20–28 in] of annual rainfall, in contrast to the roughly 100-mm [4-in] annual rainfall in the Yucca Mountain region. Although many factors, such as topographic slope, degree of incision, and eolian sedimentation affect tephra-fall erosion, areas of greater annual rainfall should experience higher erosion rates of nonconsolidated fall deposits than areas of lower annual rainfall. Thus, tephra-fall deposits in the Yucca Mountain region likely are significantly preserved for around 10,000 years, and a removal half-life of 1,000 years is selected. Removal rate equals $1/n$ 2 divided by the half-life.
ASHRMOVO	AshBulkDensity[g/cm ³]	ρ_{ash} Bulk density for volcanic ash deposited in the Fortymile Wash catchment basin and at the receptor location [g/cm ³]	constant 1.2	Data based on <i>in-situ</i> measurements of tephra deposits during the 1995 Cerro Negro eruption made at 1 km [0.6 mi] from the vent (Hill, et al., 1998, p. 1,232).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
DCAGS	IndoorShieldingFactor	Factor that accounts for reduction in external radiation when the receptor is indoors due to the shielding effect of structures; factor is used with occupancy and exposure time inputs to compute a value for SoilContamination ExposureTime for GENTPA that is consistent with exposure assumptions used by DCAGS for inhalation dose calculations	constant 0.7	Value is based on default input for the RESRAD Version 6.0 site decommissioning code (Yu, et al., 2001), which is higher than the value reported in Kennedy and Strenge (1992) and generally consistent with the upper end of the range of values provided by Beyeler, et al. (1999) for a typical residential structure.
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadAboveFresh AshBlanketHeavyDisturbance [g/m ³]	$S_{\text{ash,out-H}}$ Outdoor airborne mass load of resuspended ash due to heavy disturbance activities [g/m ³]	uniform 1.0e-3, 1.0e-2	Outdoor mass loads over ash deposits for heavy disturbance activities have been measured within this range. Measurements were taken four years after the 1995 Cerro Negro eruption in Nicaragua at a height of 1.5 m [59 in] above the tephra deposits located about 5 km [3.1 mi] from the vent (Hill, et al., 2000). Digging and driving over deposits resulted in airborne mass loads of $\sim 10^{-2}$ g/m ³ , which was assigned as the maximum value. Walking over deposits resulted in airborne mass loads of $\sim 10^{-3}$ g/m ³ , which was assigned as the minimum value. Range also supported by posteruptive measurements near Montserrat volcano by Searl, et al. (2002).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadAboveFresh AshBlanketLightDisturbance [g/m ³]	$S_{\text{ash, out-L}}$ Outdoor airborne mass load of resuspended ash due to light disturbance activities [g/m ³]	uniform 1.0e-4, 1.0e-3	Outdoor mass loads over ash deposits for light disturbance activities have been measured within this range. Measurements were taken 4 years after the 1995 Cerro Negro eruption in Nicaragua at a height of 1.5 m [59 in] above the tephra deposits located about 5 km [3.1 mi] from the vent (Hill et al., 2000). Walking over deposits resulted in airborne mass loads of $\sim 10^{-3}$ g/m ³ , which was assigned as the maximum value. Airborne mass loads over undisturbed deposits were $\sim 10^{-4}$ g/m ³ in 4 ± 2 m/s winds, which was assigned as the minimum value. Range also supported by posteruption measurements near Montserrat volcano by Searl, et al. (2002).
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadOutsideHeavy Disturbance[g/m ³]	$S_{\text{out-H}}$ Outdoor airborne mass load of resuspended soil due to heavy disturbance activities [g/m ³]	constant 0.0007	This value corresponds to the maximum value in the range of airborne mass loads for outdoor activities assuming soil conditions (Mohanty, et al., 2005, Table 5-4).
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadOutsideLight Disturbance[g/m ³]	$S_{\text{out-L}}$ Outdoor airborne mass load of resuspended soil due to light disturbance activities [g/m ³]	constant 0.0001	This value corresponds to the minimum value in the range of airborne mass loads for outdoor activities assuming soil conditions (Mohanty, et al., 2005, Table 5-4).

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadInsideHeavyDisturbance[g/m ³]	S _{in-H} Indoor airborne mass load of resuspended soil and ash due to heavy disturbance activities [g/m ³]	triangular 1.0e-4, 5.0e-4, 1.0e-3	Screening values of indoor mass loads for building renovation and residential exposure scenarios are discussed in a literature summary by Kennedy and Streng (1992). They describe a range of 0.00005 to 0.0001 g/m ³ as representing longer term average concentrations that account for airborne dust from nonradioactive sources. They further consider the range a prudently conservative estimate for radioactive dust loadings in the workplace or household. Because fine ash particles are expected to elevate normal dust loadings and this parameter is for heavy disturbance conditions, we take the recommendation of 0.0001 g/m ³ as the lower end of a triangular distribution that extends to a maximum value that is equal to the low end of outdoor mass loading for fresh ash (0.001 g/m ³) described above, with the midpoint of this range (0.0005 g/m ³) assumed to be the mode of a triangular distribution, selected to avoid overemphasizing the extreme high and low ends of the range.

Table 17-1. Reference Data for Parameters of tpa.inp Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in tpa.inp	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadInsideLightDisturbance[g/m ³]	S_{in-L} Indoor airborne mass load of resuspended soil and ash due to light disturbance activities [g/m ³]	triangular 1.0e-5, 5.0e-5, 1.0e-4	Screening values of indoor mass loads for building renovation and residential exposure scenarios are discussed in a literature summary by Kennedy and Streng (1992). They describe a range of 0.00005 to 0.0001 g/m ³ as representing longer term average concentrations that account for airborne dust from nonradioactive sources. They further consider the range a prudently conservative estimate for radioactive dust loadings in the workplace or household. Because this parameter is for light disturbance conditions that span a range of disturbance conditions (including no disturbance at all), the recommendation in Kennedy and Streng (1992) of 0.0001 g/m ³ is selected as the upper end of a triangular distribution that extends to a minimum value (0.00001 g/m ³) that encompasses a dust loading representing relatively clean air (0.00002 g/m ³), with the midpoint of this range (0.00005 g/m ³) assumed to be the mode of a triangular distribution, selected to avoid overemphasizing the extreme high and low ends of the range.
MASS LOADING AND OCCUPANCY FACTORS	AirborneMassLoadOffsite[g/m ³]	$S_{offsite}$ Offsite airborne mass load of contaminated particles [g/m ³]	constant 0.0	Offsite locations are assumed to be well beyond the eolian source region and free of contamination.
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionOutsideHeavyDisturbance[]	f_{out-H} Fraction of time receptor spends outdoors with heavy disturbance [unitless]	constant 0.125	Based on an assumption of 2.75 hr/day of moderate work and 0.25 hr/day of hard work outdoors (Mohanty, et al., 2005, Chapter 5).

Table 17-1. Reference Data for Parameters of <i>tpa.inp</i> Used by DCAGW and DCAGS (continued) <i>(Disclaimer: The listed input parameter distributions and values were provided for the release of TPA Version 5.1 and are subject to change in subsequent versions or updates to the input data.)</i>				
Input Block in <i>tpa.inp</i>	Parameter Name	Description	Distribution Type and Parameter Value(s)	Remarks
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionOutsidelLightDisturbance[]	f_{out-L} Fraction of time receptor spends outdoors with light disturbance [unitless]	constant 0.084	Based on an assumption of 2 hr/day of light work outdoors (Mohanty, et al., 2005, Chapter 5).
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionInsideHeavyDisturbance[]	f_{in-H} Fraction of time receptor spends indoors with heavy disturbance	constant 0.104	Based on an assumption of 2 hr/day of moderate work and 0.5 hr/day of hard work indoors (Mohanty, et al., 2005, Chapter 5).
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionInsidelLightDistance[]	f_{in-L} Fraction of time receptor spends indoors with light disturbance [unitless]	constant 0.583	Based on an assumption of 8 hr/day sleeping, 3 hr/day sedentary, and 3 hr/day of light work indoors (Mohanty, et al., 2005, Chapter 5).
MASS LOADING AND OCCUPANCY FACTORS	OccupancyFractionOffsite[]	$f_{offsite}$ Fraction of time receptor spends offsite [unitless]	constant 0.104	Based on an assumption of 1.25 hr/day outdoors and 1.25 hr/day indoors offsite (Mohanty, et al., 2005, Chapter 5).

17.5 Auxiliary Input Data and External Process Models

Table 17-2 lists the auxiliary input data files for DCAGW and DCAGS. The auxiliary input data files supply additional input parameters, as indicated in Table 17-2, beyond *tpa.inp* parameters, and formatting for generation of GENTPA input files.

No external process models need to be run to generate inputs for DCAGW or DCAGS calculations. However, dosimetry modeling conducted by other investigators generated the dose coefficients that are inputs for calculations in both modules (Section 17.5.1). GENTPA is integrated into TPA Version 5.1 and is discussed in previous sections.

Table 17-2. Auxiliary Input Data Files Used by DCAGW or DCAGS	
File Name	Description of Data
<i>dilution.dat</i>	Wellbore data for the saturated zone including well capture widths and well capture thicknesses by well pump rates and aquifer thicknesses, and well screen lengths by well pump rates. DCAGW uses data from this file only when the input flag PlumeCaptureModel is set to 2 (a legacy option). The reference case PlumeCaptureModel selection sets plume capture fraction to the upper bound of 1.0 and uses the water demand specified in 10 CFR 63.312(c).
<i>filename.dat</i>	Identifies filenames of all files needed for execution of GENTPA.
<i>ggenii.def, ggeniis.def</i>	Auxiliary input including Fraction of Roots in Upper Soil, Fraction of Roots in Deep Soil, Mass Loading Factor, Crop Growing Times (by crop), Crop Yields (by crop), Food Product Holdup Times (by food type), Livestock Drinking Water Fractions (by food type), Livestock Diet Fractions (by food type and feed type), and Livestock Feed Storage Times (by food type), and formatting for GENTPA input file <i>ggenii.inp</i> . Letter <i>s</i> at end of file name denotes file used for DCAGS.
<i>gdefault.def, gdefaults.def</i>	Auxiliary input including Deposition Velocity for Resuspension, Leaf Resuspension Factor, Biomass (by crop), Depth of Surface Soil, Surface Soil Density, Harvest Removal Flag, Soil Ingestion Rate, Crop Leaf Deposition Weathering Half Time, Plant Translocation Factors (by crop), Livestock Feed Translocation Factors (by feed type), Livestock Feed Consumption Rates (by feed type), Livestock Drinking Water Consumption Rates (by livestock), Plant Dry-to-Wet Ratio, and formatting for GENTPA input file <i>gdefault.inp</i> . Letter <i>s</i> at end of file name denotes file used for DCAGS.
<i>gftranss.def, gftrans.def</i>	Element-specific soil-to-plant and feed-to-animal uptake factors (International Atomic Energy Agency, 1994; LaPlante and Poor, 1997) and formatting for GENTPA input file <i>gftrans.inp</i> . Additional letter <i>s</i> at the end of the file name denotes file used for DCAGS.
<i>gnewdf.dat</i>	Age-dependent dose coefficients for ingestion and inhalation from Publication 72 (International Commission on Radiological Protection, 2002; 1996) and adult dose coefficients from Federal Guidance Report No. 11 (EPA, 1988). See Section 17.5.1.
<i>organdf.dat</i>	Organ and effective (whole body) ingestion dose coefficients for use in groundwater protection drinking water dose calculations. Values are from Federal Guidance Report No. 11 (EPA, 1988).

Table 17-2. Auxiliary Input Data Files Used by DCAGW or DCAGS (continued)	
File Name	Description of Data
<i>ggrdf.dat</i>	External dose coefficients (only ground surface coefficients are used) from Federal Guidance Report No. 12 (EPA, 1993). See Section 17.5.1.
<i>grmdlib.dat</i>	GENTPA radionuclide library including half-lives and decay chain information. This is the default data file from GENII Version 1.485 (Napier, et al., 1988) with no modification except as noted in the file header.
<i>ggamen.dat</i>	Gamma energies for plume calculations (data is not used in calculations, but file is required for GENTPA execution).
<i>gbioac1.dat</i>	Bioaccumulation data (data not used in calculations, but file is required for GENTPA execution).
<i>gdosinc2.dat</i>	No data (file is required for GENTPA execution).
<i>strmtube.dat</i>	The reference data set in TPA Version 5.1 defines three streamtubes that emanate from the water table beneath the potential repository footprint and terminate at the receptor location. DCAGW uses flow rates and dimensions from this file only when the input flag PresentDayDilutionModel is set to options 0 or 4 (both are legacy modeling options). The reference case PresentDayDilutionModel selection allows a water demand consistent with requirements in 10 CFR 63.312(c) to be used. This file is described in further detail in Chapter 18.

17.5.1 Dose Coefficient Data Files

The modular construction of the GENII Version 1.485 software that is the basis for GENTPA allows implementation of more current dosimetry options in TPA Version 5.1 than included in the original software.

The options in TPA Version 5.1 include dosimetry methods recommended by the International Commission on Radiological Protection commonly used by both United States and international regulatory agencies for radiation protection. The International Commission on Radiological Protection periodically updates and documents dosimetry models based on available scientific information and data (International Commission on Radiological Protection, 1996, 1979, 1977).

A variety of dosimetry models, data, and the resulting published sets of dose coefficients are available. Thus, differences in the dose coefficient selections provided in TPA Version 5.1 reflect the state of the science when the recommendations were made. This section provides summary information pertaining to the dose coefficients that have been selected for use in TPA Version 5.1 dose calculations. Refer to the source documents for additional detailed information and technical bases.

17.5.1.1 Internal Dose Coefficients (*gnewdf.dat*, *organdf.dat*)

The dose coefficients used in TPA Version 5.1 are selected from published results of internal dosimetry modeling (International Commission on Radiological Protection, 2002, 1996; EPA, 1988). This modeling involves a biokinetic model that evaluates the partitioning of ingested or inhaled radioactive elements within the body (i.e., blood, organs, bone, and digestive tract) supported by available biokinetic data and a dosimetric model that calculates dose to specific

tissues. These primary components of dosimetry modeling (biokinetic model, biokinetic data, dosimetric model) have evolved over time resulting in differences among available methods that can be applied to convert human intakes of radioactive material to dose.

The dosimetry modeling that forms the basis for the reference case dose coefficients in TPA Version 5.1 for individual protection calculations is described in International Commission on Radiological Protection Publication 72 (International Commission on Radiological Protection, 1996). This set of dose coefficients represents the most recent update of dosimetry recommendations by the International Commission on Radiological Protection. An alternate set of dose coefficients based on the models and data described in International Commission on Radiological Protection Publications 26 and 30 (International Commission on Radiological Protection, 1979, 1977) is also available for use in TPA Version 5.1 dose calculations. These coefficients are published in Federal Guidance Report No. 11 (EPA, 1988). Groundwater protection drinking water dose calculations use the maximum values for internal dose coefficients (by organ and for whole body) from Federal Guidance Report No. 11 (EPA, 1988).

In Publication 72 (International Commission on Radiological Protection, 1996) new dose coefficients for 31 elements, including Neptunium, Technetium, Iodine, Americium, and Plutonium were calculated using updated lung absorption data, a new human respiratory tract model, and a new biokinetic model. The new dose coefficients were calculated for three clearance classes (fast, moderate, and slow) based on the length of time the radionuclide stays in the body. Inhalation dose coefficients for the remaining 60 elements are calculated by the International Commission on Radiological Protection by using the updated human respiratory tract model and older biokinetic information based on International Commission on Radiological Protection Publication 30 regarding lung absorption and clearance (International Commission on Radiological Protection, 1996). For ingestion dose coefficients, the International Commission on Radiological Protection Publication 72 values for the 31 elements are based on updated biokinetic information regarding fractional absorption into the gastrointestinal tract and no changes from Publication 30 for the remaining 60 elements (International Commission on Radiological Protection, 1996).

The Age&Dosimetry flag in *tpa.inp* controls the age of the receptor and the selection of dosimetry coefficients tabulated in *gnewdf.dat* for use in individual protection calculations. Adult dosimetry is used based on the applicable regulations for Yucca Mountain in 10 CFR 63.312(e); however, TPA Version 5.1 includes a legacy modeling option to execute calculations for other age groups (i.e., infant, toddler, preteen, teen, adult), provided the user changes the Age&Dosimetry flag and supplies values for all applicable age-dependent biosphere input parameters (e.g., breathing rates, food consumption rates) in *tpa.inp*.

Selection of inhalation dose coefficients from International Commission on Radiological Protection Publication 72 (International Commission on Radiological Protection, 1996) for inclusion in *gnewdf.dat* is based on consideration of options regarding airborne particle size distribution and the rate of absorption from the respiratory tract to body fluids. Selected coefficients are based on a lognormal particle size distribution (International Commission on Radiological Protection, 1995) with a particle activity mean aerodynamic diameter of 10 μm [0.0004 in] (International Commission on Radiological Protection, 2002). The 10 μm [0.0004 in] assumption is generally consistent with available measurements of resuspended volcanic ash particle sizes (Hill and Connor, 2000). Regarding the rate of absorption from the respiratory tract to body fluids, which is influenced by the expected chemical form of the inhaled material,

International Commission on Radiological Protection Publication 72 provides coefficients by radionuclide for absorption classes including very fast, fast, moderate, and slow. For key radionuclides (Americium-241, Plutonium-239, Neptunium-237, Iodine-129, Technetium-99), values for inhalation dose coefficients were selected based on the assumed igneous scenario chemical form (i.e., oxidized)—a refinement based on the importance of the inhalation pathway in prior performance assessment calculations (NRC, 2005). The remaining inhalation dose coefficients were selected based on International Commission on Radiological Protection recommendations for absorption type (i.e., default recommendations for cases where no supporting chemical form data exist) (International Commission on Radiological Protection, 1996). For elements where no recommendations have been made (chlorine, yttrium, palladium, tin, samarium, bismuth, actinium, and protactinium), maximum values are used.

Selection of ingestion dose coefficients from International Commission on Radiological Protection Publication 72 for inclusion in *gnewdf.dat* is more straightforward. These coefficients are calculated using a single fractional absorption value (denoted f_1 in source documentation) for the gastrointestinal tract (International Commission on Radiological Protection, 1996). Thus, there are no options provided in the source document for selecting ingestion dose coefficients based on the chemical form of material.

Selection of dose coefficients for *gnewdf.dat* and *organdf.dat* from Federal Guidance Report No. 11 (EPA, 1988), where options are provided (based on chemical form of inhaled or ingested material), are based on the maximum absorption classes. This is a bounding selection (i.e., no higher values available from the source document). This set of dose coefficients may be useful for testing or evaluation purposes. TPA Version 5.1 has the flexibility to read any values entered into the data files if calculations with alternative coefficients or updates are needed in the future.

17.5.1.2 External Dose Coefficients (*ggrdf.dat*)

Calculation of human dose from external exposure to photons and electrons emitted by radionuclides on a contaminated ground surface is based on dosimetry coefficients provided in Federal Guidance Report No. 12 (EPA, 1993). That report is intended to be a companion report to Federal Guidance Report No. 11 (EPA, 1988), which provides inhalation and ingestion dose coefficients. No analogous companion report was provided for the dose coefficients in International Commission on Radiological Protection Publication 72 (International Commission on Radiological Protection, 1996); therefore, Federal Guidance Report No. 12 is provided as the only option for external dosimetry modeling in TPA Version 5.1.

Because external doses arise from radioactive decay of isotopes outside of the body, the types of radiation of concern for external dose (i.e., photons and electrons) are those able to penetrate skin and tissues sufficiently to deposit ionizing radiation to radiosensitive organs and tissues (EPA, 1993). An idealized model that includes uniform infinite radionuclide ground surface concentration and simplified geometries is used for estimating dose to tissues (EPA, 1993). Because the external dose is dependent on time, the coefficients represent dose per unit time-integrated concentration on the ground surface (in Sv-m²/Bq-yr).

17.6 Intermediate Outputs and Information Passed to Other Modules

DCAGW and DCAGS compute all pathway radionuclide doses for the groundwater release and the igneous eruption scenarios at every simulation timestep. Output files vary depending on TPA Version 5.1 run options selected. For example, GENTPA related output files are not produced for igneous disruptive event dose calculations if *tpa.inp* parameter AshEvolutionMode is set to 1, which runs ASHREMOB rather than DCAGS (Figure 17-1). Table 17-3 lists and describes intermediate output files for DCAGW and DCAGS.

In addition to the output files described previously, the user can specify that calculated information passed to and from DCAGW and DCAGS be saved as intermediate output for specific realizations. Tables 17-4 and 17-5 list and describe these optional intermediate output files. To specify the optional intermediate output files, the user can set *tpa.inp* parameter OutputMode (0=None, 1=All, 2=UserDefined) to a value of 1 or 2. When set to 1, all optional intermediate output for DCAGW and DCAGS are saved for all realizations. When set to 2, optional intermediate output selected are saved for realizations starting from *tpa.inp* parameter UserDefinedLowerRealizationAppended and ending with the realization specified by *tpa.inp* parameter UserDefinedUpperRealizationAppended. The user can select DCAGW optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter SelectAppendFiles to 10 for *dcagw.ech* and *dcagw.rlt*, 18 for *ggenii.cum*, 19 for *genv.cum*, or 20 for *dcfgw.cum*. The user can select DCAGS optional intermediate output by selecting the user-defined output mode and setting *tpa.inp* parameter SelectAppendFiles to 13 for *dcags.ech* and *dcags.rlt* or 20 for *dcfgs.cum*.

Table 17-3. Intermediate Output Files Created During Execution of DCAGW and DCAGS	
Output File	Contents
<i>airpkdos.res</i>	All-pathway total peak dose, peak dose time, and peak radionuclide doses from igneous release at the time of peak dose by realization. DCAGS contributes results by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> . This file is described in further detail in Chapter 19.
<i>arpkds_c.res</i>	All-pathway total peak dose, peak dose time, and peak radionuclide doses from igneous release at the time of peak dose by realization for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. DCAGS contributes results by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> . This file is described in further detail in Chapter 19.
<i>gwp_ave.res</i>	Output for groundwater protection calculations, including average groundwater concentrations (gross alpha activity including Ra-226 but excluding radon and uranium, radium-226), average organ/tissue doses (for combined beta- and photon-emitting radionuclides), and average whole body doses (for combined beta- and photon-emitting radionuclides). Averages computed over all realizations for each timestep. Generated from the reference case by DCAGW.
<i>gwpkdos.res</i>	Peak all-pathway dose from groundwater release and time of peak dose by radionuclide and for each realization. Generated from the reference case by DCAGW.

Table 17-3. Intermediate Output Files Created During Execution of DCAGW and DCAGS (continued)	
Output File	Contents
<i>gwccdf.res</i>	Groundwater release complementary cumulative distribution function for the simulation period. This is a legacy file.
<i>gwccdf_c.res</i>	Groundwater release complementary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. This is a legacy file.
<i>gwpkds_c.res</i>	Peak all-pathway dose from groundwater release and time of peak dose for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr] by radionuclide and for each realization. Generated from the reference case by DCAGW.
<i>gwpktdim.res</i>	This file contains output for groundwater protection calculations: peak groundwater concentrations and time of peak concentrations (gross alpha activity including Ra-226 but excluding radon and uranium, and radium-226), peak organ/tissue doses, and time of peak doses (for combined beta- and photon-emitting radionuclides), and peak whole body doses and time of peak doses (for combined beta- and photon-emitting radionuclides). All output is provided for each realization. Peak values are selected among all timesteps for each realization. Generated from the reference case by DCAGW.
<i>npkdoset.res</i>	Peak dose and corresponding time of peak by radionuclide for each realization.
<i>npkdst_c.res</i>	Peak dose and corresponding time of peak by radionuclide and realization for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr].
<i>pkmndose.res</i>	Dose value for each realization at the time of peak mean dose.
<i>totdose.res</i>	Time series of all pathway, all radionuclide, dose from groundwater and/or igneous release including the dilution volume for each realization. Generated from the reference case by DCAGW. Igneous contributions generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .
<i>totdos_c.res</i>	Time series of all pathway, all radionuclide, dose from groundwater and/or igneous release including the dilution volume for each realization for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. Generated from the reference case by DCAGW. Igneous contributions generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .
<i>rgsna.tpa</i>	Time history of all-pathway dose from igneous release by radionuclide, averaged among all realizations. Generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> . This file is described in further detail in Chapter 19.
<i>rgsnr.tpa</i>	Time history all-pathway dose from igneous release by radionuclide for all realizations. Generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> . This file is described in further detail in Chapter 19.
<i>rgssa.tpa</i>	Time history of all-pathway dose from igneous release summed for all radionuclides and averaged among all realizations. Generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> . This file is described in further detail in Chapter 19.

Table 17-3. Intermediate Output Files Created During Execution of DCAGW and DCAGS (continued)

Output File	Contents
<i>rgssr.tpa</i>	Time history of all-pathway dose from igneous release for all realizations summed by radionuclide. Generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> . This file is described in further detail in Chapter 19.
<i>rgwgssa.tpa</i>	Time history of dose from groundwater (DCAGW) and igneous release (DCAGS) summed for all radionuclides and averaged for all realizations. Generated by DCAGW from the reference case. Generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> . This file is described in further detail in Chapter 19.
<i>rgwna.tpa</i>	Time history all-pathway dose from groundwater release by radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwnapani.tpa</i>	Time history livestock food product (e.g., beef, poultry, egg) pathway dose from groundwater release by radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwnapdw.tpa</i>	Time history of drinking water dose from groundwater release by radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwnapext.tpa</i>	Time history of external pathway dose from groundwater release by radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwnapinh.tpa</i>	Time history of inhalation dose from groundwater release by radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwnapmlk.tpa</i>	Time history of milk pathway dose from groundwater release by radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwnappla.tpa</i>	Time history of crop ingestion pathway dose from groundwater release by radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwnr.tpa</i>	Time history of dose from groundwater release by radionuclide for all realizations. Generated from the reference case by DCAGW.
<i>rgwsa.tpa</i>	Time history of dose from groundwater release summed for all radionuclides and averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwsap.tpa</i>	Time history of dose from groundwater release by exposure pathway and radionuclide, averaged among all realizations. Generated from the reference case by DCAGW.
<i>rgwsr.tpa</i>	Time history of dose from groundwater release for all realizations summed by radionuclide. Generated from the reference case by DCAGW.
<i>gdefault.inp</i>	Default data input file written with input values from <i>tpa.inp</i> and <i>gdefault.dat</i> (for DCAGW for reference case) or <i>gdefaults.dat</i> (for DCAGS, when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i>) prior to execution of GENTPA. File is overwritten multiple times each realization.
<i>genv.in</i>	Intermediate file generated by execution of GENTPA. This file contains input to pathway calculations. File is overwritten within a TPA Version 5.1 realization every time GENTPA is executed. Generated by DCAGW from the reference case and by DCAGS when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> .

Table 17-3. Intermediate Output Files Created During Execution of DCAGW and DCAGS (continued)	
Output File	Contents
<i>genv.out</i>	Radionuclide-specific human intakes and exposure-time-weighted soil concentrations calculated by GENTPA for a single GENTPA execution. Generated by DCAGW from the reference case and by DCAGS when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> . File is overwritten multiple times per realization.
<i>gentoo.out</i>	Workspace file used by internal programs in GENTPA. Contains no useful information for the user. Generated from the reference case by DCAGW and by DCAGS when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> .
<i>gdefaults.inp</i>	Default data input file written with input values from <i>tpa.inp</i> and <i>gdefaults.dat</i> (when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i>) prior to execution of GENTPA. File is overwritten multiple times each realization.
<i>gftrans.inp</i>	Element-specific soil-to-plant and feed-to-animal uptake factors and soil leaching factors (computed by TPA Version 5.1 for each realization from inputs in <i>tpa.inp</i>). Input data for GENTPA based on values from <i>gftrans.def</i> (for DCAGW for the reference case) and <i>gftranss.def</i> (for DCAGS when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i>) with parameter additions or modifiers from <i>tpa.inp</i> . File is overwritten twice each realization when a simulation involves both DCAGW and DCAGS calculations.
<i>gftranss.inp</i>	Element-specific soil-to-plant and feed-to-animal uptake factors (International Atomic Energy Agency, 1994; LaPlante and Poor, 1997) and soil leaching factors (computed by the TPA Version 5.1 during execution from inputs in <i>tpa.inp</i>). Input data for GENTPA exposure pathway code executions for DCAGS based on values from <i>gftranss.def</i> with parameter additions and modifications from <i>tpa.inp</i> input parameters applicable to animal and plant uptake factors.
<i>ggenii.inp</i>	Primary formatted input file written with input values from <i>tpa.inp</i> and <i>ggenii.def</i> (for DCAGW for reference case) or <i>ggeniis.def</i> (for DCAGS when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> . prior to GENTPA execution. File is overwritten multiple times each realization.
<i>ggeniis.inp</i>	Primary formatted input file written with input values from <i>tpa.inp</i> and <i>ggeniis.def</i> (when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i>) prior to GENTPA execution. File is overwritten multiple times each realization.
<i>ggenii.out</i>	GENTPA-run output showing input echo for last execution of GENTPA including data files read and input parameters read from <i>ggenii.inp</i> . Generated from the reference case by DCAGW and by DCAGS when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> . File is overwritten multiple times per realization.
<i>ggeniis.out</i>	GENTPA output showing input echo for last execution including data files read and input parameters read from <i>ggeniis.inp</i> . File is overwritten multiple times per realization.
<i>gmedia.out</i>	Intermediate output from GENTPA with media-specific (e.g., soil) concentrations in the biosphere following execution of pathway models. Generated from the reference case by DCAGW and by DCAGS when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> . File is overwritten multiple times per realization.

Table 17-3. Intermediate Output Files Created During Execution of DCAGW and DCAGS (continued)	
Output File	Contents
<i>gs_cb_ad.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This file contains results for current biosphere and the farming community receptor. Generated by DCAGS by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> . File is overwritten each realization.
<i>gs_cb_ci.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This file is the result of a legacy option that is no longer supported. Generated DCAGS by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> . File is overwritten each realization.
<i>gs_pb_ad.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This file contains results for pluvial biosphere and the farming community receptor. Generated by DCAGS by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> . Files is overwritten each realization.
<i>gs_pb_ci.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This file is the result of a legacy option that is no longer supported. Generated by DCAGS by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> . File is overwritten each realization.
<i>gw_cb_ad.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This file contains results for current biosphere and the farming community receptor. Generated from the reference case by DCAGW. File is overwritten each realization.
<i>gw_cb_ci.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This file is the result of a legacy option that is no longer supported. Generated from the reference case by DCAGW. File is overwritten each realization.
<i>gw_pb_ad.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This file contains results for pluvial biosphere and the farming community receptor. Generated from the reference case by DCAGW. File is overwritten each realization.

Table 17-3. Intermediate Output Files Created During Execution of DCAGW and DCAGS (continued)

Output File	Contents
<i>gw_pb_ci.dat</i>	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This file is the result of a legacy option that is no longer supported. Generated from the reference case by DCAGW. File is overwritten each realization.
<i>gwork.buf</i>	Workspace file used by internal programs in GENTPA. Contains no useful information for the user. Generated from the reference case by DCAGW and by DCAGS when <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) is set to 1 and <i>AshEvolutionMode</i> [0=no ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> .

Table 17-4. Optional Intermediate Output Files Created During Execution of DCAGW

Output File	Contents
<i>dcagw.ech</i>	Echo of input to DCAGW including annual saturated zone groundwater flux by radionuclide, timestep, and realization. Generated when <i>tpa.inp</i> parameter <i>OutputMode</i> (0=None,1=All,2=UserDefined) is set to a value of 1, or 2 if the <i>SelectAppendFiles</i> parameter is set to a value of 10.
<i>dcagw.rlt</i>	Time series of all-pathway dose from groundwater by radionuclide and realization. Generated when <i>tpa.inp</i> parameter <i>OutputMode</i> (0=None,1=All,2=UserDefined) is set to a value of 1, or 2 if the <i>SelectAppendFiles</i> parameter is set to a value of 10.
<i>dcfgw.cum</i>	Compilation of all groundwater biosphere dose conversion factor output files (e.g., <i>gw_cb_ad.dat</i>) by climate state and realization. Generated when <i>tpa.inp</i> parameter <i>OutputMode</i> (0=None,1=All,2=UserDefined) is set to a value of 1, or 2 if the <i>SelectAppendFiles</i> parameter is set to a value of 20.
<i>genv.cum</i>	Radionuclide-specific human intakes and exposure-time-weighted soil concentrations by climate state and realization. Only applicable to DCAGW calculations. Generated from GENTPA output when <i>tpa.inp</i> parameter <i>OutputMode</i> (0=None,1=All,2=UserDefined) is set to a value of 1, or 2 if the <i>SelectAppendFiles</i> parameter is set to a value of 19.
<i>ggenii.cum</i>	Compilation of GENTPA-run output showing input echos for each GENTPA execution including data files read and input parameters read from each <i>ggenii.inp</i> file by climate state and realization. Only applicable to DCAGW calculations. Generated when <i>tpa.inp</i> parameter <i>OutputMode</i> (0=None,1=All,2=UserDefined) is set to a value of 1, or 2 if the <i>SelectAppendFiles</i> parameter is set to a value of 18.

Table 17-5. Optional Intermediate Output Files Created During Execution of DCAGS	
Output File	Contents
<i>dcfgs.cum</i>	Compilation of all ground surface biosphere dose conversion factor output files (e.g., <i>gs_cb_ad.dat</i>) by climate state for all realizations. Generated when <i>tpa.inp</i> parameter VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0, and OutputMode(0=None,1=All,2=UserDefined) to 1, or 2 if the SelectAppendFiles parameter is set to a value of 20.
<i>dcags.ech</i>	Echo of input to DCAGS including areal radionuclide activity concentrations on the ground surface by radionuclide and timestep. Generated when <i>tpa.inp</i> parameter VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and OutputMode(0=None,1=All,2=UserDefined) is set to a value of 1, or 2 if the SelectAppendFiles parameter is set to a value of 13.
<i>dcags.rlt</i>	Time series of all pathway dose from ground surface by radionuclide and by realization. Generated when <i>tpa.inp</i> parameter VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and OutputMode(0=None,1=All,2=UserDefined) is set to a value of 1, or 2 if the SelectAppendFiles parameter is set to a value of 13.

17.7 Techniques for Understanding Module Performance

While there is no single analysis that best provides insights into subsystem processes, a variety of techniques can be employed to better understand the relative effects of processes modeled by DCAGW and DCAGS. Processes with significant uncertainties are assigned probabilistic parameter distributions in *tpa.inp*, and several types of parametric sensitivity analysis techniques may be useful to understand their effects on system-level performance.

Intermediate results of biosphere calculations in DCAGW and DCAGS, biosphere dose conversion factors, are factors that proportionally scale total-system dose results. As a result, some analyses can be conducted efficiently on the biosphere calculations at the process level to gain insights to possible system-level impacts (e.g., an individual constant parameter change that results in an increase in the biosphere dose conversion factors would similarly impact total-system results for a given realization).

Single parameter importance analyses can be performed by repetitively varying input parameters associated with particular subsystem processes modeled by DCAGW or DCAGS and analyzing dose output and intermediate results for changes. Intermediate results such as annual intake values in *genv.cum* or biosphere dose conversion factor output (e.g., *gw_cb_ad.dat*, *gwdcf.cum*, *gsdcf.cum*) are useful for such analyses. Pathway results are presented at a greater level of specificity in the intake output files *genv.out* or *genv.cum*, allowing enhanced scrutiny of individual pathways prior to summation and dose conversion. A variety of files provide average and peak dose output by exposure pathway, radionuclide, and

timestep that can be useful for specific analyses (see Tables 17-3, 17-4, and 17-5 for a complete list of applicable output file options).

Single parameter importance analyses can be performed using the mean value input file (*tpameans.out*), which contains the mean or central value derived from the original input distribution specified for a parameter. Alternatively, a single parameter importance analysis could be performed by repetitively specifying smaller ranges within the parameter's original distribution in *tpa.inp*. TPA Version 5.1 supports input parameters for their provided ranges. The user should exercise care in interpreting results from simulations in which input are altered beyond their intended ranges.

Because pathway calculations include a series of environmental compartments that contaminants pass through prior to exposing the receptor, input parameters that control the magnitude of contaminant transfer can significantly affect the magnitude of the receptor dose. The depiction of the pathways and implementation approach in Figures 17-2 and 17-3 can aid the user in identifying appropriate portions of the calculations where intermediate outputs can be evaluated. Key input parameters and data that can influence pathway and dose calculations include

- Irrigation rates and irrigation times in *tpa.inp* (control the initial deposition rate from irrigation water to soil); because irrigation time represents the duration of the growing season and annual irrigation rates are constant over the season in the model, lower irrigation times will allocate the annual irrigation to a shorter period and increase deposition
- Soil distribution coefficients in *tpa.inp* (control buildup and loss rate of contaminants in soil and influence by prior irrigation time in *tpa.inp*)
- Plant transfer factors in *gftrans.def* and their scale factors in *tpa.inp* (control amount of contamination that transfer from the soil to crops)
- Food consumption rates in *tpa.inp* (directly scale intake of contaminated food)
- Mass loading and occupancy fractions in *tpa.inp* (control resuspension of contaminants from soil to air and inhalation intake)
- Dosimetry coefficients in *gnewdf.dat*, *ggrdf.dat*, and *organdf.dat* (account for the estimated dose per unit radionuclide intake and directly scale dose results)

Analysis of variability and uncertainty in biosphere dose conversion factors is done by running TPA Version 5.1 for multiple realizations with `SelectAppendFiles=0` and compiling the output by realization from *dcfgw.cum* or *dcfgs.cum*. Multivariate sensitivity analyses can be conducted by applying statistical methods to code results that analyze the effects of variation in individual input parameters on model output variation. Values for sampled input parameters by realization are output to *samplpar.res* (Chapter 19) and the headers for these parameters output to *samplpar.hdr*.

Combinations of sampled complementary input parameters can lead to more extreme results; therefore, it is useful to evaluate such combinations to ensure results are within the bounds of physical limits and expected system behavior (e.g., high soil distribution coefficient causes buildup and high plant transfer for a given radionuclide enhances transfer to plants in the model). Output evaluation by exposure pathway and computation of pathway contributions to total dose can also provide useful insights to model behavior. Biosphere dose conversion factor output is presented by pathway and can be quickly reviewed to ensure pathway contributions for various radionuclides are within reasonable bounds and are consistent with model inputs. Dose output is also provided by pathway (for DCAGW calculations only) in *rgwsap.tpa*.

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18 INPUT DATA FILES

TPA Version 5.1 is executed using one primary and several auxiliary input data files. Primary input data for TPA Version 5.1 are contained in *tpa.inp*; the auxiliary input data files provide additional information used by various modules. Whereas the user can modify input data in *tpa.inp* to specify the settings for any particular execution of TPA Version 5.1, the abstractions implemented in the corresponding modules should be carefully considered when making changes to the auxiliary input data files. The *tpa.inp* file is described in Chapter 4.

This chapter includes a single table (Table 18-1) that serves as a quick reference for the user to locate the chapters that explain the listed auxiliary input data files in detail. Table 18-1 contains four columns, including the name of the input data file, a brief description of the contents, and the relevant chapters. The “Used By Module” column cross-references the relevant chapters (Chapters 4–17) or Appendix A for detailed descriptions of how the contents of the various files are used in TPA Version 5.1.

The modules addressed in Table 18-1 include: the Infiltration Tabulator for Yucca Mountain module (ITYM),¹ the Climate and Infiltration module (UZFLOW),² the Unsaturated Zone Flow and Transport module (UZFT),³ the Saturated Zone Flow and Transport module (SZFT),⁴ the Dose Conversion Analysis for Groundwater module (DCAGW),⁵ the Near-Field Environment module (NFENV),⁶ the Abstracted Reflux model (REFLUX3),⁷ the Drip Shield Corrosion Failure module (DSFAIL),⁸ the Igneous Activity Ash Remobilization module (ASHREMOB),⁹ the Waste

¹The Infiltration Tabulator for Yucca Mountain module is referenced frequently throughout this chapter. The abbreviation ITYM will be used.

²The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

³The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

⁴The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

⁵The Dose Conversion Analysis for Groundwater module is referenced frequently throughout this chapter. The abbreviation DCAGW will be used.

⁶The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

⁷The Abstracted Reflux model is referenced frequently throughout this chapter. The abbreviation REFLUX3 will be used.

⁸The Drip Shield Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation DSFAIL will be used.

⁹The Igneous Activity Ash Remobilization module is referenced frequently throughout this chapter. The abbreviation ASHREMOB will be used.

Package Corrosion Failure module (EBSFAIL),¹⁰ the Engineered Barrier System Radionuclide Release module (EBSREL),¹¹ the Dose Conversion Analysis for Ground Surface module (DCAGS),¹² the Drip Shield and Waste Package Mechanical Failure module (MECHFAIL),¹³ and the utility modules INVENT and READER.

¹⁰The Waste Package Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

¹¹The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

¹²The Dose Conversion Analysis for Ground Surface module is referenced frequently throughout this chapter. The abbreviation DCAGS will be used.

¹³The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAIL will be used.

Table 18-1. Description of Auxiliary Input Data Files <i>(Disclaimer: The listed input data files were provided for the release of the TPA Version 5.1 code and are subject to change in subsequent versions of the TPA code or updates to the input data.)</i>			
File	Used By Module	Description	TPA User Guide Chapter(s)
<i>bunitdem.dat</i>	ITYM	Bedrock unit classification digital elevation model.	Appendix A, Appendix H of Mohanty, et al. (2002)
<i>burnup.dat</i>	INVENT	Time-dependent thermal output for boiling water reactor and pressurized water reactor spent nuclear fuel and the blend ratio per waste package.	4
<i>careadem.dat</i>	ITYM	Upslope contributing area digital elevation model.	Appendix A
<i>cdepdem.dat</i>	ITYM	Upslope average soil depth digital elevation model.	Appendix A
<i>climato1.dat</i>	UZFLOW	Normally distributed random numbers used in computing time-varying mean annual precipitation and mean annual temperature.	5
<i>climato2.dat</i>	UZFLOW	Time history of climate expressed as a relative change in mean annual precipitation and mean annual temperature from initial state to full glacial maximum.	5
<i>coefkdeq.dat</i>	UZFT SZFT	Polynomial coefficients for the surface response functions for actinide sorption and site-tailored pH ranges for discrete partial pressures of carbon dioxide.	11, 12
<i>dilution.dat</i>	DCAGW	Wellbore data for the saturated zone including well capture widths and well capture thicknesses by well pump rates and aquifer thicknesses, and well screen lengths by well pump rates. DCAGW uses data from this file only when the input flag PlumeCaptureModel is set to 2 (a legacy option). The reference case PlumeCaptureModel selection sets plume capture fraction to the upper bound of 1.0 and uses the water demand specified in 10 CFR 63.312(c).	17
<i>drythick.dat</i>	NFENV	Temporal variations in the dryout zone thickness for both degraded and intact drift cases. Used with the REFLUX3 model.	7
<i>elevdem.dat</i>	ITYM	Ground surface elevation digital elevation model.	Appendix A, Appendix H of Mohanty, et al. (2002)
<i>filename.dat</i>	DCAGW	Identifies filenames of all files needed for execution of GENTPA Version 1.0.	17
<i>fluoride.dat</i>	DSFAIL	Fluoride concentration of the seepage water as a function of time. This is a legacy file and is not supported.	8

Table 18-1. Description of Auxiliary Input Data Files (continued) <i>(Disclaimer: The listed input data files were provided for the release of the TPA Version 5.1 code and are subject to change in subsequent versions of the TPA code or updates to the input data.)</i>			
File	Used By Module	Description	TPA User Guide Chapter(s)
<i>gbioac1.dat</i>	DCAGW	Bioaccumulation data (data not used in calculations, but file is required for GENTPA Version 1.0 execution).	17
<i>gdosinc2.dat</i>	DCAGW	No data (file is required for GENTPA Version 1.0 execution).	17
<i>ggamen.dat</i>	DCAGW	Gamma energies for plume calculations (data is not used in calculations, but file is required for GENTPA Version 1.0 execution).	17
<i>ggrdf.dat</i>	DCAGW	External dose coefficients (only ground surface coefficients are used) from Federal Guidance Report No. 12 (U.S. Environmental Protection Agency, 1993).	17
<i>gnewdf.dat</i>	DCAGW	Age-dependent dose coefficients for ingestion and inhalation from ICRP Publication 72 (International Commission on Radiological Protection, 1996) and adult dose coefficients from Federal Guidance Report No. 11 (U.S. Environmental Protection Agency, 1988).	15, 17
<i>grmdlib.dat</i>	DCAGW	GENTPA Version 1.0 radionuclide library including half-lives and decay chain information.	17
<i>ia.dat</i>	READER	Hierarchical system of identifiers (subsystem, barrier, component, and parameter) for importance analysis.	4
<i>itym.dat</i>	ITYM	Miscellaneous input parameters to ITYM, including uncertainty and variability of climate, vegetation, soil, and lithology properties.	Appendix A
<i>maidtbl.dat</i>	UZFLOW	Mean of the estimated mean annual infiltration calculated within each grid block of the digital elevation model (generated by the ITYM external process module).	5, Appendix A
<i>maswtbl.dat</i>	ITYM	Table of mean annual clear-sky shortwave radiation flux as a function of ground rotation.	Appendix A, Appendix H of Mohanty, et al. (2002)
<i>nuclides.dat</i>	INVENT	Master list of the nuclides and colloids considered in TPA Version 5.1, initial inventory for spent fuel and glass waste forms, and a decay flag for groundwater protection calculations.	4
<i>organdf.dat</i>	DCAGW	Organ and effective (whole body) ingestion dose coefficients for use in groundwater protection drinking water dose calculations from Federal Guidance Report No. 11 (U.S. Environmental Protection Agency, 1988).	17
<i>remob_lut.dat</i>	ASHREMOB	Lookup table of parameters for airborne transport and deposition of contaminated tephra. Generated by the TEPHRA Version 1.0 code.	15
<i>repdes.dat</i>	READER	Repository panel and emplacement block geometry data.	4

Table 18-1. Description of Auxiliary Input Data Files (continued) <i>(Disclaimer: The listed input data files were provided for the release of the TPA Version 5.1 code and are subject to change in subsequent versions of the TPA code or updates to the input data.)</i>			
File	Used By Module	Description	TPA User Guide Chapter(s)
<i>smaidtbl.dat</i>	UZFLOW	Standard deviation of the estimated mean annual infiltration calculated within each grid block of the digital elevation model (generated by the ITYM external process module).	5
<i>soildem.dat</i>	ITYM	Soil thickness digital elevation model.	Appendix A, Appendix H of Mohanty, et al. (2002)
<i>strmtube.dat</i>	SZFT DCAGW	The reference data set in TPA Version 5.1 defines three streamtubes that emanate from the water table beneath the potential repository footprint and terminate at the receptor location. For each streamtube, <i>strmtube.dat</i> defines (i) an input flux, (ii) a set of three points defining the centerline of the streamtube inlet underneath the repository footprint, and (iii) a set of coordinates defining the width of the streamtubes at discrete distances downstream from the repository edge. For the reference case data set, sources from the unsaturated zones of Subareas 1, 6, 7, 8, and 9 contribute to the central streamtube; Subareas 2, 3, 4, and 5 contribute to the northern streamtube; and Subarea 10 contributes to the southern streamtube.	12, 17
<i>sunitdem.dat</i>	ITYM	Soil unit classification digital elevation model.	Appendix A, Appendix H of Mohanty, et al. (2002)
<i>tpanames.dat</i>	READER	Text file database of all TPA Version 5.1 input parameter names and their associated eight-character abbreviations.	4
<i>winddem.dat</i>	ITYM	Wind speed digital elevation model.	Appendix A, Appendix H of Mohanty, et al. (2002)
<i>dsfailt.def</i>	DSFAIL	Parameters for drip shield corrosion failure, including corrosion rate, drip shield thickness, and failure criterion.	8
<i>ebsfail.def</i>	EBSFAIL	Parameters for waste package corrosion failure, including some not specified in <i>tpa.inp</i> .	8
<i>ebsfilt.def</i>	EBSREL	Invert properties, including radionuclide retardation coefficient values and colloid filtration factors. Used by the legacy EBSFILT model and is not supported.	10
<i>ebsrel.def</i>	EBSREL	Default input file for engineered barrier system release calculations, and contains some input parameters not specified in <i>tpa.inp</i> , including rock parameters and diffusion rates.	10

Table 18-1. Description of Auxiliary Input Data Files (continued) <i>(Disclaimer: The listed input data files were provided for the release of the TPA Version 5.1 code and are subject to change in subsequent versions of the TPA code or updates to the input data.)</i>			
File	Used By Module	Description	TPA User Guide Chapter(s)
<i>gdefaults.def</i>	DCAGS	Auxiliary input including Deposition Velocity for Resuspension, Leaf Resuspension Factor, Biomass (by crop), Depth of Surface Soil, Surface Soil Density, Harvest Removal Flag, Soil Ingestion Rate, Crop Leaf Deposition Weathering Half Time, Plant Translocation Factors (by crop), Livestock Feed Translocation Factors (by feed type), Livestock Feed Consumption Rates (by feed type), Livestock Drinking Water Consumption Rates (by livestock), Plant Dry-to-Wet Ratio, and formatting for GENTPA input file <i>gdefault.inp</i> .	17
<i>gdefault.def</i>	DCAGW	Auxiliary input including Deposition Velocity for Resuspension, Leaf Resuspension Factor, Biomass (by crop), Depth of Surface Soil, Surface Soil Density, Harvest Removal Flag, Soil Ingestion Rate, Crop Leaf Deposition Weathering Half Time, Plant Translocation Factors (by crop), Livestock Feed Translocation Factors (by feed type), Livestock Feed Consumption Rates (by feed type), Livestock Drinking Water Consumption Rates (by livestock), Plant Dry-to-Wet Ratio, and formatting for GENTPA input file <i>gdefault.inp</i> .	17
<i>gtrans.def</i>	DCAGW	Element-specific soil-to-plant and feed-to-animal uptake factors and soil leaching factors.	17
<i>gtranss.def</i>	DCAGS	Element-specific soil-to-plant and feed-to-animal uptake factors and soil leaching factors.	17
<i>ggenii.def</i>	DCAGW	Auxiliary input including Fraction of Roots in Upper Soil, Fraction of Roots in Deep Soil, Mass Loading Factor, Crop Growing Times (by crop), Crop Yields (by crop), Food Product Holdup Times (by food type), Livestock Drinking Water Fractions (by food type), Livestock Diet Fractions (by food type and feed type), and Livestock Feed Storage Times (by food type), and formatting for GENTPA input file <i>ggenii.inp</i> .	17
<i>ggeniis.def</i>	DCAGS	Auxiliary input including Fraction of Roots in Upper Soil, Fraction of Roots in Deep Soil, Mass Loading Factor, Crop Growing Times (by crop), Crop Yields (by crop), Food Product Holdup Times (by food type), Livestock Drinking Water Fractions (by food type), Livestock Diet Fractions (by food type and feed type), and Livestock Feed Storage Times (by food type), and formatting for GENTPA input file <i>ggenii.inp</i> .	17
<i>mechfail_ds.def</i>	MECHFALL	Additional parameters related to the mechanical capacity of the drip shield.	9
<i>mechfail_wp.def</i>	MECHFALL	Additional parameters related to the mechanical capacity of the waste package.	9

Table 18-1. Description of Auxiliary Input Data Files (continued) <i>(Disclaimer: The listed input data files were provided for the release of the TPA Version 5.1 code and are subject to change in subsequent versions of the TPA code or updates to the input data.)</i>			
File	Used By Module	Description	TPA User Guide Chapter(s)
<i>wflow.def</i>	EBSREL	Time history of factors that account for flow reaching waste package and near-drift and in-drift flow diversions.	10
<i>tefkti.inp</i>	NFENV	Tabular input of temperature and relative humidity.	7

18.1 References

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U.S. Environmental Protection Agency (EPA). EPA-402-R-93-081, "External Exposures to Radionuclides in Air, Water, and Soil." Federal Guidance Report No. 12. Washington, DC: EPA, Office of Radiation and Indoor Air. 1993.

———. EPA-5201/1-88-020, "Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion." Federal Guidance Report No. 11. Washington, DC: EPA. 1988.

19 OUTPUT FILES

TPA Version 5.1 generates many intermediate output files. All output files are written in ASCII text format; they contain the results of simulations, including summaries of sampled and constant parameters, module variables, and time histories of radionuclide releases, water flows, radionuclide fluxes, and annual doses.

This chapter presents the output files in three tables: (i) primary intermediate output files (Table 19-1), (ii) optional intermediate output files (Table 19-2), and (iii) other output files (Table 19-3). These tables are expected to serve as quick references for the user to locate the chapters that explain the listed files with greater detail. Each table contains four fields: (i) the name of the output file, (ii) the module, or modules, that generate information in the output file, (iii) a brief description of the contents and the flag settings required to generate the output files produced by simulations other than the reference case, and (iv) a cross-reference to the relevant module chapter (Chapters 3 through 17).

The primary output files (Table 19-1) are identified by the extension *.res* (for result), *.abb* (for abbreviations), *.hdr* (for header), and *.tpa*. These files are the main outputs from the modules that are either passed to other modules or aggregated into the final output of the simulation. The secondary output files (Table 19-2) have extensions *.cum*, *.ech*, and *.rlt*. These files are generated by setting two parameters in *tpa.inp*: *OutputMode* (0=None, 1=All, 2=UserDefined) to 1 or 2 and *SelectAppendFiles* to the appropriate values specified in Table 3-2. Output of certain modules is written to files with extension *.cum*. Files with extensions *.rlt* and *.ech* are the output and input passed in the argument list of the modules. Other output files (Table 19-3) have extensions *.ash*, *.buf*, *.csv*, *.dat*, *.dbg*, *.dis*, *.in*, *.inp*, *.log*, *.nuc*, *.out*, *.rel*, *.src*, *.tmp*, and *.vel*. These files are described in their respective cross-referenced chapters.

The modules addressed in Tables 19-1 through 19-3 include: the Igneous Activity Ash Remobilization module (ASHREMOB),¹ the Dose Conversion Analysis for Ground Surface module (DCAGS),² the Igneous Activity Airborne Transport module (ASHPLUMO),³ the Engineered Barrier System Radionuclide Release module (EBSREL),⁴ the Unsaturated Zone Flow and Transport module (UZFT),⁵ the Saturated Zone Flow and Transport module (SZFT),⁶

¹The Igneous Activity Ash Remobilization module is referenced frequently throughout this chapter. The abbreviation ASHREMOB will be used.

²The Dose Conversion Analysis for Ground Surface module is referenced frequently throughout this chapter. The abbreviation DCAGS will be used.

³The Igneous Activity Airborne Transport module is referenced frequently throughout this chapter. The abbreviation ASHPLUMO will be used.

⁴The Engineered Barrier System Radionuclide Release module is referenced frequently throughout this chapter. The abbreviation EBSREL will be used.

⁵The Unsaturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation UZFT will be used.

⁶The Saturated Zone Flow and Transport module is referenced frequently throughout this chapter. The abbreviation SZFT will be used.

the Drip Shield Corrosion Failure module (DSFAIL),⁷ the Drip Shield and Waste Package Mechanical Failure module (MECHFAIL),⁸ the Dose Conversion Analysis for Groundwater module (DCAGW),⁹ the Climate and Infiltration module (UZFLOW),¹⁰ the Near-Field Environment module (NFENV),¹¹ the Waste Package Corrosion Failure module (EBSFAIL),¹² the Igneous Activity Deposition and Evolution of Ash module (ASHRMOVO),¹³ the Drift Degradation module (DRIFTFAIL),¹⁴ the Direct Faulting Disruptive Event module (FAULTO),¹⁵ and the Igneous Disruptive Event Involving Magma module (VOLCANO).¹⁶

⁷The Drip Shield Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation DSFAIL will be used.

⁸The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this chapter. The abbreviation MECHFAIL will be used.

⁹The Dose Conversion Analysis for Groundwater module is referenced frequently throughout this chapter. The abbreviation DCAGW will be used.

¹⁰The Climate and Infiltration module is referenced frequently throughout this chapter. The abbreviation UZFLOW will be used.

¹¹The Near-Field Environment module is referenced frequently throughout this chapter. The abbreviation NFENV will be used.

¹²The Waste Package Corrosion Failure module is referenced frequently throughout this chapter. The abbreviation EBSFAIL will be used.

¹³The Igneous Activity Deposition and Evolution of Ash module is referenced frequently throughout this chapter. The abbreviation ASHRMOVO will be used.

¹⁴The Drift Degradation module is referenced frequently throughout this chapter. The abbreviation DRIFTFAIL will be used.

¹⁵The Direct Faulting Disruptive Event module is referenced frequently throughout this chapter. The abbreviation FAULTO will be used.

¹⁶The Igneous Disruptive Event Involving Magma module is referenced frequently throughout this chapter. The abbreviation VOLCANO will be used.

Table 19-1. Description of Primary Intermediate Output Files			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>samplpar.abb</i>	READER	Abbreviations for <i>tpa.inp</i> parameter names in the same order as <i>samplpar.res</i> and <i>samplpar.hdr</i> . This file captures the abbreviations assigned to the sampled parameters in <i>tpa.inp</i> as specified in <i>tpanames.dat</i> . They are presented as one abbreviation per line to facilitate usage with many statistical software packages. Abbreviations for constant parameters are not provided.	4
<i>samplpar.hdr</i>	READER	Provides sampled parameter names and their respective abbreviations as specified in <i>tpanames.dat</i> . Abbreviations for constant parameters are not provided.	4
<i>airpkdos.res</i>	ASHREMOB DCAGS	Total peak dose, peak dose time, and peak radionuclide doses from igneous release at the time of peak dose by realization. ASHREMOB contributes results by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> (Chapter 15). This file contains all-pathway doses only if DCAGS is invoked. DCAGS contributes results by setting <i>tpa.inp</i> parameters VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 (Chapter 17).	15, 17
<i>arpkds_c.res</i>	ASHREMOB DCAGS	Total peak dose, peak dose time, and peak radionuclide doses from igneous release at the time of peak dose by realization for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. ASHREMOB contributes results by setting <i>tpa.inp</i> parameter VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> (Chapter 15). This file contains all-pathway doses only if DCAGS is invoked. DCAGS contributes results by setting <i>tpa.inp</i> parameters VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 (Chapter 17).	15, 17
<i>ashout.res</i>	ASHPLUMO	Provides output data from ASHPLUMO only when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> . Data include time of volcanic event, number of waste packages exhumed, areal ash and spent fuel density, column height, ash mass, and vent exit velocity.	16

Table 19-1. Description of Primary Intermediate Output Files (continued)			
File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>cumrel.res</i>	EBSREL UZFT SZFT	This file reports cumulative releases over the simulation period from the engineered barrier system, unsaturated zone, and saturated zone summed over all subareas in terms of Ci for each radionuclide for each realization.	10, 11, 12
<i>cumrel_c.res</i>	EBSREL UZFT SZFT	This file reports cumulative releases over the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr] from the engineered barrier system, unsaturated zone, and saturated zone summed over all subareas in terms of Ci for each radionuclide for each realization.	10, 11, 12
<i>dsfail.res</i>	DSFAIL MECHFAIL	Number of drip shields failed by corrosion and mechanical failure including time of failure for each realization.	8, 9
<i>gsccdf.res</i>	EXEC	Ground surface release complementary cumulative distribution function for the simulation period. This is a legacy file.	15, 16
<i>gsccdf_c.res</i>	EXEC	Ground surface release complementary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. This is a legacy file.	15, 16
<i>gwccdf.res</i>	EXEC	Groundwater release complementary cumulative distribution function for the simulation period. This is a legacy file.	12
<i>gwccdf_c.res</i>	EXEC	Groundwater release complementary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. This is a legacy file.	12
<i>gwp_ave.res</i>	DCAGW	Output for groundwater protection calculations including average groundwater concentrations (gross alpha activity, Ra-226), average organ/tissue doses (for combined beta- and photon-emitting radionuclides), and average whole body doses (for combined beta- and photon-emitting radionuclides). Averages computed over all realizations for each timestep.	17
<i>gwpkds.res</i>	DCAGW	Peak all-pathway dose from groundwater release and time of peak dose by radionuclide and for each realization.	17
<i>gwpkds_c.res</i>	DCAGW	Peak all-pathway dose from groundwater release and time of peak dose for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. Doses computed by radionuclide and for each realization.	17

Table 19-1. Description of Primary Intermediate Output Files (continued)

File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>gwpktime.res</i>	DCAGW	Output for groundwater protection calculations: peak groundwater concentrations and time of peak concentration calculations (gross alpha, Ra-226), peak organ/tissue doses and time of peak doses (for combined beta- and photon-emitting radionuclides), and peak whole body doses and time of peak doses (for combined beta- and photon-emitting radionuclides). All output is provided for each realization. Peak values are selected among all timesteps for each realization.	17
<i>gwtutusz.res</i>	UZFT SZFT	Groundwater travel times for each subarea and realization for the unsaturated zone, saturated zone, and combined travel time.	11, 12
<i>infilper.res</i>	UZFLOW	This file contains the flow rate after modification by each of the flow factors F_{ow} , F_{mult} , F_r , and F_d , as well as the weighted average flow rates into and out of the waste package, for every tenth timestep and all subareas. Also contains deep percolation rate averaged over all subareas at every 10 timesteps for each realization; includes data on reflux and diversion factors.	5, 10
<i>mechfail_ds.res</i>	MECHFAIL	Summary of results from MECHFAIL for mechanical drip shield failure for each realization and each subarea.	9
<i>mechfail_wp.res</i>	MECHFAIL	Summary of results from MECHFAIL for mechanical waste package failure for each realization and each subarea.	9
<i>nearfld.res</i>	NFENV	Subarea averaged values for waste package temperature, relative humidity, and chloride concentration at the waste package surface at every tenth timestep.	7
<i>npkdoset.res</i>	ASHREMOB DCAGW DCAGS	Peak dose and corresponding time of peak by radionuclide for each realization.	15, 17
<i>npkdst_c.res</i>	ASHREMOB DCAGW DCAGS	Peak dose and corresponding time of peak by radionuclide and realization for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr].	15, 17
<i>pkmndose.res</i>	ASHREMOB DCAGW DCAGS	Dose value for each realization at the time of peak mean dose.	15, 17
<i>pkreltime.res</i>	EBSREL	Engineered barrier system peak release rate and time of peak release for the simulation period by nuclide and subarea for each realization.	10

Table 19-1. Description of Primary Intermediate Output Files (continued)			
File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>pkrltm_c.res</i>	EBSREL	Engineered barrier system peak release rate and time of peak release for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr] by nuclide and subarea for each realization.	10
<i>relccdf.res</i>	SZFT ASHREMOB ASHPLUMO	Total release complimentary cumulative distribution function for the simulation period.	12, 15, 16
<i>relgwgs.res</i>	SZFT ASHREMOB ASHPLUMO	Groundwater, ground surface, and total release for the simulation period; values for each realization.	12, 15, 16
<i>rlccdf_c.res</i>	SZFT ASHREMOB ASHPLUMO	Total release complimentary cumulative distribution function for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr].	12, 15, 16
<i>rlgwgs_c.res</i>	SZFT ASHREMOB ASHPLUMO	Groundwater, ground surface, and total release for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]; values for each realization.	12, 15, 16
<i>samplpar.res</i>	READER	Sampled values of <i>tpa.inp</i> parameters that are assigned nonconstant sample distributions. A vector of sampled values is provided for each realization.	4
<i>totdose.res</i>	ASHREMOB DCAGW DCAGS	Time series of radionuclide dose and dilution volume for each realization. Igneous contributions are generated by ASHREMOB by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> . This file contains all-pathway doses only if DCAGS is invoked. Igneous contributions are generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	15, 17
<i>totdos_c.res</i>	ASHREMOB DCAGW DCAGS	Time series of radionuclide dose and dilution volume for each realization for the period specified by <i>tpa.inp</i> parameter DurationOfCompliancePeriod[yr]. Igneous contributions generated by ASHREMOB by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> . This file contains all-pathway doses only if DCAGS is invoked. Igneous contributions generated by DCAGS by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	15, 17

Table 19-1. Description of Primary Intermediate Output Files (continued)			
File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>wpsfail.res</i>	EBSFAIL MECHFAL FAULTO VOLCANO	For each realization and subarea, this file presents a table of six different waste package failure modes and the number of failed packages that is also available for groundwater release by each mode in order of failure time. Failure modes include initial failure, general corrosion, localized corrosion, mechanical failure, faulting, and igneous activity.	8, 9, 13, 14
<i>rgsna.tpa</i>	ASHREMOB DCAGS	Time history of dose from igneous release by radionuclide, averaged among all realizations. ASHREMOB contributes results by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> (Chapter 15). This file contains all-pathway doses only if DCAGS is invoked. DCAGS contributes results by setting <i>tpa.inp</i> parameters VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 (Chapter 17).	15, 17
<i>rgsnr.tpa</i>	ASHREMOB DCAGS	Time history of dose from igneous release by radionuclide for all realizations. ASHREMOB contributes results by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> (See Chapter 15). This file contains all-pathway doses only if DCAGS is invoked. DCAGS contributes results by setting <i>tpa.inp</i> parameters VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 (Chapter 17).	15, 17
<i>rgssa.tpa</i>	ASHREMOB DCAGS	Time history of all-pathway dose from igneous release summed for all radionuclides and averaged among all realizations. ASHREMOB contributes results by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> (Chapter 15). This file contains all-pathway doses only if DCAGS is invoked. DCAGS contributes results by setting <i>tpa.inp</i> parameters VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 (Chapter 17).	15, 17
<i>rgssr.tpa</i>	ASHREMOB DCAGS	Time history of dose from igneous release for all realizations summed by radionuclide. ASHREMOB contributes results by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> (Chapter 15). This file contains all-pathway doses only if DCAGS is invoked. DCAGS contributes results by setting <i>tpa.inp</i> parameters VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 (Chapter 17).	15, 17

Table 19-1. Description of Primary Intermediate Output Files (continued)

File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>rgwgssa.tpa</i>	ASHREMOB DCAGW DCAGS	Time history of dose from groundwater and igneous release summed for all radionuclides and averaged for all realizations. ASHREMOB contributes results by setting <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) to 1 in <i>tpa.inp</i> (Chapter 15). This file contains all-pathway doses only if DCAGS is invoked. DCAGS contributes results by setting <i>tpa.inp</i> parameters <i>VolcanismDisruptiveScenarioFlag</i> (yes=1,no=0) to 1 and <i>AshEvolutionMode</i> [0=no_ashremob,1=ashremob] to 0 (Chapter 17).	15, 17
<i>rgwna.tpa</i>	DCAGW	Time history dose from groundwater release by radionuclide, averaged among all realizations.	17
<i>rgwnapani.tpa</i>	DCAGW	Time history livestock food product (e.g., beef, poultry, egg) pathway dose from groundwater release by radionuclide, averaged among all realizations.	17
<i>rgwnapdw.tpa</i>	DCAGW	Time history of drinking water dose from groundwater release by radionuclide, averaged among all realizations.	17
<i>rgwnapext.tpa</i>	DCAGW	Time history of external pathway dose from groundwater release by radionuclide, averaged among all realizations.	17
<i>rgwnapinh.tpa</i>	DCAGW	Time history of inhalation dose from groundwater release by radionuclide, averaged among all realizations.	17
<i>rgwnapmlk.tpa</i>	DCAGW	Time history of milk pathway dose from groundwater release by radionuclide, averaged among all realizations.	17
<i>rgwnappla.tpa</i>	DCAGW	Time history of crop ingestion pathway dose from groundwater release by radionuclide, averaged among all realizations.	17
<i>rgwnr.tpa</i>	DCAGW	Time history of dose from groundwater release by radionuclide for all realizations.	17
<i>rgwsa.tpa</i>	DCAGW	Time history of dose from groundwater release summed for all radionuclides and averaged among all realizations.	17
<i>rgwsap.tpa</i>	DCAGW	Time history of dose from groundwater release by exposure pathway and radionuclide, averaged among all realizations.	17
<i>rgwsr.tpa</i>	DCAGW	Time history of dose from groundwater release for all realizations summed by radionuclide.	17

Table 19-2. Description of Optional Intermediate Output Files			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>ashplume.cum</i>	ASHPLUMO	Cumulative output of <i>ashplume.out</i> over all realizations. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	16
<i>dcfgs.cum</i>	DCAGS	Compilation of all ground surface biosphere dose conversion factor output files (e.g., <i>gs_cb_ad.dat</i>) by climate state for all realizations. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	17
<i>dcfgw.cum</i>	DCAGW	Compilation of all groundwater biosphere dose conversion factor output files (e.g., <i>gw_cb_ad.dat</i>) by climate state for all realizations.	17
<i>ebsrel.cum</i>	EBSREL	Waste package corrosion failure times for each subarea and realization from RELEASET.	10
<i>failt.cum</i>	EBSFAIL	Waste package outer container thickness versus time for the millannealed region due to various corrosion processes including localized corrosion; corrosion potential and critical potential for localized corrosion as a function of emplacement time for each subarea and realization.	8
<i>genv.cum</i>	DCAGW DCAGS	Radionuclide-specific human intakes and exposure-time-weighted soil concentrations calculated by GENTPA pathway modeling by climate state for all realizations. Generated by DCAGS when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> .	17
<i>ggenii.cum</i>	DCAGW	Compilation of GENTPA-run output by climate state and realization showing input echoes for each GENTPA exposure pathway model execution including data files read and input parameters read from each <i>ggenii.inp</i> .	17
<i>infilper.cum</i>	UZFLOW EBSREL	Provides average deep percolation for each subarea; includes data on reflux and diversion factors. Identical to <i>infilper.res</i> except that every timestep is reported.	5, 10
<i>nefiialluv.cum</i>	SZFT	Saturated alluvium flow and radionuclide transport input parameters for NEFMKS for each subarea in each realization. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .	12

Table 19-2. Description of Optional Intermediate Output Files (continued)			
File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>nefiituff.cum</i>	SZFT	Saturated tuff flow and radionuclide transport input parameters for NEFMKS for each subarea in each realization. Generated by setting <code>SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)</code> to 1 in <i>tpa.inp</i> .	12
<i>nefiisz.cum</i>	SZFT	This file is identical to <i>nefiisz.inp</i> except that information for every timestep is reported.	12
<i>nefiuiz.cum</i>	UZFT	Unsaturated zone flow and radionuclide transport input parameters for NEFMKS for each subarea in each realization.	11
<i>releasef.cum</i>	EBSREL	Contents of all <i>releasef.out</i> files for each waste form type, subarea, and realization.	10
<i>ashplumo.ech</i>	ASHPLUMO	Metric tonnes of uranium ejected for all subareas in each realization. Echoes input passed to ASHPLUMO. Generated by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> .	16
<i>ashrmovo.ech</i>	ASHRMOVO	Timestep and surface areal spent fuel density for all subareas in each realization. Echoes input passed to ASHRMOVO. Generated by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> .	16
<i>dcags.ech</i>	DCAGS	Echoes input to DCAGS, including areal radionuclide activity concentrations on the ground surface by radionuclide and timestep for all subareas in each realization. Generated by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 in <i>tpa.inp</i> .	17
<i>dcagw.ech</i>	DCAGW	Echoes input to DCAGW, including annual saturated zone groundwater flux by radionuclide and timestep for all subareas in each realization.	17
<i>driftfail.ech</i>	DRIFTFAIL	Echoes input passed to DRIFTFAIL for every realization, including characteristic values of seismic events used to evaluate drift degradation.	6
<i>dsfail.ech</i>	DSFAIL	Echoes input, such as realization number and subarea, passed to DSFAIL.	8
<i>ebfail.ech</i>	EBSFAIL	Echoes input, such as temperature, relative humidity, pH, and fraction of drip shields failed, passed to EBSFAIL for each subarea of every realization.	8
<i>ebrel.ech</i>	EBSREL	Echoes input passed to EBSREL for each subarea of every realization.	10

Table 19-2. Description of Optional Intermediate Output Files (continued)			
File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>faulto.ech</i>	FAULTO	Timesteps and number of subareas for all subareas in each realization. Echoes input passed to FAULTO. Generated by setting FaultingDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> .	13
<i>mechfail.ech</i>	MECHFAIL	Echoes input passed to MECHFAIL. Information includes realization number, subarea, number of timesteps, static and seismic demands, and drip shield and waste package thickness.	9
<i>nfenv.ech</i>	NFENV	Timestep and flow rate per waste package for each subarea at all times (this file echoes inputs to NFENV).	7
<i>szft.ech</i>	SZFT	UZFT releases passed to SZFT are included in this file, and includes all radionuclides in all subareas at every timestep.	12
<i>uzflow.ech</i>	UZFLOW	Timesteps that are mapped to UZFLOW output (this file echoes input values passed to UZFLOW).	5
<i>uzft.ech</i>	UZFT	Echoes the input values that are passed to UZFT by EBSREL. For each subarea at each timestep in each realization, provides a list of flow values and radionuclide release values into the lower unsaturated zone (below the repository).	11
<i>volcano.ech</i>	VOLCANO	Timestep information input to VOLCANO for all subareas in each realization. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> .	14
<i>ashplumo.rlt</i>	ASHPLUMO	Output from ASHPLUMO including ash and spent fuel areal densities. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	16
<i>ashrmovo.rlt</i>	ASHRMOVO	Output from ASHRMOVO including ground surface release by time and by nuclide. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	16
<i>dcags.rlt</i>	DCAGS	Time series of all-pathway dose from ground surface by radionuclide and by realization. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> .	17
<i>dcagw.rlt</i>	DCAGW	Time series of all-pathway dose from groundwater by radionuclide and realization.	17

Table 19-2. Description of Optional Intermediate Output Files (continued)			
File	Generated by Module	Description	TPA User Guide Chapter(s)
<i>driftfail.rlt</i>	DRIFTFAIL	This file contains the outputs generated by DRIFTFAIL for all subareas in each realization evaluated during the stimulation. The output includes times at which drifts fill with rubble, vertical pressures at the time of seismic events, and the drift geometries and vertical pressures resulting from drift degradation.	6
<i>dsfail.rlt</i>	DSFAIL	Contains results of drip shield corrosion calculations for each subarea and realization.	8
<i>ebsfail.rlt</i>	EBSFAIL	Contains results for the fraction of waste packages failed versus time and waste package outer container wall thickness versus time for each subarea and realization.	8
<i>ebsrel.rlt</i>	EBSREL	Contains EBSREL radionuclide release rates from the engineered barrier system for all radionuclide species (dissolved and colloidal), all timesteps, all subareas, and all realizations. It also indicates whether release was solubility controlled and includes information on waste package breaches, water contact times, and radionuclide inventories.	10
<i>faulto.rlt</i>	FAULTO	Time history of fraction of waste packages failed by faulting events for each subarea in each realization. Generated by setting FaultingDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> .	13
<i>mechfail.rlt</i>	MECHFAIL	Contains the output parameters of each subarea for all timesteps for both the drip shield and waste package performance. The information includes time step, drip shield and waste package failures due to static or dynamic loading and corrosion.	9
<i>nfenv.rlt</i>	NFENV	Rock wall temperature, waste package and drip shield temperatures, relative humidity, pH, and chloride, carbonate, nitrate and sulfate concentrations for each subarea for all timesteps.	7
<i>szft.rlt</i>	SZFT	The time history of radionuclide releases calculated by SZFT is provided by this file.	12
<i>uzflow.rlt</i>	UZFLOW	Volumetric deep percolation flow rates into each subarea for each timestep in each realization.	5
<i>uzft.rlt</i>	UZFT	Presents the radionuclide release rate from the unsaturated zone in curies per year at each timestep in each subarea for each realization.	11
<i>volcano.rlt</i>	VOLCANO	Inventory ejected, inventory of intrusive waste package failures by subarea, and time history of fraction of waste packages failed from volcanic activity for each subarea in each realization. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> .	14

Table 19-3. Description of Other Output Files			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>infile.ash</i>	ASHPLUMO	ASHPLUMO utilizes the parameters specified in the ASHPLUMO section of <i>tpa.inp</i> to write <i>infile.ash</i> . The <i>infile.ash</i> file is overwritten every time ASHPLUMO executes the standalone code ASHPLUME. Consequently, values in <i>infile.ash</i> are from the final realization. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	16
<i>gwork.buf</i>	DCAGW DCAGS	Workspace file used by internal programs in GENTPA. Contains no useful information for the user.	17
<i>lhs.csv</i>	SAMPLER	(Empty file)	—
<i>chlrdmf.dat</i>	EBSFAIL	Contains chloride concentration information versus time from NFENV and is used as input to EBSFAIL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.	8
<i>driftfail.dat</i>	DRIFTFAIL	Time histories of vertical pressures and geometries for the degraded drift. File is overwritten for each subarea calculation.	6
<i>drifts.dat</i>	READER	Drift endpoint coordinates and number of waste packages in each drift in the repository.	4
<i>dsfailt.dat</i>	DSFAIL	Drip shield failure information and time history of drip shield thickness. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.	8, 13, 14
<i>ebsflo.dat</i>	EBSREL	Provides flow diversion data at each timestep. This file is input to the RELEASET standalone code; values reflect the final subarea and realization.	10
<i>ebsglass.dat</i>	EBSREL	Provides glass waste form release rates for each nuclide at each timestep. Values in this file reflect the final subarea and realization.	10
<i>ebsnef.dat</i>	EBSREL	Waste package release rates for all aqueous and colloidal nuclides, plus water flow rate. Input to EBSFILT, a legacy model which is no longer supported. Values in this file reflect the final subarea and realization.	10
<i>ebsnef2.dat</i>	EBSREL	Waste package release rates for all aqueous and colloidal nuclides, plus water flow rate. Output from EBSFILT a legacy model that is no longer supported.	10
<i>ebssf.dat</i>	EBSREL	Provides spent fuel waste form release rates for each nuclide at each timestep. Values in this file reflect the final subarea and realization.	10

Table 19-3. Description of Other Output Files (continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>ebstrh.dat</i>	EBSFAIL	Contains weld and waste package failure summary data. Also contains temperatures, relative humidity, pH, and inhibitor information versus time information from NFENV. Time, temperatures, and summary data are input to EBSREL. Within the summary data, weld corrosion breaching time and waste package surface corrosion breaching time are used by EBSREL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.	8
<i>gs_cb_ad.dat</i>	DCAGS	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This file contains results for current biosphere and the farming community receptor. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	17
<i>gs_cb_ci.dat</i>	DCAGS	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This is a legacy file and is no longer supported. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	17
<i>gs_pb_ad.dat</i>	DCAGS	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This file contains results for pluvial biosphere and the farming community receptor. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	17

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>gs_pb_ci.dat</i>	DCAGS	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in ground surface soil and ash at the receptor location (e.g., biosphere dose conversion factors). A separate file is produced by climate state and receptor type. This is a legacy file. Generated by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> .	17
<i>gw_cb_ad.dat</i>	DCAGW	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This file contains results for current biosphere and the farming community receptor.	17
<i>gw_cb_ci.dat</i>	DCAGW	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This is a legacy file and is no longer supported.	17
<i>gw_pb_ad.dat</i>	DCAGW	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This files contains results for pluvial biosphere and the farming community receptor.	17
<i>gw_pb_ci.dat</i>	DCAGW	Intermediate output of annual dose to the receptor by exposure pathway and radionuclide per unit concentration in receptor well water (e.g., biosphere dose conversion factors). Separate files are produced by climate state and receptor type. This is a legacy file and is no longer supported.	17
<i>maxrel.dat</i>	EBSREL	Written by the RELEASET standalone code, this file contains the maximum fractional release of all radionuclides (prior to colloid allocation), and the time of each maximum release. Values in this file reflect the final subarea and realization.	10

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>mechfail_ds.dat</i>	MECHFAIL	Contains the timesteps for the subarea indicating whether drip shield failure occurs due to static loading, dynamic loading, or corrosion for both rock types. A summary shows the drip shield failure times, static and seismic demands at the time of failure (e.g., vertical pressure) and drip shield capacity parameters. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.	9
<i>mechfail_wp.dat</i>	MECHFAIL	This intermediate file computes information about the waste packages exhibiting mechanical failure in MECHFAIL. The file contains the time steps for the subarea indicating whether waste package failure occurs due to static or dynamic loading. A summary shows the waste package failure times, vertical pressure, waste package thickness, contact angle, contact length, and peak ground acceleration. This file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains the input information for the last subarea of the last realization.	9
<i>sotnef.dat</i>	UZFT SZFT	Written by UZFT as an input file for NEFMKS transport calculations. The file provides NEFMKS with the time-dependent source term (radionuclide releases) data from EBSREL, after adjusting the source term to account for (i) flux splitting, if there is a bypass fraction at that timestep and (ii) the filtration of colloids in the unsaturated zone rock matrix (i.e., less of J-species). UZFT saves a copy of <i>sotnef.dat</i> as <i>nefiuz.src</i> , which is a more informative file name. Both files are overwritten each time a subarea calculation is performed by UZFT. In addition, <i>sotnef.dat</i> is overwritten by SZFT during saturated zone transport calculations (Chapter 12). At the end of a simulation, <i>nefiuz.src</i> will reflect the input source term information for the unsaturated zone transport calculation for the last subarea of the last realization, and <i>sotnef.dat</i> will reflect the corresponding saturated zone transport calculation for that subarea and realization.	11, 12

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>wpflow.dat</i>	EBSREL	Contains the time history of seepage factors for flow diversion (F_{mult}), flow contacting waste packages (F_{ow}), fraction of subarea wetted (F_{wet}), rubble diversion (F_r), failed drip shield diversion (F_d), and breached waste package diversion by corrosion (F_{wc}), mechanical events 1 and 2 (F_{wm1} and F_{wm2}), and initially defective waste package diversion (F_{id}) used in RELEASET. Values in this file reflect the final subarea and realization.	10
<i>driftfail.dbg</i>	DRIFTFAIL	Debug information for drift failure. This file contains a list of the timesteps, and the seismic event properties: time of events, peak ground acceleration and rubble compaction factor.	6
<i>dsfail.dbg</i>	DSFAIL	Debug information for drip shield corrosion failure.	8
<i>ebsfilt.dbg</i>	EBSFILT	Debug information for invert transport. Generated by setting InvertBypass(0=ebsfilt,1=bypass-ebsfilt) to 0 in <i>tpa.inp</i> . This is a legacy file and is no longer supported.	10
<i>echofail.dbg</i>	EBSFAIL	Debug information for waste package corrosion failure. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.	8
<i>mechfail_ds.dbg</i>	MECHFAIL	Debug information for drip shield mechanical failure. This file contains error messages that occur during the execution of MECHFAIL of the last realization.	9
<i>mechfail_wp.dbg</i>	MECHFAIL	Debug information for waste package mechanical failure. This file contains error messages that occur during the execution of MECHFAIL of the last realization.	9
<i>thermal.dbg</i>	NFENV	Reports time, drip shield and waste package temperatures, rubble temperature, rubble thickness, and conductance of different legs modeled in Thermal Mode 1 and 2.	7
<i>wpsfail.dbg</i>	EBSFAIL	Debug information for waste package failure. This file presents a table of five different waste package failure modes in time order for each realization. The subarea of failure is also noted.	8
<i>nefii.dis</i>	UZFT SZFT	Contains radionuclide discharge from last NEFMKS run of a simulation; typically the last saturated zone transport calculation from the last subarea of the last realization.	11, 12
<i>nefiialluv.dis</i>	SZFT	Contains time histories for radionuclide discharge rates from last saturated alluvium NEFMKS run of a simulation; typically the last subarea of the last realization. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .	12

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>nefiituff.dis</i>	SZFT	Contains time histories for radionuclide discharge rates from last saturated tuff NEFMKS run of a simulation; typically the last subarea of the last realization. Generated by setting <code>SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)</code> to 1 in <i>tpa.inp</i> .	12
<i>nefiisz.dis</i>	SZFT	This is a copy of the <i>nefi.dis</i> output file produced by NEFMKS during the saturated zone transport calculation. It contains a time history of radionuclide discharge from the saturated zone during the simulation period for each radionuclide decay chain specified in <i>tpa.inp</i> . This file is overwritten each time a subarea calculation is performed; at the end of simulation this file will reflect the saturated zone transport calculation for the last subarea.	12
<i>nefiuz.dis</i>	UZFT	This is a copy of <i>nefi.dis</i> , an output file that provides a time history of radionuclide discharge from the unsaturated zone during the simulation period for each radionuclide decay chain specified in <i>tpa.inp</i> , as calculated by NEFMKS. This file is overwritten each time a subarea calculation is performed. At end of a simulation, <i>nefiuz.dis</i> will contain the radionuclide releases for the last unsaturated zone subarea calculated by NEFMKS in the last realization. Note that if UZFT applies flux splitting in the calculations for this subarea, the radionuclide releases reported in <i>nefiuz.dis</i> will include only the fraction of the flow that was used in the NEFMKS transport calculations. However, a time history for the combined (matrix fraction plus bypass fraction) unsaturated zone radionuclide releases is provided in the intermediate output file <i>nefiisz.src</i> (Chapter 10).	11
<i>ashplume.in</i>	ASHPLUMO	Intermediate file generated as a part of the stochastic sampling routine. Generated by setting <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> to 0 in <i>tpa.inp</i> .	16
<i>genv.in</i>	DCAGW DCAGS	Intermediate file generated by execution of the first of two programs (ENVIN.EXE; ENV.EXE) comprising GENTPA exposure pathway code. This file contains input to ENV.EXE pathway calculations. File is overwritten within a TPA realization every time GENTPA is executed.	17
<i>deltaec.inp</i>	EBSFAIL	The change in critical potential as a function of time.	8
<i>driftfail.inp</i>	DRIFTFAIL	Drift and engineered barrier geometries and rock properties as input for DRIFTFAIL. File is overwritten for each subarea calculation.	6

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>dsfailt.inp</i>	DSFAIL	Sampled input values provided to DSFAILT. This file is generated using the template file <i>dsfailt.def</i> and the input parameter values are specified in the DSFAIL and EBSFAIL sections of <i>tpa.inp</i> .	8
<i>ebsfail.inp</i>	EBSFAIL	Input parameters used by EBSFAIL. This file is generated using the template file <i>ebsfail.def</i> and the input parameter values specified in the EBSFAIL section of <i>tpa.inp</i> .	8
<i>ebsfilt.inp</i>	EBSREL	Invert transport properties (radionuclide retardation factors, colloid filtration factors, etc.). Generated by setting InvertBypass(0=ebsfilt,1=bypass-ebsfilt) to 0 in <i>tpa.inp</i> . This is a legacy file and is no longer supported.	10
<i>ebsrel.inp</i>	EBSREL	Input file for RELEASET. The file includes waste package breach numbers and times, wetted fraction of the subarea, waste package and waste form physical characteristics, temperature, flow factors from <i>ebsflo.dat</i> , leaching parameters, water contact mode data, inventory, cladding parameters, and diffusion parameters. This file corresponds to <i>ebsrelglass.inp</i> or <i>ebsrelsf.inp</i> , depending on the modeled waste form. Values in this file reflect the final subarea, realization, and waste form.	10
<i>ebsrelglass.inp</i>	EBSREL	This RELEASET input file for glass waste form corresponds to <i>ebsrel.inp</i> . Values in this file reflect the final subarea and realization.	10
<i>ebsrelsf.inp</i>	EBSREL	This RELEASET input file for spent nuclear fuel corresponds to <i>ebsrel.inp</i> . Values in this file reflect the final subarea and realization.	10
<i>ebstrhc.inp</i>	EBSFAIL	This file contains temperature, pH, and inhibitor information versus time from NFENV and is used as input to EBSFAIL. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.	8
<i>gdefault.inp</i>	DCAGW	Default data input file written with input values from <i>tpa.inp</i> and <i>gdefault.dat</i> (for DCAGW for reference case) or <i>gdefaults.dat</i> (for DCAGS, when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i>) prior to execution of GENTPA. File is overwritten multiple times each realization.	17
<i>gdefaults.inp</i>	DCAGS	Default data input file written with input values from <i>tpa.inp</i> and <i>gdefaults.dat</i> (when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i>) prior to execution of GENTPA. File is overwritten multiple times each realization.	17

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>gftrans.inp</i>	DCAGW	Element-specific soil-to-plant and feed-to-animal uptake factors (International Atomic Energy Agency, 1994; LaPlante and Poor, 1997) and soil leaching factors (computed by the TPA Version 5.1 during execution from inputs in <i>tpa.inp</i>). Input data for GENTPA exposure pathway code executions for DCAGW based on values from <i>gftrans.def</i> with parameter additions and modifications from <i>tpa.inp</i> input parameters applicable to biosphere soil leaching and animal and plant uptake factors.	17
<i>gftranss.inp</i>	DCAGS	Element-specific soil-to-plant and feed-to-animal uptake factors (International Atomic Energy Agency, 1994; LaPlante and Poor, 1997) and soil leaching factors (computed by the TPA Version 5.1 during execution from inputs in <i>tpa.inp</i>). Input data for GENTPA exposure pathway code executions for DCAGS based on values from <i>gftranss.def</i> with parameter additions and modifications from <i>tpa.inp</i> input parameters applicable to animal and plant uptake factors.	17
<i>ggenii.inp</i>	DCAGW	Primary formatted input file written with input values from <i>tpa.inp</i> and <i>ggenii.def</i> (for DCAGW for reference case) or <i>ggeniis.def</i> (for DCAGS when <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> is set to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> is set to 0 in <i>tpa.inp</i> prior to GENTPA execution. File is overwritten multiple times each realization.	17
<i>ggeniis.inp</i>	DCAGS	Primary formatted input file written with input values from <i>tpa.inp</i> and <i>ggeniis.def</i> (when <code>VolcanismDisruptiveScenarioFlag(yes=1,no=0)</code> is set to 1 and <code>AshEvolutionMode[0=no_ashremob,1=ashremob]</code> is set to 0 in <i>tpa.inp</i> prior to GENTPA execution. File is overwritten multiple times each realization.	17
<i>lhs.inp</i>	SAMPLER	Input data for SNLLHS. Contains all sampled parameters for all realizations.	3, 4
<i>mechfail.inp</i>	MECHFAIL	Input data for MECHFAIL. This file copies data from <i>mechfail_ds.inp</i> and <i>mechfail_wp.inp</i> .	9
<i>mechfail_ds.inp</i>	MECHFAIL	Input data for MECHFAIL containing parameters from <i>tpa.inp</i> and <i>mechfail_ds.def</i> .	9
<i>mechfail_wp.inp</i>	MECHFAIL	Input data for MECHFAIL containing parameters from <i>tpa.inp</i> and <i>mechfail_wp.def</i> .	9
<i>nefii.inp</i>	UZFT SZFT	Defines flow path and transport characteristics for NEFMKS standalone code.	11, 12

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>nefiialluv.inp</i>	SZFT	Input information for the saturated alluvium NEFMKS transport calculation for the last subarea. File is overwritten each time a subarea calculation is performed. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .	12
<i>nefiituff.inp</i>	SZFT	Input information for the saturated tuff NEFMKS transport calculation for the last subarea. File is overwritten each time a subarea calculation is performed. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .	12
<i>nefiisz.inp</i>	SZFT	This is a copy of <i>nefii.inp</i> for NEFMKS; it defines flow path and transport characteristics. This file is overwritten each time a subarea calculation is performed; at the end of simulation, this file will reflect the saturated zone transport calculation for the last subarea.	12
<i>nefiuz.inp</i>	UZFT	This is a copy of <i>nefii.inp</i> , the main input file for NEFMKS for unsaturated zone transport calculations. It defines unsaturated zone flow path and transport characteristics, including (i) number of NEFMKS legs and leg lengths, (ii) calculated dispersivity for each leg, (iii) decay chain attributes and (iv) colloid-adjusted retardation factors (RD) for each transport leg. This file is overwritten each time a subarea calculation is performed. At the end of a simulation, <i>nefiuz.inp</i> will contain the input information for the unsaturated zone transport calculation for the last subarea of the last realization.	11
<i>nefmks.log</i>	SZFT	Logs calls to NEFMKS by SZFT by printing "szft" once for each call. Used for diagnostics only. Generated only when parameter SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 1 in <i>tpa.inp</i> .	12
<i>ebspac.nuc</i>	EBSREL	This RELEASET input file contains initial radionuclide inventory per waste package, molecular weights, half-lives, and decay chain data from INVENT (Chapter 4), and solubility limits, invert retardation factors, and gap fractions specified in the EBSREL section of <i>tpa.inp</i> . The file corresponds to <i>ebspacglass.nuc</i> or <i>ebspacsf.nuc</i> , depending on the modeled waste form. Values in this file reflect the final realization and waste form.	10

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>ebspacglass.nuc</i>	EBSREL	This RELEASET input file (for glass waste form) contains initial radionuclide inventory per waste package, molecular weights, half-lives, and decay chain data from INVENT (Chapter 4), and solubility limits, invert retardation factors, and gap fractions specified in the EBSREL section of <i>tpa.inp</i> . Values in this file reflect the final realization and waste form.	10
<i>ebspacsf.nuc</i>	EBSREL	This RELEASET input file (for spent nuclear fuel waste form) contains initial radionuclide inventory per waste package, molecular weights, half-lives, and decay chain data from INVENT (Chapter 4), and solubility limits, invert retardation factors, and gap fractions specified in the EBSREL section of <i>tpa.inp</i> . Values in this file reflect the final realization and waste form.	10
<i>ashremob.out</i>	ASHREMOB	Time histories for airborne mass loads for each source region, initial deposit at receptor location during light and heavy disturbance activities, fluvial and eolian remobilization, airborne concentrations of high-level waste, and total outdoor particle loads during light and heavy disturbance activities. File is rewritten for each realization. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 in <i>tpa.inp</i> and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0.	15
<i>ashcmd.out</i>	ASHPLUMO	Input data summary for ASHPLUME. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	16
<i>ashplume.out</i>	ASHPLUMO	Output from ASHPLUME calculations includes results for twenty parameters. Generated by setting VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] to 0 in <i>tpa.inp</i> .	16
<i>cumrelse.out</i>	EBSREL	Output from RELEASET; contains time history of radionuclide quantity outside the waste package for a given subarea. Values in this file reflect the final subarea and realization.	10
<i>diagnose.out</i>	EBSREL	Diagnostic information for RELEASET.	10
<i>ebscld.out</i>	EBSREL	Written in EBSREL, this file contains colloidal J-species release rates. Reflects the final subarea and realization.	10
<i>ebsfilt.out</i>	EBSREL	Screen output from the last execution of EBSFILT. Generated by setting InvertBypass(0=ebsfilt,1=bypass-ebsfilt) to 0 in <i>tpa.inp</i> . This is a legacy file and is no longer supported.	10

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>ebsnef.out</i>	EBSREL	This RELEASET output file contains time-dependent waste package radionuclide release rates, affected flag (indicating whether release was solubility limited), and water flow rate q_{out} . Values in this file reflect the final subarea and realization.	10
<i>failt.out</i>	EBSFAIL	Output from FAILT corrosion calculations. Corrosion failure information for the waste package outer container surface and welds. File is overwritten for each subarea calculation. Contains information for the last subarea of the last realization.	8
<i>frac_rel.out</i>	EBSREL	Radionuclide fractional release output. Same information as <i>ebsnef.dat</i> .	10
<i>gencorrfail.out</i>	EBSFAIL	Time history of corrosion potentials for general corrosion. File is overwritten for each subarea calculation. Typically contains information for the last subarea of the last realization.	8
<i>gentoo.out</i>	DCAGW DCAGS	Workspace file used by internal programs in GENTPA. Contains no useful information for the user. Generated by DCAGS when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> .	17
<i>genv.out</i>	DCAGW DCAGS	Radionuclide-specific human intakes and exposure-time-weighted soil concentrations calculated by GENTPA exposure pathway code for a single execution. Overwritten multiple times per realization. Generated by DCAGS when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> .	17
<i>ggenii.out</i>	DCAGW	GENTPA output showing input echo for last execution including data files read and input parameters read from <i>ggenii.inp</i> file. File is overwritten multiple times per realization.	17
<i>ggeniis.out</i>	DCAGS	GENTPA output showing input echo for last execution including data files read and input parameters read from <i>ggeniis.inp</i> . File is overwritten multiple times per realization.	17
<i>gmedia.out</i>	DCAGW DCAGS	Intermediate output from GENTPA with media-specific (e.g., soil) concentrations in the biosphere following execution of pathway models. File is overwritten multiple times per realization. Generated by DCAGS when VolcanismDisruptiveScenarioFlag(yes=1,no=0) is set to 1 and AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 0 in <i>tpa.inp</i> .	17

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>inv1000.out</i>	EBSREL	This file is written by RELEASET and contains the inventory of the groundwater nuclides at 1,000 years and the initial inventory per waste package from <i>ebspac.nuc</i> . Reflects the final subarea and realization.	10
<i>lhs.out</i>	SAMPLER	Contains all of the sampled parameters for all realizations. The block format of the file enables the efficient reading of the data in the SAMPLER utility module. All of the parameters for a given realization are grouped into a single block of data values.	3, 4
<i>lhse.out</i>	SAMPLER	Captures the screen output of the SNLLHS standalone code.	3, 4
<i>nefiialluv.out</i>	SZFT	This is a copy of the <i>nefii.out</i> output file produced by <i>nefmks.out</i> during the saturated tuff transport calculation. It contains a summary of all NEFMKS input and output. It is overwritten each time a subarea calculation is performed; at end of simulation, this file will reflect the saturated zone transport calculation for the last subarea. Generated only when parameter SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 1 in <i>tpa.inp</i> .	12
<i>nefiituff.out</i>	SZFT	This is a copy of <i>nefii.out</i> produced by <i>nefmks.out</i> during the saturated tuff transport calculation. It contains a summary of all NEFMKS input and output. It is overwritten each time a subarea calculation is performed; at end of simulation, this file will reflect the saturated zone transport calculation for the last subarea. Generated only when parameter SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) is set to 1 in <i>tpa.inp</i> .	12
<i>nefii.out</i>	UZFT SZFT	Provides a summary of all NEFMKS input and output. Overwritten each time NEFMKS is called.	11, 12
<i>nefiisz.out</i>	SZFT	This is a copy of the <i>nefii.out</i> output file produced by NEFMKS during the saturated zone transport calculation. It contains a summary of all NEFMKS input and output. It is overwritten each time a subarea calculation is performed; at end of simulation, this file will reflect the saturated zone transport calculation for the last subarea.	12

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>nefiuz.out</i>	UZFT	This is a copy of <i>nefi.out</i> output file that contains a summary of NEFMKS input and output, including the average or the time-dependent velocities that are passed to NEFMKS depending on which value is specified in <i>tpa.inp</i> for the parameter UZVelocity[0=average,1=time-dependent]. The file is overwritten each time a subarea calculation is performed. At the end of a simulation, <i>nefiuz.out</i> will contain the output for the unsaturated transport calculation for the last subarea of the last realization.	11
<i>relcum.out</i>	EBSREL	This file contains output from RELEASET, including number of breached waste packages per class, the time at which liquid water contacts the waste form, waste package water fill times, and radionuclide inventory data. The inventory values represent quantities inside the waste package if release had not occurred, cumulative quantities released from waste form but not from the waste package, and cumulative quantities released from the engineered barrier system. The file corresponds to <i>relcumglass.out</i> or <i>relcumsf.out</i> , depending on the modeled waste form. Values in this file reflect the final subarea, realization, and waste form.	10
<i>relcumglass.out</i>	EBSREL	This RELEASET output file for glass waste form corresponds to <i>relcum.out</i> . Values in this file reflect the final subarea and realization.	10
<i>relcumsf.out</i>	EBSREL	This RELEASET output file for spent nuclear fuel corresponds to <i>relcum.out</i> . Values in this file reflect the final subarea and realization.	10
<i>releaset.out</i>	EBSREL	This file contains screen output from the last execution of EBSREL. It contains only debugging information and reflects the final subarea and realization.	10
<i>relfrac.out</i>	EBSREL	This RELEASET output file, used by EBSREL, contains the time of maximum release rate for each radionuclide, the maximum normalized release rate for each radionuclide (prior to colloidal species allocation), and waste package water fill times. Values in this file reflect the final subarea and realization.	10
<i>rel_flow.out</i>	EBSREL	Written in RELEASET, this file contains the weld surface fraction, weld failure flag and time, waste package general corrosion flag and breach time, and waste package localized corrosion failure flag and time. Reflects the final subarea and realization.	10
<i>sz_kdrd.out</i>	SZFT	This file provides a report of intermediate results of calculated values for saturated zone radionuclide distribution coefficients and the sampled parameters contributing to those calculations.	12

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>sz_revers.out</i>	SZFT	This file reports the saturated zone retardation factors after corrections to account for effects of reversible sorption to colloids. For each radionuclide, values are reported for mobile and immobile regions for both the tuff and alluvium transport legs and for each subarea.	12
<i>tpamax.out</i>	READER	File produced by TPA Version 5.1 that is a version of <i>tpa.inp</i> with all parameters set to constant values that reflect the maximum value of the sample distribution.	4
<i>tpameans.out</i>	READER	File produced by TPA Version 5.1 that is a version of <i>tpa.inp</i> with all parameters set to constant values that reflect the mean value of the sample distribution (approximated for parameter distributions that do not have a closed-form analytical expression for mean value).	4
<i>tpamin.out</i>	READER	File produced by TPA Version 5.1 that is a version of <i>tpa.inp</i> with all parameters set to constant values that reflect the minimum value of the sample distribution.	4
<i>trelease.out</i>	EBSREL	This file is generated by RELEASET and contains the quantity of a radionuclide outside the waste package as a function of the internal RELEASET timesteps. Values in this file reflect the final subarea and realization.	10
<i>uz_kdrd.out</i>	UZFT	For every realization in a simulation, this file shows the matrix and fracture sorption coefficient (K_D) values calculated by UZFT for six actinides (americium, neptunium, plutonium, thorium, uranium and curium) for every hydrostratigraphic layer in the unsaturated zone. It also shows the calculated fracture retardation factors (R_D) for the same actinides and lists the sampled parameter values from <i>tpa.inp</i> used in K_D and R_D calculations. The calculated values in <i>uz_kdrd.out</i> are not adjusted for the effects of sorption to colloids. Results are shown only for the first subarea processed in each realization.	11
<i>uz_revers.out</i>	UZFT	This file reports the adjusted retardation factors (R_D^{eff}) for all radionuclides after corrections to account for effects of reversible sorption to colloids. For each radionuclide, values are reported for each subarea in each realization, but the values are calculated only for the specific hydrostratigraphic layers that were used as transport legs in NEFMKS.	11

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>weldfail.out</i>	EBSFAIL	This file contains corrosion potential and critical potential versus time for the welded regions and is generated by EBSFAIL. This file also contain the residual thickness of the welded region due to various corrosion processes including localized corrosion. The file is overwritten each time a subarea calculation is performed; at the end of a simulation, the file contains information for the last subarea of the last realization.	8
<i>wpfillstats.out</i>	EBSREL	This file contains the number of waste packages into which water flows and waste package fill time data for each subarea and realization.	10
<i>nefi.rel</i>	UZFT SZFT	This is an intermediate output that reports cumulative releases over the simulation period from a saturated or unsaturated zone transport calculation. Overwritten each time NEFMKS is called. At end of each simulation, this file will reflect the saturated zone transport calculation for the last subarea and is used to develop the <i>cumrel.res</i> file.	11, 12
<i>nefiialluv.src</i>	SZFT	Copy of <i>sotnef.dat</i> .	12
<i>nefiituff.src</i>	SZFT	Copy of <i>sotnef.dat</i> .	12
<i>nefiisz.src</i>	SZFT	Copy of the <i>sotnef.dat</i> generated by SZFT for the saturated zone transport calculation. Overwritten each time NEFMKS is called. At the end of each simulation, this file will reflect the last subarea of the last realization run.	12
<i>nefiuz.src</i>	UZFT	Input file for NEFMKS transport calculations. The file provides NEFMKS with the time-dependent source term (radionuclide releases) data from EBSREL, after adjusting the source term to account for (i) flux splitting, if there is a bypass fraction at that timestep and (ii) the filtration of colloids in the unsaturated zone rock matrix (i.e., less of J-species). UZFT saves a copy of <i>sotnef.dat</i> as <i>nefiuz.src</i> , which is a more informative file name. Both files are overwritten each time a subarea calculation is performed by UZFT. At the end of a simulation, <i>nefiuz.src</i> will reflect the input source term information for the unsaturated zone transport calculation for the last subarea of the last realization.	11
<i>tpasys.tmp</i>	EXEC	Contains system path for folder containing TPA Version 5.1 used for the simulation.	4
<i>cp.tpa</i>	SAMPLER	List of all constant parameters and their values from <i>tpa.inp</i> .	4

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>mv.tpa</i>	EXEC	Module variables are stored for each realization. This file captures the parameter names of the module variables generated by various modules of the TPA Version 5.1 code, as well as the values used for each realization. Calculated physical quantities are passed among modules using this mechanism.	4
<i>sp.tpa</i>	SAMPLER	Number of sampled parameters and sampled parameter values.	3
<i>spquery.tpa</i>	SAMPLER	List of each parameter indicating the number of times the parameter is accessed per realization.	4
<i>nefi.vel</i>	UZFT SZFT	Time-varying velocity input file for NEFMKS used for unsaturated zone and saturated zone radionuclide transport calculations.	11, 12
<i>nefiialluv.vel</i>	SZFT	Copy of <i>nefi.vel</i> generated by SZFT for the saturated alluvium transport calculation. Overwritten each time NEFMKS is called. At the end of each simulation, this file will reflect the last subarea of the last realization run. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .	12
<i>nefiituff.vel</i>	SZFT	Copy of <i>nefi.vel</i> generated by SZFT for the saturated tuff transport calculation. Overwritten each time NEFMKS is called. At the end of each simulation, this file will reflect the last subarea of the last realization run. Generated by setting SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes) to 1 in <i>tpa.inp</i> .	12
<i>nefiisz.vel</i>	SZFT	This is a copy of the <i>nefi.vel</i> input file for NEFMKS, which defines the time-varying velocity during the simulation period. This file is overwritten each time a subarea calculation is performed; at the end of simulation, this file will reflect the saturated zone transport calculation for the last subarea.	12

Table 19-3. Description of Other Output Files(continued)			
File	Generated By Module	Description	TPA User Guide Chapter(s)
<i>nefiuz.vel</i>	UZFT	This is a copy of <i>nefi.vel</i> , an input file for NEFMKS. It provides the unsaturated zone time-varying water velocities that were developed for NEFMKS using hydrologic parameters and selection criteria specified in <i>tpa.inp</i> and the time history of deep percolation determined in UZFLOW. Velocities in <i>nefiuz.vel</i> are reported in feet per year [1 ft = 0.305 m]. If the flag UZVelocity[0 or 1] in <i>tpa.inp</i> is set to 0 (i.e., constant velocities), the time-varying velocities are not used in NEFMKS, but the values are still listed in <i>nefiuz.vel</i> . This file is overwritten each time a subarea calculation is performed. At the end of a simulation, <i>nefiuz.vel</i> will contain the input velocity for the unsaturated zone transport calculation for the last subarea of the last realization.	11

19.1 References

International Atomic Energy Agency. "Handbook of Parameter Values for the Prediction of Coefficients: Workers and Members Radionuclide Transfer in Temperate Environments." Technical Report Series No. 364. Vienna, Austria: International Atomic Energy Agency. 1994.

LaPlante, P.A. and K. Poor. "Information and Analysis to Support Selection of Critical Groups and Reference Biospheres for Yucca Mountain Exposure Scenarios." CNWRA 97-009. San Antonio, Texas: CNWRA. 1997.

APPENDIX A

INFILTRATION TABULATOR FOR YUCCA MOUNTAIN EXTERNAL PROCESS MODEL DESCRIPTION

INFILTRATION TABULATOR FOR YUCCA MOUNTAIN EXTERNAL PROCESS MODEL DESCRIPTION

The Infiltration Tabulator for Yucca Mountain (ITYM)¹ external process model calculates the net amount of water infiltrating from the ground surface into the unsaturated zone above the repository. Specifically, ITYM determines the spatial variation of percolation water flux below the rooting zone for a set of climatic states. ITYM execution is completed prior to initiating a TPA Version 5.1 simulation. The resulting information is used by the Climate and Infiltration (UZFLOW)² module in TPA Version 5.1 to estimate the temporal and spatial variation of deep percolation at the repository horizon in the absence of thermal effects.

A user's guide to ITYM is documented in Appendix H of the TPA Version 4.0 User's Guide (Mohanty, et al., 2002). The version of ITYM documented by Mohanty, et al. (2002) has been modified to consider overland flow and to provide additional output files to UZFLOW. These changes are documented in this appendix. Other than these changes, the input files for the reference case are the same as described by Mohanty, et al. (2002). Additional information on modeling of climate change and its effect on percolation flux can be found in Stothoff and Walter (2007) and Stothoff (1999).

A.1 Modifications to Infiltration Due to Overland Flow

The abstractions developed using simulations do not consider water that moves into a grid cell through overland flow (runon), although they do implicitly account for runoff by assuming that water does not pond (hence runs off). The effect of runon is accounted for by locally increasing the effective value for mean annual precipitation (MAP)³ based on upslope conditions.

The KINEROS2 simulator (Smith, et al., 1995; Woolhiser, et al., 1990) was used to simulate storm runoff for several storms. These simulations were used to derive a regression model relating upslope contributing area, average upslope soil depth, and effective increase in MAP due to overland flow under present-day conditions in Upper Split Wash, a small watershed at Yucca Mountain. The relationship has the form

$$E_i = 4.097 + 0.300A_{ri} - 10.4hav_i \quad (\text{A-1})$$

where E_i is the excess MAP due to runon [mm/yr], A_{ri} is the upslope contributing area divided by grid-cell area, and hav_i is the area-averaged upslope soil depth [m]. The A_{ri} parameter is

¹The Infiltration Tabulator for Yucca Mountain module is referenced frequently throughout this appendix. The abbreviation ITYM will be used.

²Climate and Infiltration is referenced frequently throughout this appendix. The abbreviation UZFLOW will be used.

³Mean annual precipitation is referenced frequently throughout this appendix. The abbreviation MAP will be used.

calculated for each grid cell by dividing the value in the DEM file⁴ (*careadem.dat*) by the area of the grid cell, and the *hav_i* parameter is provided in the DEM file *cdepdem.dat*.

A.2 Input Files for Infiltration Tabulator for Yucca Mountain External Process Model

The reference set of input files used for ITYM in TPA Version 5.1 has a slightly different set of parameters in *itym.dat* and two new distributed-parameter files. These differences are discussed in the following sections.

A.2.1 Control Parameters

Control parameters specify characteristics of the output table, the names of associated data files, and reference values. Each keyword in *itym.inp* has one associated parameter. The keywords related to output files replace the description by Mohanty, et al. (2002) with the new keyword/parameter descriptions shown in Table A–1.

The output files are DTBL files,⁵ indicated by DTBL in the name of the file. Each combination of MAP and mean annual temperature (MAT)⁶ considered in the ITYM simulation generates a new coverage for the DTBL file; thus a DTBL file can be quite large. The DTBL files consist of pixel-by-pixel statistics of mean annual infiltration (MAI)⁷ for all realizations. The available output files include the mean and standard deviation of both MAI and log(MAI). An output DTBL file is only generated if the corresponding keyword is provided.

Table A–1. New Control Parameters Used to Define an Infiltration Tabulator Yucca Mountain Run			
Keyword	Type	Restrictions	Description
Reference Values			
zDTBLmai	char	name of file	DTBL* file name for the mean of MAI†
zDTBLsmai	char	name of file	DTBL* file name for the standard deviation of MAI†
zDTBLmay	char	name of file	DTBL* file name for the mean of log MAI†
zDTBLsmay	char	name of file	DTBL* file name for the standard deviation of log MAI†

⁴Files with the same format and grid as the Digital Elevation Model file used to describe ground-surface elevation (*elevdem.dat*) are referred to as DEM files throughout this appendix.

⁵Files that consist of a table of DEM files are referred to as DTBL files throughout this appendix.

⁶Mean annual temperature is referenced frequently throughout this appendix. The abbreviation MAT will be used.

⁷Mean annual infiltration is referenced frequently throughout this appendix. The abbreviation MAI will be used.

Table A–1. New Control Parameters Used to Define an Infiltration Tabulator Yucca Mountain Run (continued)			
Keyword	Type	Restrictions	Description
Reference Values			
do_MAI_DTBL	integer	1 or 0	1 to output the mean of MAI†, 0 otherwise
do_sMAI_DTBL	integer	1 or 0	1 to output the standard deviation of MAI†, 0 otherwise
do_MAY_DTBL	integer	1 or 0	1 to output the mean of log MAI†, 0 otherwise
do_sMAY_DTBL	integer	1 or 0	1 to output the standard deviation of log MAI†, 0 otherwise
*A DTBL file contains several DEM-format outputs in a table. †Mean Annual Infiltration (MAI)			

A.2.2 External Files

Several parameters are inherently variable across the site and cannot be easily specified through linear relationships. These parameters are typically entered as DEM-format files all registered to the same grid. Other information is most conveniently defined as tabular inputs. Keywords defining file names containing DEM coverages that are not documented by Mohanty, et al. (2002) are presented in Table A–2.

Upslope contributing area and average soil depth are the only new DEM files not described by Mohanty, et al. (2002). These quantities are derived directly from the ground surface DEM and the soil thickness DEM using a flow-routing model.

Table A–2. Commands Defining External Files Used to Define Spatially Distributed Parameters and Tabular Information			
Keyword	File Name	Data Type	Description
zCareaDEM	careadem.dat	real	Upslope contributing area [m ²] DEM file*
zCdepDEM	cdepdem.dat	real	Upslope average soil depth [m] DEM file*
*File in the same format as the Digital Elevation Model (DEM) file describing elevation			

A.2.3 Auxiliary Files Supplied to ITYM

All auxiliary files are located in the *data* subdirectory. In addition to auxiliary data files, ITYM has other useful files in the *itym* subdirectory. A brief description of the contents, use, and either a complete or partial listing follows for the new auxiliary data files.

A.2.3.1 File name: *careadem.dat*

ITYM obtains upslope contributing area from the data file *careadem.dat*. This DEM file assigns a contributing area to each pixel in the repository discretization based on independent calculations of overland flow using a flow-routing scheme. The same discretization is used for all other DEM files listed in Table A–2. The discretization consists of 199 columns and 300 rows with the lower left grid coordinate (545010, 4074000) expressed in UTM NAD27 easting and northing (m). The grid size is 30 × 30 m [98 × 98 ft]. Upslope contributing area data correspond to pixels beginning at the upper left-hand (northwest) corner of the grid and continuing to the right every 30 m [98 ft]. The second row of pixels from the top of the grid moving left to right comprises the next set of upslope contributing areas, and so forth for all 300 rows of soil types. The first 15 lines and last 5 lines of *careadem.dat* are provided in Sample A–1.

Sample A–1

DEM of upslope contributing area for each pixel; used in ITYM preprocessor software.

```
NROWS 300
NCOLS 199
XLLCORNER 545010
YLLCORNER 4074000
CELLSIZE 30
NODATA_VALUE -9999
132.962
1090.82
1234.18
241.903
11525.6
40978.6
41490.2
35103.7
35575.9
.
.
.
93.8056
121.219
73.1133
137.273
63.1389
```

A.2.3.2 File name: *cdepdem.dat*

ITYM obtains average upslope soil depth from the data file *cdepdem.dat*. This DEM file assigns the average upslope soil depth to each pixel in the repository discretization based on the average soil depth encountered by the flow-routing scheme used for *careadem.dat*. The same discretization is used for all other DEM files listed in Table A–2. The discretization consists of 199 columns and 300 rows with the lower left grid coordinate (545010, 4074000) expressed in UTM NAD27 easting and northing (m). The grid size is 30 × 30 m [98 × 98 ft]. Upslope soil depth data correspond to pixels beginning at the upper left-hand (northwest) corner of the grid and continuing to the right every 30 m. The second row of pixels from the top of the grid moving left to right comprises the next set of soil types, and so forth for all 300

rows of soil types. The first 15 lines and last 5 lines of *cdepdem.dat* are provided in Sample A–2.

Sample A–2

```
# DEM of upslope soil depth for each pixel; used in ITYM preprocessor software.
NROWS 300
NCOLS 199
XLLCORNER 545010
YLLCORNER 4074000
CELLSIZE 30
NODATA_VALUE -9999
1.12909
0.799209
3.94997
5.91172
3.52102
0.10177
0.086721
0.114273
.
.
.
5.01199
4.1582
7.69001
4.51291
10.3097
```

A.2.3.3 Input Control File for Infiltration Tabulator Yucca Mountain

The input control file for running ITYM contains many records that generally should not be modified. The parameters listed in Table A–2 control the size and the range of MAP and MAT used to generate *maidtbl.dat* and *smaidtbl.dat* and are generally the only parameters that should be changed. The first 41 lines and the last 5 lines of the input control file *itym.dat* are provided below in Sample A–3.

Sample A–3

```
# Input control file itym.dat for ITYM preprocessor software version 1.0, TPA 4.0
##### Size of Tables #####

num_MAP_table      4
num_MAT_table      4
num_pixel_merge     4
num_realize_per_table 500

##### Options #####

PathwaySum    MaxOnly
RegrForm      TPA4
```

zElevDEM	elevdem.dat
zWindDEM	winddem.dat
zSoilDEM	soildem.dat
zBUnitDEM	bunitdem.dat
zSUnitDEM	sunitdem.dat
zCareaDEM	careadem.dat
zCdepDEM	cdepdem.dat
zMASWtbl	maswtbl.dat
zDTBLmai	maidtbl.dat
zDTBLsmai	smaidtbl.dat
zDTBLmay	maydtbl.dat
zDTBLsmay	smaydtbl.dat

MergeIDListNum	0
do_MAI_DTBL	1
do_MAY_DTBL	0
do_sMAI_DTBL	1
do_sMAY_DTBL	0

Minimum, Maximum, and Typical Values

MAP_min[mm/yr]	50
MAP_max[mm/yr]	800
MAT_min[degreeC]	0
MAT_max[degreeC]	22
base_elev[km]	1.4
randomseed	5.05187067d8

#Do not change any record below this line

```

.
.
.
MergeSet
MergeDEMNameID tr
MergeVolCase tr carfill soilfill unfilled
MergeSet

```

A.3 References

Mohanty, S., T.J. McCartin, and D. Esh. "Total-system Performance Assessment (TPA) Version 4.0 Code: Module Descriptions and User's Guide." San Antonio, Texas: CNWRA. 2002.

Smith, R.E., D.C. Goodrich, D.A. Woolhiser, and C.L. Unkrich. "KINEROS—A KINematic Runoff and EROSION Model." *Computer Models of Watershed Hydrology*. V.P. Singh, ed. Highlands Ranch, Colorado: Water Resources Publications. pp. 697–732. 1995.

Stothoff, S. "Infiltration Abstractions for Shallow Soil Over Fractured Bedrock in a Semiarid Climate." San Antonio, Texas: CNWRA. 1999.

Stothoff, S. and G. Walter. "Long-Term-Average Infiltration at Yucca Mountain, Nevada: Million-Year Estimates." CNWRA 2007-003. San Antonio, Texas: CNWRA. 2007.

Woolhiser, D.A., R.E. Smith, and D.C. Goodrich. "KINEROS, KINematic Runoff and EROSION Model: Documentation and User Manual." ARS-77. Washington, DC: U.S. Department of Agriculture. 1990.

APPENDIX B

GOVERNING EQUATIONS FOR TEMPERATURE CALCULATIONS

APPENDIX B

Appendix B describes the equations for temperature and heat transfer calculations for Thermal Mode 1 and Thermal Mode 2 described in Sections 7.3.1.2.1 and 7.3.1.2.2. The network models described here are an expansion of the implementation of Chapter 7, and the *tpa.inp* parameters used in this appendix are described in Table 7-1

B.1 Thermal Conductance Through Invert Leg in Thermal Mode 1

The simplified radial geometry used to represent indrift component and rubble for Thermal Mode 1 is illustrated in Figure B-1(a). The heat transfer through different pathways or legs is solved using a thermal network approach as shown in Figure B-1(b). The only mode of heat transfer through the invert leg is conduction. Legs A and B will have conduction through the accumulated rubble and combined convection with radiation through the air gap depending on the presence of rubble and air. Figure B-1(b) shows the network for a generalized scenario assuming both air and rubble are present in Legs A and B. Appropriate thermal-network schematics for a particular situation where rubble or air is not present in a particular segment can be constructed from Figure B-1(b) by neglecting the corresponding branch. Figure B-1 implies the simplification that conduction through the drip shield need not be included in the calculation. This simplification is reasonable because of the small thickness and high thermal conductivity of the drip shield. It is important, however, to include the drip shield in the algorithm to physically separate heat transfer processes beneath and above the drip shield, at least prior to the rubble covering the drip shield.

$$G_{Total} = G_{invert} + G_{leg-A} + G_{leg-B} \quad (B-1)$$

where

G_{invert} — effective thermal conductance for the invert leg [W/°C]

G_{leg-A} — effective thermal conductance for Leg A [W/°C]

G_{leg-B} — effective thermal conductance for Leg B [W/°C]

The expression for thermal conductance through the invert is given by

$$G_{Invert} = \frac{2\pi K_{invert} (1 - f_c) L_{WP}}{\ln\left(\frac{D_{RW}}{D_{WP}}\right)} \quad (B-2)$$

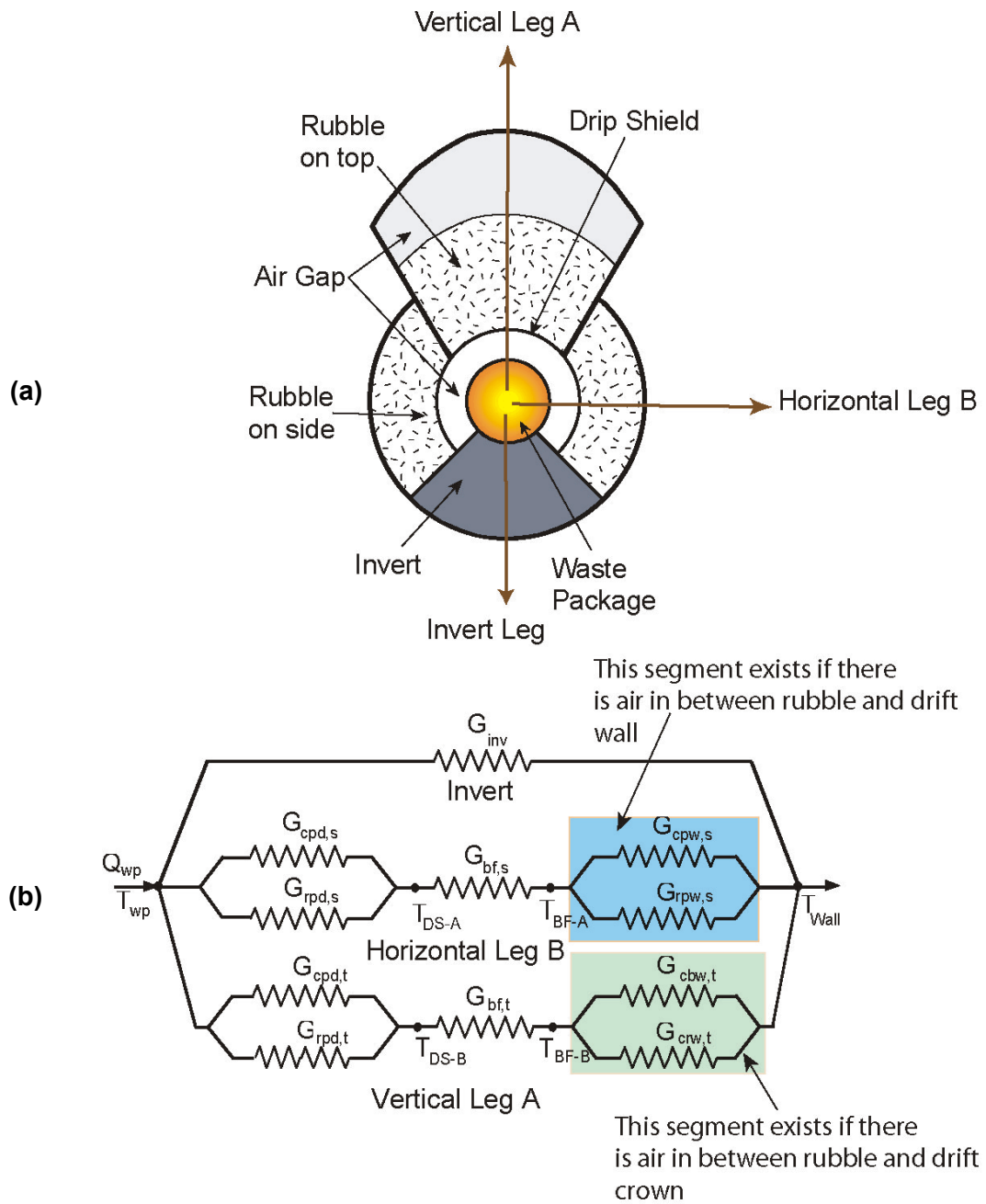


Figure B–1. Simplified Radial Geometry and Corresponding Thermal Network for Thermal Mode 1

where

- f_c — fraction of the waste package surface contributing to radiative/convective heat transfer based on the *tpa.inp* parameter CircumferentialFractionNotCoveredByFloor[]
- K_{invert} — effective thermal conductivity of invert material [W/(m–°C)] as specified by the *tpa.inp* parameter ThermalConductivityOfFloor [W/(m–C)]
- L_{WP} — length of waste package [m] as specified by the *tpa.inp* parameter WPLength[m]
- D_{WP} — waste package outer diameter [m] as specified by the *tpa.inp* parameter WPDiameter[m]
- D_{RW} — rock wall diameter [m] as specified by the *tpa.inp* parameter EmplacementDriftDiameter[m]

B.1.1 Thermal Conductance Through Vertical Leg A in Thermal Mode 1

The expression for thermal conductance through Leg A is given by

$$G_{leg-A} = \frac{1}{\frac{1}{G_{cpd,t} + G_{rpd,t}} + \frac{1}{G_{bf,t}} + \frac{1}{G_{cbw,t} + G_{rbw,t}}} \quad (B-3)$$

where

- $G_{cpd,t}$ — effective thermal conductance due to convection in air between the waste package and drip shield in Leg A [W/°C]; this is given by

$$G_{cpd,t} = \frac{2\pi K_{nc} f_{wedge} L_{WP}}{\ln\left(\frac{D_{DS}}{D_{WP}}\right)} \quad (B-4)$$

where

- f_{wedge} — fraction of the waste package surface that constitutes the crown wedge based on the *tpa.inp* parameter FractionAllowedToDegrade[]
- K_{nc} — equivalent thermal conductivity due to convection as specified by the *tpa.inp* parameter Cond_EqvForNaturalConvection[W/(m–C)]

- D_{DS} — drip shield inner diameter [m] as specified by the *tpa.inp* parameter DripShieldEqvIntDia[m]
- $G_{rpd, t}$ — effective thermal conductance due to radiation between waste package and drip shield in Leg A [W/°C]; this is given by

$$G_{rpd, t} = \frac{\pi \sigma f_{wedge} L_{WP} 4(273.15 + T_{Wall})^3}{\frac{1}{\epsilon_{WP} D_{WP}} + \frac{1 - \epsilon_{DS}}{\epsilon_{DS} D_{DS}}} \quad (B-5)$$

where

- σ — Stefan-Boltzmann constant [5.67×10^{-8} W/(m²K⁴)]
- ϵ_{wp} — emissivity of the waste package surface as specified by the *tpa.inp* parameter EmissivityOfWastePackage[-]
- ϵ_{DS} — emissivity of the drip shield surface as specified by the *tpa.inp* parameter EmissivityOfDripShield[-]
- T_{Wall} — drift wall temperature provided from the mountain-scale heat transfer equations
- $G_{cbw, t}$ — effective thermal conductance due to convection in air between rubble and drift wall in Leg A [W/°C]; this is given by

$$G_{cbw, t} = \frac{2\pi K_{nc} f_{wedge} L_{WP}}{\ln\left(\frac{D_{Wall}}{D_{BF}}\right)} \quad (B-6)$$

where

- D_{BF} — rubble outer diameter [m] obtained from the Drip Shield and Waste Package Mechanical Failure module (MECHFAL)¹
- D_{Wall} — wall inner diameter for Leg A or the Crown Diameter [m]
Note: The crown diameter D_{Wall} is different from the original rock wall diameter D_{RW} . D_{Wall} depends on the amount of rubble generated due to drift degradation and the ceiling of the degraded drift
- $G_{rbw, t}$ — effective thermal conductance due to radiation between rubble and drift wall in Leg A [W/°C]; this is given by

¹The Drip Shield and Waste Package Mechanical Failure module is referenced frequently throughout this appendix. The abbreviation MECHFAL will be used.

$$G_{rbw,t} = \frac{\pi \sigma f_{wedge} L_{WP} 4(273.15 + T_{Wall})^3}{\frac{1}{\epsilon_{BF} D_{BF}} + \frac{1 - \epsilon_{Wall}}{\epsilon_{Wall} D_{Wall}}} \quad (B-7)$$

where

- ϵ_{Wall} — emissivity of the drift wall as specified by the *tpa.inp* parameter EmissivityOfDriftWall[-]
- $G_{bf,t}$ — effective thermal conductance due to conduction through the rubble material in Leg A [W/°C]; this is given by

$$G_{bf,t} = \frac{2\pi K_{BF} f_{wedge} L_{WP}}{\ln\left(\frac{D_{BF}}{D_{DS} + 2t_{DS}}\right)} \quad (B-8)$$

where

- K_{BF} — effective thermal conductivity of rubble material as specified by the *tpa.inp* parameter ThermalConductivityOfBackfillModelOne[W/(m-C)]
- t_{DS} — drip shield thickness [m] as specified by the *tpa.inp* parameter DripShieldThickness[m]

B.1.2 Thermal Conductance Through Horizontal Leg B in Thermal Mode 1

The expression for thermal conductance through Leg B is given by

$$G_{leg-B} = \frac{1}{\frac{1}{G_{cpd,s} + G_{rpd,s}} + \frac{1}{G_{bf,s}} + \frac{1}{G_{cbw,s} + G_{rbw,s}}} \quad (B-9)$$

where

- $G_{cpd,s}$ — effective thermal conductance due to convection in air between the waste package and drip shield in Leg B [W/°C]; this is given by

$$G_{cpd,s} = \frac{2\pi K_{nc} (f_c - f_{wedge}) L_{WP}}{\ln\left(\frac{D_{DS}}{D_{WP}}\right)} \quad (B-10)$$

where

$G_{rpd, s}$ — effective thermal conductance due to radiation between the waste package and drip shield in Leg B [W/°C]; this is given by

$$G_{rpd, s} = \frac{\pi\sigma(f_c - f_{wedge})L_{WP}4(273.15 + T_{Wall})^3}{\frac{1}{\epsilon_{WP}D_{WP}} + \frac{1 - \epsilon_{DS}}{\epsilon_{DS}D_{DS}}} \quad (B-11)$$

where

$G_{cbw, t}$ — effective thermal conductance due to convection in air between rubble and drift wall in Leg B [W/°C]; this is given by

$$G_{cbw, t} = \frac{2\pi K_{nc}(f_c - f_{wedge})L_{WP}}{\ln\left(\frac{D_{Wall-B}}{D_{BF-B}}\right)} \quad (B-12)$$

where

D_{BF-B} — backfill outer diameter in the horizontal direction along Leg B [m] available from MECHFAIL

D_{Wall-B} — wall inner diameter in the horizontal direction for Leg B [m] available from MECHFAIL. Note: D_{Wall-B} is different from the original rock wall diameter D_{RW} and wall diameter in the vertical direction along Leg A D_{wall} .

$G_{rbw, s}$ — effective thermal conductance due to radiation between rubble and drift wall in Leg B [W/°C]; this is given by

$$G_{rbw, s} = \frac{\pi\sigma(f_c - f_{wedge})L_{WP}4(273.15 + T_{Wall})^3}{\frac{1}{\epsilon_{BF}D_{BF-B}} + \frac{1 - \epsilon_{Wall}}{\epsilon_{Wall}D_{Wall-B}}} \quad (B-13)$$

where

$G_{bf, s}$ — effective thermal conductance due to conduction through the rubble material in Leg B [W/°C]; this is given by

$$G_{bf, s} = \frac{2\pi K_{BF}(f_c - f_{wedge})L_{WP}}{\ln\left(\frac{D_{BF-B}}{D_{DS} + 2t_{DS}}\right)} \quad (B-14)$$

B.1.3 Calculation of Temperature Profile in Thermal Mode 1

The thermal conductance values along with the drift wall temperature and waste package heat load at a certain time is used to compute the temperature profile. The following equations describe how temperatures are computed at different locations:

Waste package temperature, T_{WP}

$$T_{WP} = T_{Wall} + \frac{Q_{WP}}{G_{Total}} \quad (B-15)$$

where

- Q_{WP} — time-dependent total thermal output for a waste package adjusted for ventilation during the preclosure period [W]
- T_{WP} — waste package temperature [°C]
- G_{Total} — total calculated conductance [W/°C]

Drip shield temperature along Leg A, T_{DS-A} [°C]

$$T_{DS-A} = T_{Wall} - \frac{Q_{WP} \frac{G_{leg-A}}{G_{Total}}}{G_{rpd,t} + G_{cpd,t}} \quad (B-16)$$

where

- G_{leg-A} — total calculated conductance for Leg A

Drip shield temperature along Leg B, T_{DS-B} [°C]

$$T_{DS-B} = T_{WP} - \frac{Q_{WP} \frac{G_{leg-B}}{G_{Total}}}{G_{rpd,s} + G_{cpd,s}} \quad (B-17)$$

where

- G_{leg-B} — total calculated conductance for Leg B

Temperature at rubble outer surface along Leg A, T_{BF-A} [°C]

$$T_{BF-A} = T_{DS-A} - \frac{Q_{WP} \frac{G_{leg-A}}{G_{Total}}}{G_{bf,t}} \quad (B-18)$$

Temperature at rubble outer surface along Leg B, T_{BF-B} [°C]

$$T_{BF-B} = T_{DS-B} - \frac{Q_{WP} \frac{G_{leg-B}}{G_{Total}}}{G_{bf,s}} \quad (B-19)$$

B.2 Thermal Conductance Through Invert Leg in Thermal Mode 2

Thermal Mode 2 represents the rubble as a uniformly accumulated mass around the drip shield. The simplified radial geometry used for Thermal Mode 2 is illustrated in Figure B-2(a). The outer radius of the rubble thickness is determined from the volume of accumulated rubble. The thermal network diagram for heat transfer analysis in Thermal Mode 2 is shown in Figure B-2(b). This diagram provides the most generalized abstracted scenario. Special cases could be constructed from this diagram by replacing appropriate branches.

$$G_{Total} = G_{invert} + G_{leg-C} \quad (B-20)$$

where

- G_{invert} — effective thermal conductance for the invert leg [W/°C]
- G_{leg-C} — effective thermal conductance for Leg C [W/°C]

The expression for thermal conductance through invert is given by Eq. (B-1).

B.2.1 Thermal Conductance Through Vertical Leg C in Thermal Mode 2

The expression for thermal conductance through Leg C is given by

$$G_{leg-C} = \frac{1}{\frac{1}{G_{cpd} + G_{rpd}} + \frac{1}{G_{bf}} + \frac{1}{G_{cbw} + G_{rbw}}} \quad (B-21)$$

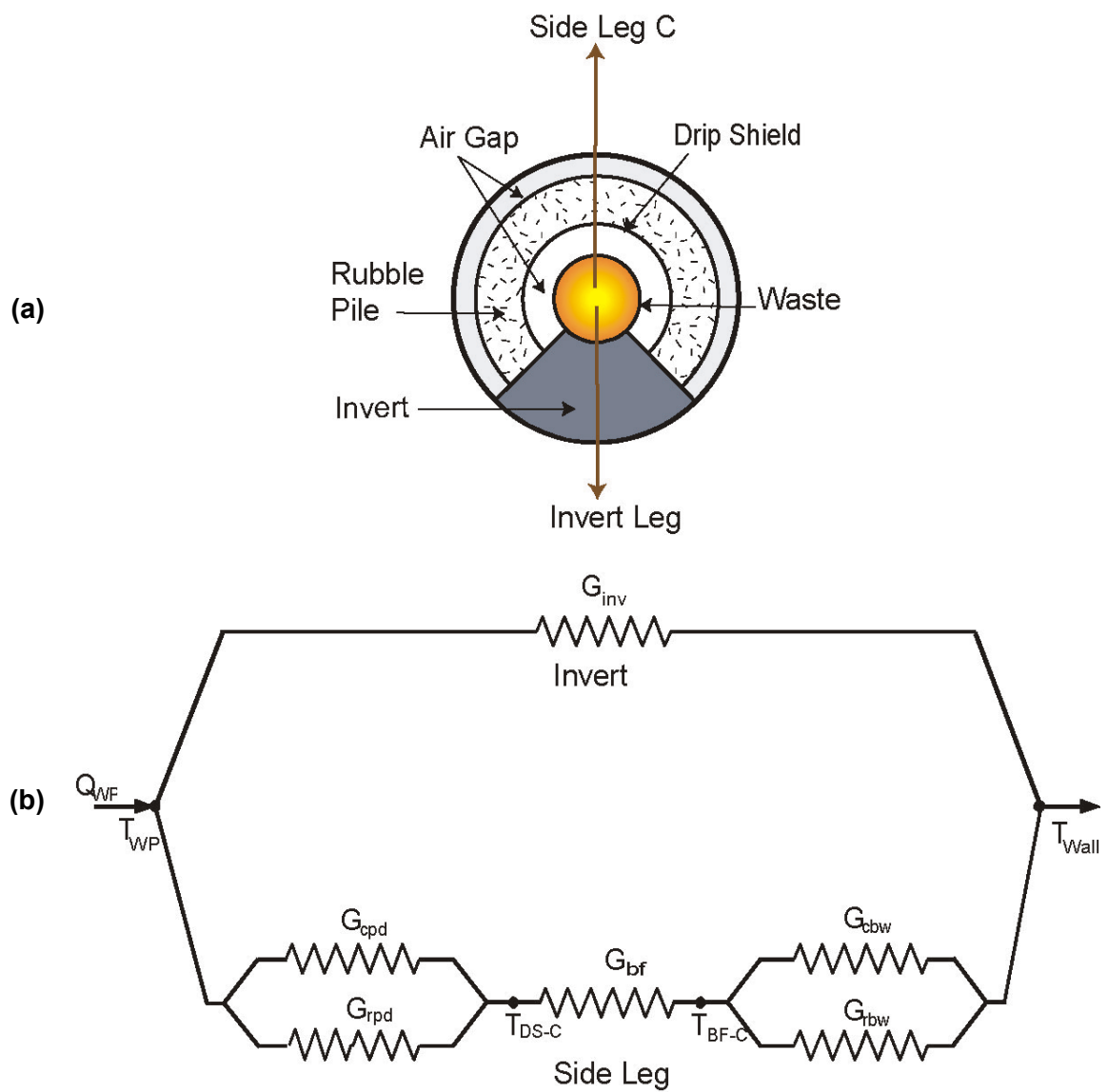


Figure B-2. Simplified Radial Geometry and Corresponding Thermal Network for Thermal Mode 2

$$G_{cpd} = \frac{2\pi K_{nc} f_c L_{WP}}{\ln\left(\frac{D_{DS}}{D_{WP}}\right)} \quad (B-22)$$

$$G_{rpd} = \frac{\pi \sigma f_c L_{WP} 4(273.15 + T_{Wall})^3}{\frac{1}{\epsilon_{WP} D_{WP}} + \frac{1 - \epsilon_{DS}}{\epsilon_{DS} D_{DS}}} \quad (B-23)$$

$$G_{cpd} = \frac{2\pi K_{nc} f_c L_{WP}}{\ln\left(\frac{D_{Wall}}{D_{BF}}\right)} \quad (B-24)$$

$$G_{rbw} = \frac{\pi \sigma f_c L_{WP} 4(273.15 + T_{Wall})^3}{\frac{1}{\epsilon_{BF} D_{BF}} + \frac{1 - \epsilon_{Wall}}{\epsilon_{Wall} D_{Wall}}} \quad (B-25)$$

$$G_{bf} = \frac{2\pi K_{BF} f_c L_{WP}}{\ln\left(\frac{D_{BF}}{D_{DS} + 2t_{DS}}\right)} \quad (B-26)$$

B.2.2 Calculation of Temperature Profile in Thermal Mode 2

The thermal conductance values along with the drift wall temperature and waste package heat load at a certain time are used to compute the temperature profile. The following equations describe how temperatures are computed at different locations.

Waste package temperature, T_{WP} [°C]

$$T_{WP} = T_{Wall} + \frac{Q_{WP}}{G_{Total}} \quad (B-27)$$

Drip shield temperature along Leg C, T_{DS-C} [°C]

$$T_{DS-C} = T_{WP} - \frac{Q_{WP} \left(1 - \frac{G_{invert}}{G_{Total}} \right)}{G_{rpd} + G_{cpd}} \quad (B-28)$$

Temperature at rubble outer surface along Leg C, T_{BF-C} [°C]

$$T_{BF-C} = T_{DS-C} - \frac{Q_{WP} \left(1 - \frac{G_{invert}}{G_{Total}} \right)}{G_{bf}} \quad (B-29)$$